

# **USER GUIDE**

**Clarity Software** 

ENG

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Author: DR

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

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

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

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

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

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

 Note:
 Notifies the reader of relevant information.

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

#### Marks the problem statement or trouble question.

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

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

# **1** Installation

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

# **1.1 Installing Clarity**

These are the basic steps you have to follow for the <u>First installation</u> of Clarity.

## First installation of the software (since version 7.0)

1. Install the software BEFORE connecting any hardware.

More Info:

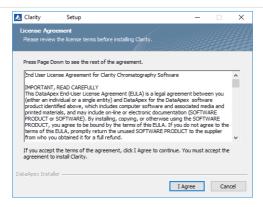
- The software can be installed by inserting the installation USB and running install.exe or by downloading the installation from the download center at our website.
- On administered systems use "*Run as Administrator*" from intended User account. Administered systems are managed by an administrator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



2. Select the language.

Installer L	anguage X
	Please select a language.
	English
	OK Cancel

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



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

🔼 Clarity Setup		-		×
Choose Install Location Choose the folder in which to install Clarity.				
Setup will install Clarity in the following directo	ry.			
In Windows 7, 8.1 and 10 never install Clarity function properly.	in the Program Files folde	r as it ma	iy not	
Destination Folder				
C:\Clarity		Brow	se	
Space required: 972.8MB				
Space available: 70.1GB				
DataApex Installer				
	< Back Next	>	Cano	el

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

Clarity Setup	-		×
Data location Folder setting for your projects			
Set location for your data files - projects, chromatograms, methods, etc.			
C:\Clarity\DataFiles	E	Browse	
DetaApex Installer	>	Cance	ł

6. Select the type of installation.

#### More Info:

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

Choose which features of Cla Check the components you w install. Click Next to continue	ant to install and uncheck the components you don't w	ant to
Select the type of install:	Typical	$\sim$
Or, select the optional components you wish to install:	Program Files     Program Files     Program Files     DeMO projects     C Control     Of Control     Instrument Control Framework (ICF)	^ ~
Space required: 970.3MB	Description Position your mouse over a component to see its description.	

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

🛃 Clarity Setup	-		$\times$
Hardware Setup Select the acquisition device			
Which A/D acquisition device would you like to set as default?			
None (select when using Clarity Offline or Digital acquisition)	)		
◯ Colibrick (external USB box)			
O INT7 (internal PCI card)			
O INT9 (internal PCI card)			
O U-PAD2 (external USB box)			
O Net-PAD (external TCP/IP box)			
DataApex Installer			
< Back Ne	ext >	Can	cel

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

🔼 Clarity Setup		-		$\times$
Choose Start Menu Folder Choose a Start Menu folder for the Clarity shortcuts.				
Select the Start Menu folder in which you would like to cre can also enter a name to create a new folder.	ate the progr	am's shor	tcuts. You	
Clarity				
Accessibility Accessibility Administrative Tools Maintenance Startup System Tools Windows PowerShell				
Do not create shortcuts				
DataApex Installer				
< Bac	k Inst	tall	Cance	ł

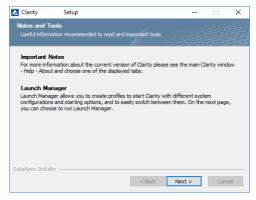
9. Enter the User code corresponding to your hardware key or leave blank for a 30 day trial mode.

More Info:

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

🔼 Clarity User Code		×
2	Setup requires you to enter your User Code. In case of an improper Us Code the station will not start until the valid one is entered. If you leave the User Code field blank, the station will start in 30 Days Trial Mode. The Trial mode allows the Clarity station to be fully operatio for 100 sessions or 30 days from first opening (whatever comes first). Detected HW Key: User code: 1	
	< Back Next > Skip	

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



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

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

🔼 Clarity	Setup	– 🗆 ×
	******	Completing the Clarity Setup
	1111	Clarity has been installed on your computer.
		Click Finish to dose Setup.
	· · · · · · · · · · · · · · · · · · ·	Run Clarity
		Run Launch Manager
		Show Readme
لۇر.	A STATE	Show What's New
and the second		Make IQ Report
AClarit	y	DataApex Website
		< Back Einish Cancel

# **1.2 Updating Clarity Software**

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

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

More Info:

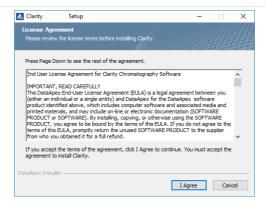
- On administered systems use *"Run as Administrator"* from intended User account. Administered systems are managed by an administrator and users using the PC may not have administrator privileges. Insufficient privileges may result in:
  - Clarity not being installed.
  - When installed from Administrator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



3. Select the language.



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



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

More Info:

In both cases your data and configuration will be preserved.

🔼 Clarity Setup	-		$\times$
Previous Version A previous version has been found			
Existing installation of Clarity found in C:\Clarity			
Update existing installation (recommended). Uninstall will be performed first.			
◯ Install to different location.			
Your data and configuration will be preserved in bo	th cases.		
DataApex Installer			
< Back	Next >	Cano	cel

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

More Info:

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

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

🔣 Clarity Uninstall		-		$\times$
Uninstall Clarity Remove Clarity from your co	mputer.			
Clarity will be uninstalled fro	m the following folder. Click Next to	continue.		
Uninstalling from: C:\Cla	ity\			
DataApex Installer		Next >	Can	cel
Clarity Uninstall Choose Components Choose which features of Cl	arity you want to uninstall.	-		×
Check the components you uninstall. Click Uninstall to st	want to uninstall and uncheck the co art the uninstallation.	omponents you	don't want	to
Select components to uninstall:	Uninstall Hardware Drivers     Uninstall Application Fil     Remove All DEMO projects     Uninstall Aglient ICF			
Space required: 0.0KB	Description Position your mouse over a co description.	mponent to see	its	
DataApex Installer ————	< Back	Uninstall	Can	cel

8. Finish Clarity uninstall.

Clarity Uninstall	– 🗆 × Clarity was Uninstalled
Clarity™	Clarity has been uninstalled from your computer. Click Finish to close Setup.
	< Back Finish Cancel

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

#### More Info:

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

📐 Clarity	Setup		-		$\times$
Choose Insta Choose the fi	all Location older in which to install Clari	ty.			
Setup will inst	tall Clarity in the following di	rectory.			
In Windows 7 function prop	7, 8.1 and 10 never install C erly.	larity in the Program Files	folder as it m	ay not	
Destination	Folder				
C:\Clarit	y		Brow	wse	
Space require Space availab DataApex Instal	ble: 70.1GB				
		< Back	Next >	Cano	el
🔼 Clarity	Setup		-		×
Upgrade	Setup previous version of Clarity				×
Upgrade Upgrade the		figuration files.			×
Upgrade Upgrade the Destination fo	previous version of Clarity	-			×
Upgrade Upgrade the Destination fo	previous version of Clarity older contains data and con	ortant data files	-		×
Upgrade Upgrade the Destination fo © Kee O Ove	previous version of Clarity older contains data and con p the configuration and imp	ortant data files g	-		×
Upgrade Upgrade the Destination fo © Kee O Ove	previous version of Clarity older contains data and con p the configuration and imp envrite all files without askin	ortant data files g			×
Upgrade Upgrade the Destination fo © Kee O Ove	previous version of Clarity older contains data and con p the configuration and imp envrite all files without askin	ortant data files g	_		×
Upgrade Upgrade the Destination fo © Kee O Ove	previous version of Clarity older contains data and con p the configuration and imp envrite all files without askin	ortant data files g	_		×
Upgrade Upgrade the Destination fo © Kee O Ove	previous version of Clarity older contains data and con p the configuration and imp erwrite all files without askin before overwriting any imp	ortant data files g	- Next >	Canc	

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

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

Clarity Setup	-		$\times$
Data location Folder setting for your projects			
Set location for your data files - projects, chromatograms, methods, etc.			
Current data location: C:\Clarity\DataFiles			
○ Change data location to:			
C:\Clarity\DataFiles		Browse	
All data files present in the current location will be moved to the selected	direct	bry.	
DataApex Installer	>	Cano	el

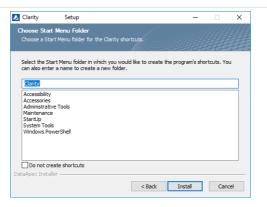
11. Select type of installation.

#### More Info:

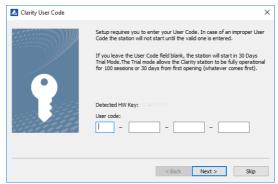
In most cases "Typical" should be selected. A "Custom" installation is necessary for Agilent HPLC control via ICF, CTC PAL, Shimadzu LC-10/20 system, Master GC, ESA Coulochem III and possibly some others.

🔼 Clarity Setup	-		×
Choose Components Choose which features of Cla	rrity you want to install.		
Check the components you w install. Click Next to continue	ant to install and uncheck the components you d	on't want to	
Select the type of install:	Typical	`	~
Or, select the optional components you wish to install:	Program Files     Program Files     DEMO projects     E    E    Control     Or GC Control     Torsument Control Framework (ICF)     Description		
Space required: 970.3MB	Position your mouse over a component to se description.	e its	
narawhey trongligt	< Back Next >	Cance	el

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



13. Confirm the User code.



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

🔼 Clarity Setup	-		×
Notes and Tools Useful information recommended to read and important tools			
Important Notes For more information about the current version of Clarity please see th - Help - About and choose one of the displayed tabs.	e main C	Clarity wind	low
Launch Manager Launch Manager allows you to create profiles to start Clarity with diffe configurations and starting options, and to easily switch between them you can choose to run Launch Manager.			<del>2</del> ,
DataApex Installer < Back Nex	:t >	Can	cel

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

#### More Info:

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

🔼 Clarity Setu	×
	Completing the Clarity Setup
	Clarity has been installed on your computer.
	Click Finish to close Setup.
	Run Clarity
	Run Launch Manager
	Show Readme
and the second	Show What's New
	Make IQ Report
AClarity	DataApex Website
	< Back Einlish Cancel

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

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

### 1.3 Installing an internal card

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

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





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

# **1.4 Installing Colibrick**

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



1. Install Clarity first.

- The drivers will be installed automatically during the installation of Clarity. Ensure that you have Administrator access rights in your Windows OS before you proceed with the installation.
- The *Colibrick* device is identified by its S/N. If you exchange it by another one later, it will be also necessary to reconfigure it in the *Clarity System Configuration* dialog.
- 2. Connect Colibrick to a USB port in your computer. It will be detected automatically.



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



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



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

# 1.5 Installing a Rockey USB dongle

Currently supplied RkNDUSB HW keys use the HID (Human interface device) technology and do not require any drivers.

For old RkUSB keys the drivers will be installed automatically during the installation of Clarity. If the installation did not proceed as expected or you have an old version of Windows, follow the procedure below.

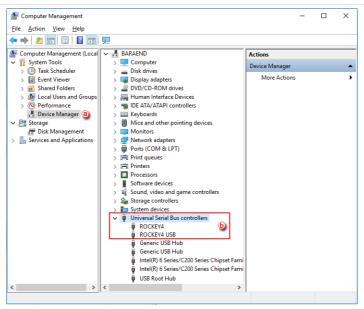


- 1. Install Clarity first.
- 2. Connect the USB dongle to a USB port on the computer.
- 3. Install the Rockey drivers by running INSTDRV.EXE in C:\CLARITY\BIN\HW\_DRIVERS\ROCKEY\. The following window will appear.
- 4. Select the Install USB driver option and click on Next to finish the installation.

👸 Setup Wizard		×
ROCKEY Driver Installation		
COLORED CO.	Iv Install USB driver	
	☐ Install parallel driver	
	Not Detect print-busy-mode	
Ø	$\mathbf C$ . Detect the print-busy-mode	
	Prev Next Cancel	

5. Verify that the driver has been installed correctly

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



If this does not work, try the following procedure after the installation of Clarity:

After connecting the dongle, **Windows** will detect a new **Plug and Play** device and the Found New Hardware Wizard will appear.

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

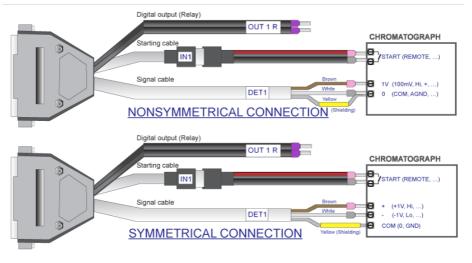
#### 3. Verify that the driver has been installed correctly

More Info:

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

# 1.6 Connecting a chromatograph analogue output to Clarity

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



- 1. Install your A/D converter card as explained in Installing an internal card or an external A/D converter like *Colibrick*, Installing Colibrick.
- 2. Switch off your chromatograph.
- 3. **Connect the bare wires to the chromatograph** depending on your equipment, configuration and the following guidelines.

More Info:

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

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

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

# **1.7 Installing Multicom**

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



1. Install *Clarity* <u>first</u> selecting the *Multicom* driver under *Utils* at the end of the components list.

#### More Info:

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

Choose which features of Cla	arity you want to install.	
Check the components you w install. Click Next to continue	vant to install and uncheck the components you do	on't want to
Select the type of install:	Custom	~
Or, select the optional components you wish to install:	Universal Drivers	^
	Opt-USB Driver	~
Space required: 1.0 GB	Position your mouse over a component to se description.	e its

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

More Info: The "Found New Hardware" message will appear on the Windows taskbar

and the LED diodes on the *MultiCOM* will be turned on one by one. Finally the message "New hardware is installed and ready to use" will appear.

- 3. Connect your devices to the *Multicom* RS232 ports.
- 4. Start *Clarity* and then add each device to a specific *Clarity Instrument* as explained in Adding a new device.
- 5. Select the appropriate port from the list during the device setup.

<u>R</u> ub	y Script:	Utils\Uni_Drivers\FLOM\FL	OMPumps.rb		
<u>P</u> or	t:	COM1		~	Autodetect
		COM1 COM3			
		COM4 COM5			
1	LC Name	COM6			LC 1
2		COM7			1
3	Do not Stop wh				
4	Auxiliary Pump				
5	Maximum High	Pressure Limit [MPa]			40
6	Maximum flow	[ml]			10

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

More Info:

#### Green LED status:

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

# 2 Configuring the Chromatography Station

Chapters covering settings in the System Configuration dialog.

# 2.1 Obtaining information about Clarity configuration

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

- 1. **Open the** *About* **window:** select *Help About...* on the *Main* window.
- 2. Switch to the System Files tab (a). Note that it may take a while for Clarity to generate the report.
- 3. Go to the first table (b) to find info about:
  - Clarity SW version
  - Number of purchased instrument licenses
  - Extensions available
  - The allowed control modules
  - Acquisition and hardware devices
- Go to the files table c to find information about the drivers and its status.
   More Info:

If the status is other than OK there may be an issue with the driver. The version of the drivers developed by DataApex should be the same as that of Clarity.

Date	06.08.2018, 14:05			
Serial number of application				
User Code	CONTRACTOR OF TAXABLE PARTY.			
Version of application	Clarity version 8.1.0.15			
Build date of application	03.08.2018, 10:48			
Instruments	All			
Extensions	SST; GPC; PDA; EA; CE	; MS; NGA; DHA;	GCxGC; MS	G-TOF
Controls	GC; LC; AS			
Certification file	C:\Clarity\Bin\iq.chk			
Checksum of cert. file	4AA4481C9E084B64			
Date of cert. file	03.08.2018, 12:55			
User	endrsbar			
System Acquisition and hardware dev	Microsoft Windows 10 Vices Key Rockey 4ND 088-0 Colibrick 1808			
Acquisition and hardware dev	Key Rockey 4ND 088-0			
Acquisition and hardware dev	Key Rockey 4ND 088-0			
Acquisition and hardware dev	rices Key Rockey 4ND 088-0 Colibrick 1808	0888+38911/000	d:192AFA0	1
Acquisition and hardware dev Files	rices Key Rockey 4ND 088-0 Colibrick 1808	0888+38911/000	d:192AFA0	11 File 03.08.2
Files	key Rockey 4ND 088-C Colibrick 1808	0888+38911/000	Size 38225 385536	11 File 03.08.2
Files	key Rockey AND 088-C Colbrick 1808 Path c:\clarity\binutis umi_drivesladvantec C:\Clarity\Bin	Version - 5.0.20.1	Size 38225 385536	File 03.08.2 03.08.2 03.08.2
Acquisition and hardware dev Files File advantecch1122scfc.rb AdviencOMS.dl Adviencommen.dl	Key Rockey 4ND 088-C Collarick 1808 Path c:\clarty\binutils umi_driversiadvantec C:\clarty\Bin	Version - 5.0.20.1 5.0.20.1	Size 38225 385536 16384	File 03.08.2 03.08.2 03.08.2 03.08.2
Acquisition and hardware dev Files File advantecchf122scfc.rb AdvionCOmmon.dl AdvionCOmmon.dl	Key Rockey 4ND 088-C Collbrick 1808 Path c:\clartybiniutis um, driversiadvantec C:\clartybin C:\clartybin C:\clartybin	Version - 5.0.20.1 5.0.20.1	Size 38225 385536 16384 321536	File 03.08.2 03.08.2 03.08.2 03.08.2

# 2.2 Setting the number and type of instruments

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

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

• Set the Instrument Type field (b) depending on the type of the device, GC or LC.

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

User Guide

System Configuration			<u>^</u>	— 🗆 🗙	
Setup Control Modules		Number of In	nstruments: 4 📮 🥘		
	5/N 4739		Instrument 2 Instrument 3 Instrument 2 Instrument 3 Instrument Type Setting Type GC GL GC GPC GPC GPC GPC	Instrument 4  Options MS ToF DHA NGA PDA  K Cancel V 1 V 1 V 1 V 1 V 1 V 1 V 1 V 1 V 1 V	X Help
Add Remove About	Setup	Units Setup	OK Cano	el Help	

# 2.3 Adding a new device

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

User Guide

System Configuration	×
Setup Control Modules	Number of Instruments:
Name Used	3 Instrument 1 3 Instrument 2 3 Instrument 3
AS LC	Name
GC Detector	Instrument 1
Balance	GC
Capillary Electrophoresis	Name     From       AS     GC       GC     Detector       Thermostat     Valve       Valve     Auxiliary
	Data Inputs & Outputs Device Number Ext. Start Dig. Input:
	Ready Dig. Output:
	Miscellaneous Settings Units Setup Method Options
Add Remove About Setup	OK Cancel Help

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

More Info:	
	If on the status column, says the module is not installed, you could install it by re-installing Clarity, clicking on <i>Custom Install</i> and selecting the module you
	wish to install.

3. Select the device and click on Add. (b)

	I	🗌 Instal	led Only Filter: All	~		8
Name		Status	Vendor	Comme	٦	
-	Marathon	installed	Spark Holland	Filter field		
~	Master AS	installed	Dani	part d Type any part of module	/ Dani	
~	Master DHS	installed	Dani		/ Dani	
~	Master SHS	installed	Dani	Static name or descriptions	/ Dani	
~	Midas	installed	Spark Holland			
×	PAL	not installed	CTC	Combi PAL, Combi-xt PAL, Combi		
×	PAL3	not installed	CTC	CTC PAL3 autosamplers controlled Testing		
~	PN5300	installed	Postnova Analytics			
~	ProStar 400	installed	Varian			
-	ProStar 410	installed	Varian			
~	S 6250	installed	Schambeck SFD GmbH	Autosampler Develope	d by Sykam	
-	S 6300	installed	Schambeck SFD GmbH	Autosampler Develope	d by Sykam	
~	S5200	installed	Schambeck SFD GmbH			
~	S5200	installed	Sykam			
-	S5250	installed	Sykam	Autosampler, also as part of the S Develope	d by Sykam	
~	S5300	installed	Sykam	Autosampler, also as part of the S Develope	d by Sykam	
-	Triathlon	installed	Spark Holland			
-	Valco Valve set as AS	installed	VICI Valco	Multiposition valve used as autosa		
~	YL2x00H	installed	YL Instrument	YL2000H, YL2000HT, YL2100H		
-	YL3x00A	installed	YL Instrument	YL3000A, YL3100A, YL3200A		
~	YL9150	installed	YL Instrum			
~	YL9151	installed				
🗆 🗰 🗖			Available Contr			
		installed	Modules list	A, G1311A, G1312A, G131		
-	212-LC	installed	Iviodules list	pump by UNI Ruby script		
	2250	installed	L			
~	30x	installed	Gilson	302-307		
	AAA500	inetallad	Indoe	Tection F	Nevelonard hy Tr	0000

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

User Guide

System Configuration			×
Setup Control Modules	Nu	mber of Instruments: 4	
Name Used	Instrument 1	3 Instrument 2 3 Instrument 3	🔇 Instrument 4
AS Detector C C C C C Colbindc A Colbindc - 1 Instrument 1 A Colbindc - 3 Instrument 1 A Colbindc - 4 Instrument 1 Balance Thermostat Valve C Capillary Electrophoresis Auxiliary	Name Instrument 1 Instrument Typ GC Name A S GC Detector A Colo A Col	Prom Prom Prot Collbrick rick - 1 Collbrick rick - 2 Collbrick rick - 4 Collbrick stat	
	- Data Inputs & O	Device	Number
	Ext. Start Dig. In		~ [1] ~
	Ready Dig. Outp		~ 1 ~
	Miscellaneous Se Units		thod Options
Add Remove About Setup.	)	OK	Cancel Help

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

# 2.4 Configuring a device

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

User Guide

System Configuration					×
Setup Contro	ol Modules		umber of Instruments:	4 ▲	
Name	Jsed	🔇 Instrument 1	a 3 Instrument 2	) Instrument 3 🚯 Inst	rument 4
Colbrick - 2	Instrument 1 Instrument 1 Instrument 1	Name Instrument 1 Instrument Typ GC Name AS	e		
Balance Thermostat Valve Capillary Electrophoresis		-> Get -A, Coli -A, Coli 	vrick - 1 vrick - 2 vrick - 3 vrick - 4 ostat	Colibrick Colibrick Colibrick Colibrick	
		Data Inputs & C		Device	Number
		Ready Dig. Outp			× 1 ×
		Miscellaneous S Units	ettings : Setup	Method Op	otions
Add Remove Ab	out <u>S</u> etup			OK Cancel	Help

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

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

DataApex Colibric	k Setup		×
Device:	Colibrick (Serial No: 1808)		~
Channel 1			
Name	Colibrick - 1	Inversion of Sig	nal 🗹 Bipolar
Quantity:	Voltage	Units: mV	Set Units
Coefficient:	1 mV / 1 mV	Autoprefix: Yes	
Synchronize	Start with Digital Input		Digital Input 1 $$
Channel 2	-	1	
Name	Colibrick - 2	Inversion of Sig	nal 🗹 Bipolar
Quantity:	Voltage	Units: mV	Set Units
Coefficient:	1 mV / 1 mV	Autoprefix: Yes	
Synchronize	Start with Digital Input		Digital Input 1 $$
Channel 3		1-	
Name	Colibrick - 3	Inversion of Sig	nal 🗹 Bipolar
Quantity:	Voltage	Units: mV	Set Units
Coefficient:	1 mV / 1 mV	Autoprefix: Yes	
Synchronize	Start with Digital Input		Digital Input 1 $$
Channel 4		-	
Name	Colibrick - 4	Inversion of Sig	nal 🗹 Bipolar
Quantity:	Voltage	Units: mV	Set Units
Coefficient:	1 mV / 1 mV	Autoprefix: Yes	
Synchronize	Start with Digital Input		Digital Input 1 $$
Device Setup			
Digital	Input Names Change		ly Frequency
-			50 Hz
Digital C	Output Names Change	(	) 60 Hz
		ОК	Cancel Help

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

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

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

- 1. Enter the System Configuration dialog: select System Configuration... on the Main window.
- 2. Set up the options for sending the method to the instrument: in the group *Miscellaneous Settings* click on *Method Options* button. (a)

User Guide

System Configuration								$\times$
Setup Cont	rol Modules		Nur	nber of Instrume	ents: 1			
Name	Used	s/N	3 Instrument 1	Instrument	2 O Instrument 3	C Instrumer	nt 4	
AS Detector Detector An Detector 1 An Detector 1 An Detector 1 An Colbrick - 1 An Colbrick - 2 An Colbrick - 3 An Colbrick - 3 An Colbrick - 4 Balance Thermostat Valve Traction Collector Capillary Electrophoresis Auxiliary	Instrument 1	1808	 Name Instrument 1 Instrument Type GC Name GC GC GC GC GC GC A, Detecto CA, Det	r tor 1 stat	From Altech 3300 E	1.50		_
			Data Inputs & Ou		Device		Number	
			Ext. Start Dig. Inp Ready Dig. Outpu		ltech 3300 ELSD	~	1 ~	
					itteen 5500 ELSD	~	- ~	
			Miscellaneous Set Units S	-	M	ethod Options	b	
Add Remove A	bout	Setup		[	ОК	Cancel	Help	

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

Method Sending Options	×
After Each Method Change: Send Method to Instrument Do Not Send Method to Instrument	
The method is changed each time after: - logging to the Instrument window, - opening a different method in the Method field of the Single Analysis dialog, - editing a method opened in the Method field of the Single Analysis dialog.	
OK Cancel Help	

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

# 2.6 Assigning digital input and output to start acquisition

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

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

## AS + GC set - ACTIVE sequence

Variant A - Autosamplers started by closing the contacts.

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

System Configuration	×
Setup Control Modules	Number of Instruments: 4
	Data Inputs & Outputs     Device     A     Number       Ext. Start Dig. Input:     Colibrick     1        Ready Dig. Output:     Colibridk     1        Miscellaneous Settings     Units Setup     Method Options
Add Remove About Setup	OK Cancel Help

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

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

Digital Ou	Digital Outputs of Colibrick (SN:1808)					
Output ino.	Initial State:	Current State:	Descriptions:			
1	● <i>✓</i> _ <sup>−</sup>	● <i>✓</i> _	Digital Output 1			
2	<u> </u>	<u> </u>	Digital Output 2			
3	<u> </u>	<b>•</b>	Digital Output 3			
4	<u> </u>	0./_	Digital Output 4			
5	0	0	Digital Output 5			
6	0	0	Digital Output 6			
7	0	0	Digital Output 7			
8	0	0	Digital Output 8			
			Close Help			

Variant B - Autosamplers started by opening the contacts.

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

Digital Outputs of Colibrick (SN:1808)					
Output no.	Initial State:	Current State:	Descriptions:		
1	0-1	<u> </u>	Digital Output 1		
2	<u> </u>	<u> </u>	Digital Output 2		
3	<u> </u>	<u> </u>	Digital Output 3		
4	<u> </u>	<u> </u>	Digital Output 4		
5	0	•	Digital Output 5		
6	0	0	Digital Output 6		
7	0	0	Digital Output 7		
8	0	0	Digital Output 8		
			Close Help		

#### AS + LC set - ACTIVE sequence

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

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

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

		o1 (MODIFIED)	_					-			×
		88			6		<b>S</b>	2			
N	ew Open	Save Save a			lit trail		l method by e-mail	Help			
m	mon for all detec	tors		_							
-			Input	•				Output	•		
	Name	Type	Source	Input	Value	Units	Output Type	Output	Paran	neter	Store
	Start detector	Acq Begin					Colibrick	Digital Output 2	Pulse		
	Start pump	Acg Begin					Colibrick	Digital Output 3	Pulse	•	
	ent Table Mea	surement Acquisi	tion Integration	Calculation	1 Advance	ed ed					>
c   Ev	ent Table Mean	surement Acquisi	tion Integration	Calculation	n Advance	ed					>

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

- 1. Enter System Configuration dialog: Click System Configuration... or on icon.
- 2. Add the required autosampler and assign it to the instrument according to "Add new device" and "Configuring a device".
- 3. In *Ext. Start Dig. Input* line set **Device** to *Colibrick* and **Number** to 1.
- 4. In Ready Dig. Output line set Device to Colibrick and Number to -- (8).

Data Inputs & Outputs	Device		Number
Ext. Start Dig. Input:	Colibrick	$\sim$	1
Ready Dig. Output:	Colibrick	~	E
Miscellaneous Settings			
Units Setup		Method Options	5
	ОК	Cancel	Help

#### AS + GC set - PASSIVE sequence

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

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

#### AS + LC set - PASSIVE sequence

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

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

Data Inputs & Outputs	Device	Device		
Ext. Start Dig. Input:	Colibrick	$\sim$	E×	
Ready Dig. Output:	Colibrick	$\sim$	1	
Miscellaneous Settings				
Units Setup		Method Options	;	

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

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

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

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

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

Refer to the corresponding Clarity Control manual.

## 2.7 Setting a custom image and a name for an instrument

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

User Guide

System Configuration					×
Setup Co	ontrol Modules		Number of Instru	uments: 4	
Name	Used	0	Instrument 1 🏹 🚱 Instrume	ent 2 🚯 Instrument 3 🚯 Ins	trument 4
AS LC Detector Detector A. Colbrick -/A. Colbrick - 1 -/A. Colbrick - 2	Instrument 1	In	me strument 1 Instrument Type		
A Collinit - 2 - A Collinit - 3 - A Collinit - 4 - Balance - Thermostat - Valve - Fraction Collector - Capillary Electrophoresis - Auxiliary	Instrument 1 Instrument 1	> <	AS GC GC Detector - A, Colbrid: - 1 - A, Colbrid: - 2 - A, Colbrid: - 2 - A, Colbrid: - 3 - A, Colbrid: - 4 - A, Colbr	From Colibridk Colibridk Colibridk Colibridk	
		Da	ata Inputs & Outputs	Device	Number
		Ex	t. Start Dig. Input:	Colibrick	~ 1 ~
		Re	ady Dig. Output:	Colibrick	~ 1 ~
		Mi	iscellaneous Settings		
			Units Setup	Method O	ptions
Add Remove	About Setup			OK Cancel	Help

- 2. Click on the Instrument 1..4 tab to select the instrument .@
- 3. Type the name of the instrument in the *Name* field **b**.
- 4. Click on the image labeled *Image for Opened Instrument*© to change the image.

Instrument Image Setup		×
	Custom Image HP6590.bmp	

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

# **3 Configuring the User Accounts**

Chapters describing how to use *User Accounts* in **Clarity**, how to restrict some operations for defined users and how to set shared settings for a group of users.

## 3.1 Configuring the User Accounts

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

1. **Open the User Accounts window:** click on  $rac{2}{4}$  or choose System - User Accounts.

More Info:

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

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

More Info:

- Leave blank for unprotected mode all users will share a common desktop file.
- The desktop file (user profile) stores information about the last used project, table and graph settings, the files opened last, etc.
- 3. Set the minimum password length and life time (b).
- 4. Fill in the User Access Rights section ⓒ in accordance to your company rules for GLP (Good Laboratory Practice) and CFR PART 11 compliance.

User Accounts			×
User List (a) New Delete		Password Restrictions - Comr Min. Length LifeTime Expiration Warning Password Reuse Auto Lock	for All         (Chars.)           1         •         (Days)           5         •         (Days)           1         •         (Days)           1         •         (Days)           1         •         (Days)           10         •         (min)
User User Name Tom Desktop File Tom Description Other Users Can © Read & Write O Read O No Access	Access To Access	User Info Password: Password Changed: Last Login: Change I Certificate No certificates assigned to t	Blank Password
User Access Rights Open User Accounts G Open Configuration Edit Unromatogram Edit Chromatogram Projects Import Chromatogram	Edit Sequence     Edit Report Style     Select Nethod     Open Audit Trail Settings     Archive / Restore     Post Run Settings     Start Acquisition	Select Certificate Certificate For Exporting'	Clear Certificate To PDF

## 3.2 Creating a new user account

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

The User's name will be placed on the headers of the files created while working in the station.

3. Enter the desktop file name. ©

More Info:

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

- 4. Write here a user detailed description. d
- 5. Click OK to accept the changes.

User Accounts			×
User List Tereza Tom Delete		Password Restrictions - Comm Min. Length LifeTime Expiration Warning Password Reuse Auto Lock	1         \$         [Chars.]           1         \$         [Days]           5         \$         [Days]           1         \$         [Days]           5         \$         [Days]           1         \$         [Days]
User Liser Name (a) Annel Desktop File (C) Description (d)	User Details for:	User Info Password: Password Changed: Last Login:	Blank
Other Users Can	Access To Instrument 1 Instrument 2 Instrument 3 Instrument 4	Certificate No certificates assigned to the	
User Access Rights Open User Accounts Open Configuration Edit Method Edit Chromatogram Edit Calibration Projects Import Chromatogram	Edit Sequence     Edit Report Style     Select Method     Open Audit Trail Settings     Archive (Restore     Post Run Settings     Start Acquisition	Select Certificate Certificate For Exporting T	Clear Certificate o PDF
	OK Cancel	Help	

## 3.3 Deleting a user account

- 1. **Open the User Accounts window:** click on  $\stackrel{\bullet}{=}$  or choose System User Accounts.
- 2. To delete a user, select the user on the User List and then click on the Delete button (a).
- 3. Click on the OK button to accept the changes.

User Accounts			×
User List Anne John Tereza Tom Dejete		Password Restrictions - Comm Min. Length LifeTime Expiration Warning Password Reuse Auto Lock	for All         [Chars.]           1         \$         [Days]           5         \$         [Days]           1         \$         [Days]           1         \$         [Days]           1         \$         [Days]           10         \$         [min]
User User Name Abral Desktop File share Description Other Users Can	ed Agcess To	User Info Password: Password Changed: Last Login: Change P	Submitted 10. August 2018 Yassword
Read & Write     Read     No Access	<ul> <li>✓ Instrument <u>1</u></li> <li>✓ Instrument <u>2</u></li> <li>✓ Instrument <u>3</u></li> <li>✓ Instrument <u>4</u></li> </ul>	Certificate No certificates assigned to the	he selected user
User Access Rights Open User Accounts Open Configuration Edit Method Edit Chromatogram Edit Calibration Projects Import Chromatogram	Edit Sequence     Edit Report Style     Select Method     Open Audit Trail Settings     Archive / Restore     Post Run Settings     Start Acquisition	Select Certificate Certificate For Exporting 1	Clear Certificate
	OK Cancel	Help	

## 3.4 Sharing settings among users

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

More Info:

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

4. Click OK to accept the changes.

User Accounts				×
User List Anne John Tereza Tom		Password Restrictions - Commo		[Chars.] [Days] [Days]
New Delete		Password Reuse Auto Lock	1 + 10 +	[Days] [Days] [min]
User User Name John Desktop File Shared Description	User Details for: John	User Info Password: Password Changed: Last Login:	Submitted 10. August 2	10 18
Other Users Can	Access To Instrument 1 Instrument 2 Instrument 3 Instrument 4	Certificate No certificates assigned to the		:r
User Access Rights	Edit Sequence     Edit Report Style     Select Method     Open Audit Trail Settings     Archive / Restore     Yost Run Settings     Start Acquisition	Select Certificate Certificate For Exporting To	Clear Cer PDF	tificate
	OK Cancel	Help		

## 3.5 Restricting access

In Clarity it is possible to:

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

	Password Restrictions - Commor Min. Length	n for All	
Tereza Tom	LifeTime Expiration Warning Password Reuse Auto Lock	1     *       1     *       5     *       1     *       10     *	[Chars.] [Days] [Days] [Days] [min]
User User Name Abraham Program	Jser Info Password: Password Changed: Last Login: Change Pas Certificate No certificate assigned to the		
○ No Access     ☑ Instrument 4       User Access Rights     ☑ Edit Sequence       ○ Open User Accounts     ☑ Edit Report Style       ☑ Edit Method     ☑ Select Method       ☑ Edit Colloration     ☑ Ardive / Restore       ☑ Edit Calibration     ☑ Ardive / Restore       ☑ Projects     ☑ Post Run Settings       ☑ Import Chromatogram     ☑ Start Acquisition	Select Certificate	Clear Cer	

## 3.6 Setting a password for the first time

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

\land Clarity			- ×
System Instruments View Hel	p		
LInstrument 1	Instrument 2	Instrument 3	Instrument 4
	Login Dialog X		
	Choose User Name and Enter Password		
For Help, press F1	Select Project:		
	All Possible Instruments OK Cancel Help		
	Clarity You are logging in for the first th	× me, please enter your password.	

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

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

## 3.7 Changing a user password

- 1. **Open the User Accounts window:** click on  $\stackrel{\bullet}{=}$  or choose System User Accounts.
- 2. Select the user on the Users list and then click on Change password (a).
- 3. Type the new password, confirm it and then click OK.

User List		Password Restrictions - Co	mmon for All
Anne		Min. Length	1 * [Chars.]
Tereza		LifeTime	1 🔶 [Days]
		Expiration Warning	5 🌲 [Days]
New		Password Reuse	1 🗘 [Days]
Deļete		Auto Lock	10 🔶 [min]
	Use New Password	×	
Jser	Enter new password		
User Name Anne	Enter new password		Submitted
Desktop File Anne		Changed:	10. August 2018
Description	Confirm (retype) the password		
Other Users Can	Acc	Chang	e Password
Read & Write	ØK OK	Cancel	
Read		2	
O No Access	✓ Instrument <u>4</u>	No certificates assigned t	o the selected user
User Access Rights			
Open User Accounts	Edit Sequence		
Open Configuration	Edit Report Style	Select Certificate	Clear Certificate
Edit Method Edit Chromatogram	Select Method Open Audit Trail Settings	Certificate For Exportin	g To PDF
Edit Chromatogram	Archive / Restore		
	Post Run Settings		

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

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

	Analyst Name	Anne	
	Desktop File	Anne	
			Change Password (b)
Othe	er Users Can 🛛 🜖		A
_			New Password
0	Write		
0	Read		Enter new password
User	Access Rights		
0	Open User Accounts		Confirm (retype) the password
0	Open Configuration		
ø	Edit Method		
0	Edit Chromatogram		OK Cancel
0	Edit Calibration		OK Calicel
Ø	Projects		Post Run Settings
0	Import Chromatogra	m	Start Acquisition
Certi	ificate		
	Sel	ect Certificate	. Clear Certificate

## 3.8 Logging in without a password

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

📐 Clarity System Instruments View Help	2		- x
Instrument 1	Login Dialog X Choose User Name and Enter Password Tom Select Project: MyProject All Possible Instruments OK Cancel Help	Instrument 3	Instrument 4

# 4 Method Setup

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

## 4.1 Setting up a method

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

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

#### Template Method vs. Chromatogram Method

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

#### Method Setup window

- The title of the Method Setup dialog displays a method that is currently opened. If you make any changes, the method becomes (MODIFIED)
- The upper part of the Method Setup dialog displays a set of icons with which it's possible to create a new method, open existing method, save method, save method as, open report setup, open method audit trail, send method by e-mail or open help.
- Upon pressing the OK button it will be automatically saved and Method Setup dialog will close.

### Send Method

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

the 🕨 icon.

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

### **Method Development**

You can edit or develop any method without changing the current method until you send the new on by pressing *Send Method* 

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

1. Set the measurement conditions.

#### More Info:

Here you can disable or enable Autostop and set the run time for the analysis (a) as well as configure the external signal start and stop settings(b). Also you can describe some options of the method and add a note (c).

Method Setup Demo	1				_		×
New Open	Save Save as	Report setup	Audit trail	Send method by e-mail	<b>?</b> Help		
Common for all detects Method Description CKW 21.06.04 Column Mobile Phase Flow Rate Pressure	Cptima 624 Stickstoff 90 ml/min 1,2 bar				C Enable Autostop Run Time:	<b>a</b>	
Detection Temperature Note	ECD 45 °C - 5 min, 8 °C/	min, 125 °C - 0 min,	30 °C/min, 230	) °C - 5 min	External Start/Stop     O Start Only     @ Start - Restart     O Start - Stop     O Up	<b>b</b>	
Event Table Measu		Integration Calcu	llation Advan	ced	Down	ے عوام Metho	d

#### 2. Set the Data Acquisition parameters.

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

New       Open       Save       Save as       Repot setup       Audit trail       Send method by email       Help         Select Detector       Colibrid: -1       Imable       Imable       Imable       Imable         Colibrid: -1       Imable       Colibrid: -1       Imable       Imable       Imable         Colibrid: -1       Imable       Colibrid: -1       Imable       Imable       Imable         Colibrid: Detector       Colibrid: -1       Imable       Imable       Imable       Imable         Sample Rate       12123 mV       Imable       Imable       Imable       Imable       Imable         Configuration:       Bipolar       Imable       Imable       Imable       Imable       Imable	Method Setup Demo	51					_	×
Colbrick Detector Method Method Properties Range 12123 mV V Sample Rate 25 Hz V	New Open				Send method by	-		
Method Properties Range 12123 mV V Sample Rate 25 Hz V	Select Detector	Colibr	ick - 1	~ 🗹	Enabled			
	Rz Sample F	ange 12123 mV Rate 25 Hz	<b></b> b	ctor Method				
Det Status Demo Mode: Ready Det Status Event Table Measurement Acquisition Integration Calculation Advanced To OK Cancel	Event Table Measu		Integration Calc	ulation Advan	ced	Det Status		

3. Set the Signal Integration parameters.

#### More Info:

When using a multi-detector configuration, there is a specific integration table for each detector.

All operations are editable and programmable in time. If you aren't able to edit tab parameters the current detector probably isn't *Enabled*.

The integration parameters are optimized for a sample rate of 10 Hz and a 10000 mV range.

	ve as	Report setu	p Audit tra		? Help		
ect Detector	Colibr	rick - 1	~	Enabled			
		Integration	Table				
Chromatogram Operation	Grp.	Time A [min]	Time B [min]	Value			^
Global Peak Width				0.500 min			
Global Threshold				2.0000 mV			
Global Filter - Bunching				1			
Min, Area		0.000	0.000	100.000 mV.s			
Baseline - Valley		7.860	48.066				
Baseline - Lock		0.000	14.712				
Baseline - Lock		15.317	19.549				
Peak - End		14.900	0.570				
Peak - End		20.300	0.490				
Baseline - Together		19.807	20.339				
Baseline - Lock		24.675	25.697				
Peak - End		25.833	0.581				
Peak - End		25.833	0.600				
Baseline - Lock		29.359	31.642				
Peak - End		32.833	0.776				
Peak - Start		36.417	-0.495				
Peak - Start		37.983	-0.440				
Peak - End		38.900	0.007				
Peak - Start		40.067	-0.582				
Peak - End		40.067	1.328				
Peak - End		42.767	1.228				~
vent Table Measurement Ac	quisition	Integration	Calculation A	dvanced			

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

#### More Info:

- In this tab you can create New... calibration file or Set... the one created previously (a) and configure the different settings related to it.
- After data acquisition, chromatograms from unknown samples will be calibrated and chromatograms from calibration standards may be used to automatically re-calibrate the attached calibration file.
- *Clone...* b button will create a copy of a current calibration file. By using the *Save As* dialog you can select the name and location of the new calibration file. The copy will then be linked to the method.
- If it is desired to have no calibration in the method you can use the None button.
- In this tab you can also choose how you want the results to appear in the reports d and set Calculation Type e to see detail about each type invoke help (F1).

Method Setup Pah_epa	– 🗆 X
	d method by Help
Common for all detectors	
Calibration File (Peak Table)         PAH_EPA         View           Set         (a)         New         Clone         (b)         None         (c)	Scale Use Scale Factor Scale Factor 1
Calculations ISTD ( Integration Algorithm 8.0 ~	Units ul
Author         None           Description         PAHs by M2P (resp. EPA)	Unidentified Peaks Response Base: Area V
Created Modified 30/03/1995 18:36:11 01/12/2018 18:32:38	Response Factor 0 [Am/Rsp]
Report in Result Table () Hide ISTD Peaks All Peaks	Calibration Cloning In Sequence
All Identified Peaks     All Paralle in Collimation	[hanie]
All Peaks in Calibration	
Cancel	Send Method

5. Configure the settings in the additional tabs.

More Info:

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

### 4.2 Saving the chromatogram method as a template method

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

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

More Info:

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

Ξ

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

You can protect your chromatograph column from sudden pressure changes by setting up a Sequence together with three different methods, Startup, Shutdown and Analysis to ensure a slow flow rate increase and decrease on your LC pump. This option is only available for some pumps controlled by Zebrick, CB20 D/A converters or UNI Ruby scripts.

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

### **Startup Method**

2. From the Instrument window Open the Method Setup window using the

Method - Method Setup command or the Method Setup icon.

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

7. Click OK to accept the changes. More Info:

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

Method Setup Startup (MODIFIED)		- 🗆 X
New Open Save Save as Report setup /	udit trail Send method by e-mail	
Gradient Table		
Time [min]         A [%]         Flow [mL/min]           1         Initial         100.0         0.000           2         2.00         100.0         1.000           3	Standby Flow C Time to Standby Standby Time	1     mL/min       0     min       0     min
A         [%]           1.0         6           0.6         6           0.0         0.5           1.0         1.5           2.0         7           1.0         1.5           1.0         1.5           1.0         1.5           1.0         1.5	Idle State O Pump Off O Initial O Standby (a) Options	
Event Table LC Gradient Measurement Acquisition Integra	tion Calculation Advanced	Send Method

#### **Analysis Method**

#### 8. Repeat steps 2 to 6 but this time:

- Save the Method under the name Analysis.
- Set the Idle State to Initial. d
- Set the *Initial Flow* and the *Flow* on the second row (e) to the previous *Standby* value. (f)
- Set the Time to the total duration of your analysis. (e)

1ethod S	etup Ana	ilysis (N	IODIFIED)							×
New	Open	Save	Save as		C t trail	Send method by e-mail	? Help			
			Gradient T	able						
	Time [min] Initial 5.00	A [%] 100.0 100.0	Flow [mL/min] 1.000 1.000	0		Standby Flow Time to Standby Standby Time	Ð	1 0 0	mL/min min min	
Flow	min] A 1.5- 1.0- 0.5- 0.0 0	1	2 Time	[%] -80 0 -80 0 -80 0 -80 0 -20 0 3 4 5 [min]		Idle State Pump Off Initial Standby Initial - Standby Options				
Event Ta		Gradient	Measurem	ent Acquisition Integration	n Calcul	ation Advanced			Send Met	hod

### Shutdown Method

#### 9. Repeat steps 2 to 6 but this time:

- Save the *Method* under the name *Shutdown*
- Set the *Idle State* to *Initial Standby*.
- On the second row, set the *Flow* to 0 and the *Time* to obtain the appropriate flow rate decrease for your column. (h)
- Set the *Standby Flow* to 0. ()

Method	l Setup Shu	tdown	(MODIFIED	)					_		×
New	Open	Save	Save as			C trail	Send method by e-mail	Help			
			Gradient 1	[able							
1 2 3	Time [min] Initial 2.00	A [%] 100.0 100.0	Flow [mL/min] 1.000 0.000	D			Standby Flow Time to Standby Standby Time	Û	0	mL/min min min	
[ml	/min] A 1.0- 0.8- 0.6- 0.4- 0.2- 0.0 0.0	0.	5 1.0 Time		-[%] -80 Composition -40 etition -20 o 2.0 [min]	-	Idle State Pump Off Initial Standby initial - Standby Options	9			
Event		Gradient ancel	Measuren	nent Acquisition	Integration	Calcul	ation Advanced		3	S <u>e</u> nd Met	hod

#### Sequence

#### 10. Set up a Sequence as explained in Running a Sequence and:

- On the first row set the Sample Type column as Bypass () and the Method Name () to Startup.
- On the last row set the Sample Type column as Bypass and the Method Name to Shutdown.
- Set as many rows as you need in between according to the conditions of your analysis or sequence and set the *Method Name* to *Analysis*.

Fil											_									
_	😑 (f)	l 🔝	🙆 🗖 🔹	<b>P</b> C.	*	b 🖬 🛛 🖂	▶	I is			0	۵ 🗹 🖌	8 · ①	k k						
	Status	Run	SV	EV	I/V	Sample ID	Sample	Sample Amount	ISTD1 Amount	Sample Dilut.	Inj.Vol. [µL]	File Name	Sample Type Li	Method With Name	Report Style	Open	Open Calib.	Print		
		-	1	1			%Q	0.000	0.000	1.000		%q_%R	Bypass	Startup						
		>	2	2	1		%Q	0.000	0.000	1.000		%q_%R	Standard	Analysis		~				
	_	-	3	3			%Q	0.000	0.000	1.000		%q_%R	Standard	Analysis		~				
		>>		4			%Q %Q	0.000	0.000	1.000		%q_%R %q %R	Standard Bypass	Analysis Shutdown		~				
		-	3		-		1002	0.000	0.000	1.000	0.000	ved_vex	bypass	Shutdown						

# **5 Data Acquisition**

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

## 5.1 Running a single analysis

1. Open the Single Analysis dialog: select Analysis - Single from the Instrument

window or click on

Sample ID (a)	68224			
Sample	PAH-water			
Comments				
Amount	0		ISTD1 Amount	0
Dilution	1		Inj. Volume [µL]	0
Sample Type	Unknown	$\sim$	Level	1
Method	D:\clarity\DataFiles\WORK4\	Default4		Edit Method
Method Report Style	D:\clarity\DataFiles\WORK4\} Analysis	Default4		Edit Report Style
Report Style nalysis Post Run Set iontrol Send method	Analysis tings User Variables			
Report Style nalysis Post Run Set iontrol Send method	Analysis tings User Variables			Edit Report Style

- Fill in the information on the sample into the Sample ID and/or Sample fields

   a.
- 3. Fill in the Chromatogram File Name (b).

More Info:

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

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

#### More Info:

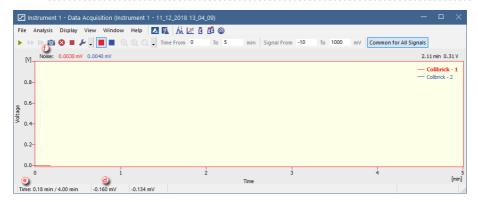
Also it can be triggered by *External Start* from the Chromatograph. The Instrument will get to the *RUNNING* state and the *Single Analysis* dialog will close. The state is visible in the status line on the *Instrument* window.

5. Open the Data Acquisition window to monitor the analysis: select Analysis -

Data Acquisition or click on the Instrument window.

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

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



## 5.2 Pre-evaluating a chromatogram during acquisition

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

on con the Instrument window.

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

More Info:

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

More Info:

🔝 Inst	trument 1	I - Data Acquisitio	n (Instrumen	nt 1 - 11_12_2018	13_04_09)						-	
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Time: 0.	.18 min / 4	.00 min -0.160	mV -0.13	14 mV								

## 5.3 Creating and running a sequence

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

ß	Instrum	ient 1 - :	Sequer	ice D:\c	larity\D	ataFiles\DE	MO1\Se	quence test2	(MODIFIED)									-		×
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									Single Analy:	sis: Ready	- Ready t	o start run V	ial: 1 / Inj	j.: 1		File Nam	e:			

4. Check the checkbox in the first (empty) row in the Run column ©.

The first row will be pre-filled with default basic information on the analysis (such as the method file used).

- 5. Fill in the Sample ID and/or Sample columns.
- 6. Fill in the File Name . (e)

More Info:

You can use variables, for example, %q (*Sample ID*) as a part of the file name. Hold the mouse pointer over the file name field to see resulting name. For more info on variables go to "Chromatogram File Name" in the **Clarity Reference Guide**.

- 7. The SV (Starting Vial) and EV (End Vial) rows (f) will be pre-filled with numbers corresponding to the sample position in the autosampler tray, if you are using an autosampler.
- 8. Fill in volume of the injection in the Inj. Vol. column (g).

- 9. Tick any of the **Open**, **Open Calib.** or **Print options** (b) in case you wish to open measured chromatogram, open measured standard or print the results after each measurement of a sample.
- 10. **Repeat the steps 4-8** for any rows you need to add to the Sequence Table.
- 11. Check the validity of the sequence: select Sequence Check Sequence or click on 82.

More Info:

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

- 12. Save the sequence: select *File Save* or click on 😿 .
- 13. **Run the prepared sequence:** select *Sequence Run* or click on ▶ ().

#### More Info:

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

# **6 Device Monitor**

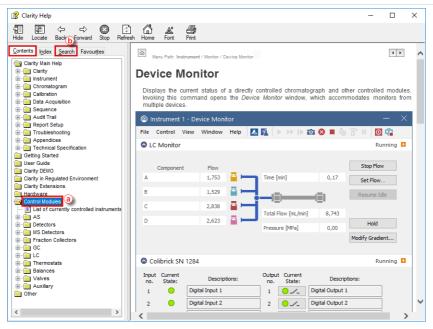
The **Device Monitor** window serves firstly to show the current status of each control module and secondly for direct control of the device.

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

Ø Instrument 1 - Device Monitor
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7 7 Digital Output 7
8 8 Digital Output 8
© DEMO Demo Mode: Ready ♥
For Help, press F1

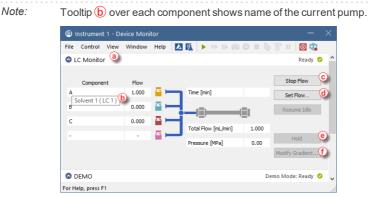
## 6.1 How to set parameters during run

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



## 6.2 How to directly control LC gradient pumps during run

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



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

changed using the Set flow (d) window. When using the *Stop Flow* or *Set Flow* button, gradient cannot be restored and the set flow will be used for the rest of acquisition.

For selected pump models (typically those controlled by Clarity in real time) are available further commands to amend the gradient conditions during run.

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

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

#### How to change gradient

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

Note:

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

Gradent Table           Imme         A         B         C         Flow [mL/min]           1         Initial         10,0         10,0         20,0         60,0         1,000           2         1,00         10,0         20,0         60,0         1,000         1000           3         3,00         0,0         1,000         1,000         1000         1000           5                  1         Initial         10,0         10,0         20,0         60,0         1,000	LC C	ontrol Man	ual Flov	v					$\times$
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								OK Cance	1

# 7 Chromatogram Editing

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

## 7.1 Modifying a peak not integrated correctly

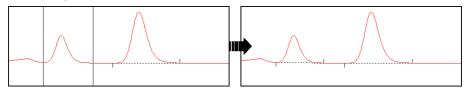
- 1. If you want to re-calculate a peak integrated incorrectly, follow the steps in section Remove a peak from integration. Then add the peak as explained on section Add a new peak.
- 2. If you need to change the position of beginning and / or end of the peak, go to section Modifying the beginning and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

## 7.2 Adding a new peak manually

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

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



## 7.3 Modifying the beginning and the end of a peak

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

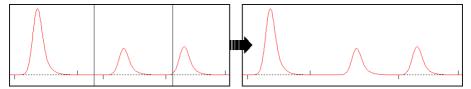
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For Help, press F1 Overlay	~~	For He	elp, press l	F1																Ove	rlay /

## 7.4 Removing a peak from integration manually

- 1. Open the *Chromatogram* window and then the chromatogram.
- 2. Launch the Lock command: select Chromatogram Baseline Lock on the main menu or in the context menu (right mouse-click in the chromatogram curve area) or click on № in the Baseline toolbar (a).
- 3. Click once before and after (b) the apex of particular peak.

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

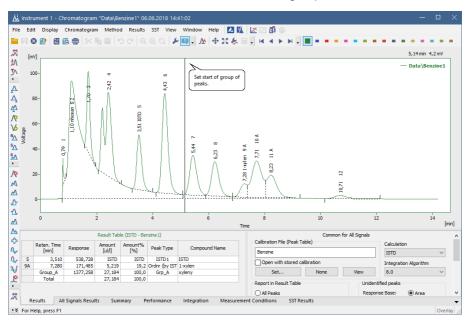


## 7.5 Adding a peak to a group

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

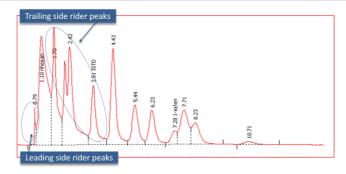
Groups	×
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- 3. Select an existing group from the list and click the Add button.
- Click on the chromatogram for the first time to select the start point and second time for selecting the end point of the interval. Peaks with apexes found in the interval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

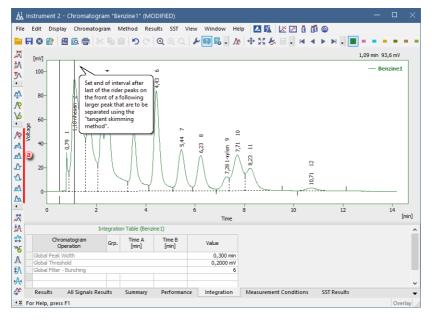


## 7.6 Separating rider peaks by tangent

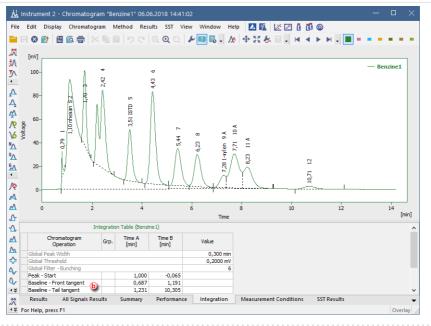
Rider peaks are small peaks which are not well resolved from a large and asymmetrical neighbor but sit on its leading or trailing side.



1. Open the Chromatogram window and then the chromatogram.



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



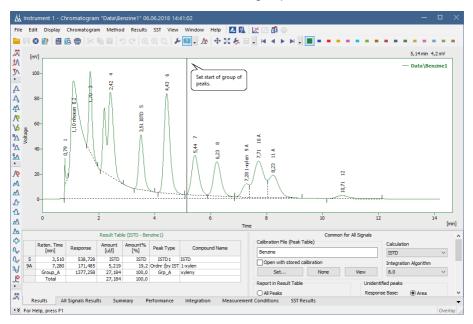
You can also use the Tangent Slope Ratio and Tangent Area Ratio under *Chromatogram - Separation* to establish a threshold for the separation of rider peaks based in those two parameters.

## 7.7 Removing a peak from a group

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

Groups	×
ID A	
Existing Groups:	
A xyleny	
Add Delete Cancel Help	

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

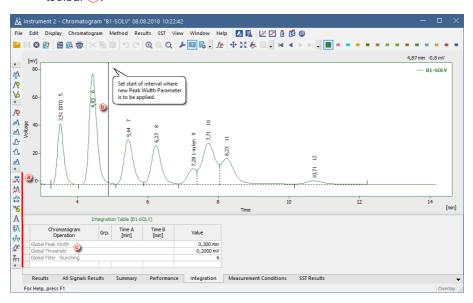


## 7.8 Modifying Minimum Width and Threshold

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

#### For setting the Local Peak Width or Threshold:

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

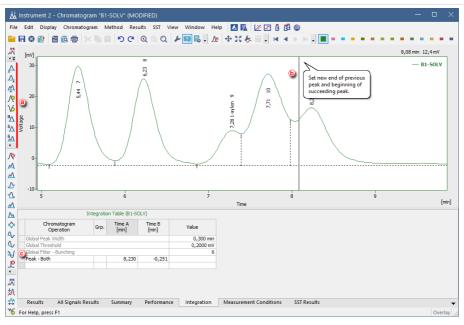


#### For setting the Global Peak Width or Threshold:

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

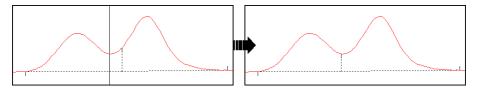
## 7.9 Changing the position of a peak separating line

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



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

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



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

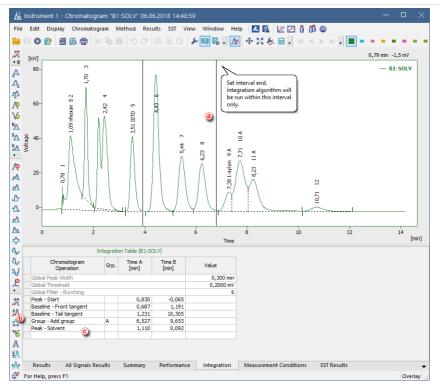
## 7.10 Setting the integration interval

- 1. Open the Chromatogram window and then the chromatogram.
- 2. Set the interval on which to apply the integration (a): select Chromatogram -

Integration - Integration Interval or click to the toolbar (b).

More Info: Subsequent uses of the same command will add further integration intervals to

the previously selected.



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

## 7.11 Adding text and lines to a chromatogram

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

		₩	Global Threshold									
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			Peak								PERSOI	
			Integration	-								
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			Create Label	•	Text		4					
0-			Remove Label(s)	•	Line		2,56					
-			Merge	T								
	L			- 6				-	1		-	1
	0	_	Set Signal Names		2			3	4	5	6	Inte
								Time			(n	nin]

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

#### More Info:

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

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

• Click the OK button to accept the settings.

Text Label	×
Text Ethanol	OK Cancel
Font	Orientation Help
Assign to Workplace Active Signal	Anchor (Text Alignment)  Text Alignment  Text Alignment

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

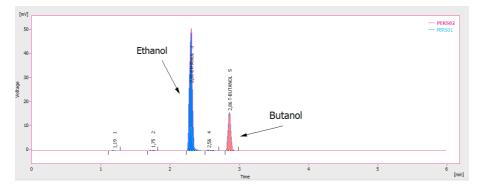
- Select whether you want to add an arrow tip at the beginning, end or at both ends of the line.
- Select the color by clicking on the Color button.
- Enter the Line Width.
- Select the Line Style.
- Assign to the workplace, if you want the line to stay in the same location regardless of the chromatogram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

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

• Click the OK button to accept the settings.



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



#### 7.12 Saving the chromatogram method as a template method

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

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

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

## 8 Calibration

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

## 8.1 Creating a new calibration

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

1. Open the Calibration window: choose Window - Calibration on the

12	Instri	ument 1 - C	alibratio	n Nonan	ne < E	STD											—		×
File	Elle Edit Display Calibration View Window Help 🔼 🛝 🖞 🗗 🖉 🞯 🐨 🎯																		
		1 🖬 🛛	盘 🔯	<b>*</b> *		5	C <sup>1</sup>		R.		紧 1	\$	Automatic	• Ca	libration	• ,/	े 🗖	» ▼	
							Cali	bration Su	ummary Tal	ble (ESTD - N	loname	- Signal	1)						
	Used Compound Reten. Left Right Peak Named Is ISTD Use ISTD Peak Color LOD LOQ Response Resp. Level 1 Use ISTD Peak Color LOD LOQ Response Resp. Level 1																		
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	Compo	unde																	
L																			•
For	Help, p	oress F1																	//

Instrument window or click on

- 2. Create a new calibration file: select File New or click on 📘 (a) .
- 3. Fill in the calibration name in the New File dialog and click OK.
- 4. Open the Calibration Options dialog: choose Calibration Options... or click on 🗾 🜔

Calibration Description:				
			Display Mode	
l			ESTD	~
Number of Signals	1 ~		Recalibration	
Calibration	e Mode		○ Replace	
	<b>A</b>		Average	
<u>A</u> utomatic	<u>C</u> alibrate		No. of Points	
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Apply on	Curve Check		Weight	_
On All Signals	Deviation			
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Units			0,25	
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Default Injected Volume	0		uL	
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	ported presidente			

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

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

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

More Info:

Select Calibration - Add All or click on  $\mathcal{R}$  to add all peaks or the Add Peak  $\mathcal{R}$ /

Add Group  $\Re$  icons to add specific peaks (h). Regardless of the set Current Level (g) the peaks will be added to the first free level.

🛃 Inst	rument 1 - C	alibration	n Nonam	ne < E	STD (N	NODIFIE	D)									—	
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or Help,	press F1																

12. If you selected *Automatic* calibration:

- Name the peaks identified in the Calibration Summary Table (i) by their retention times by typing the Compound Name for each peak. No peak name may be used more than once.
- Fill in the Amount () for each compound into the Calibration Summary Table.

More Info:

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

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		Compound	Reten.	Left	Right	Peak	Named						Response	Resp.	0	Lev	el 1	
	Used	Name	Time	Window	Window		Groups	Is ISTD	Use ISTD	Peak Color	LOD	LOQ	Base	Factor	Response	Amount	Resp. Fact	Rec No.
1	•	Peak 15,000	15,000	0,200 mi	0,200 mi	Ord		None			0,000	0,000	A	0,0000	6207,993	0,000	0,0000	
2	-	Peak 19,800	19,800	0,200 mi	0,200 mi	Ord		None			0,000	0,000	A	0,0000	1320,158	0,000	0,0000	
3	•	Peak 20,367	20,367	0,200 mi	0,200 mi	Ord		None			0,000	0,000	A	0,0000	4266,108	0,000	0,0000	
4	-	Peak 22,250			0,200 mi			None			0,000	0,000	A	0,0000	2415,335	0,000	0,0000	
5	•	Peak 24,033	24,033	0,200 mi	0,200 mi	Ord		None			0,000			0,0000	9089,145	0,000	0,0000	
5	-	Peak 25,950			0,200 mi			None			0,000	0,000	A	0,0000	956,3875	0,000	0,0000	
1	-	Peak 27,500	27,500	0,200 mi	0,200 mi	Ord		None			0,000	0,000	A	0,0000	2767,424	0,000	0,0000	
	-	Peak 31,833	31,833	0,200 mi	0,200 mi	Ord		None			0,000	0,000	A	0,0000	5538,981	0,000	0,0000	
	-	Peak 32,867	32,867	0,200 mi	0,200 mi	Ord		None			0,000	0,000	Α	0,0000	2723,449	0,000	0,0000	
)	-	Peak 36,400	36,400	0,200 mi	0,200 mi	Ord		None			0,000	0,000	A	0,0000	2495,424	0,000	0,0000	
1	-	Peak 38,017	38,017	0,200 mi	0,200 mi	Ord		None			0,000	0,000	Α	0,0000	######	0,000	0,0000	
2	-	Peak 40,100	40,100	0,200 mi	0,200 mi	Ord		None			0,000	0,000	A	0,0000	9049,470	0,000	0,0000	
3	-	Peak 42,767	42,767	0,200 mi	0,200 mi	Ord		None			0,000	0,000	Α	0,0000	5680,966	0,000	0,0000	
4	-	Peak 46,017	46,017	0,200 mi	0,200 mi	Ord		None			0,000	0,000	A	0,0000	3450,639	0,000	0,0000	
5	-	Peak 47,500	47,500	0,200 mi	0,200 mi	Ord		None			0,000	0,000	A	0,0000	698,4496	0,000	0,0000	
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- 13. If you selected *Manual* calibration:
  - Fill in the Amount, the Compound Name and set any other parameters related to the peak on the Calibrate Peak window. This window will open once for each one of the peaks processed.

Calibration - Add Peak	×
Level	Compound
First Free Level 3 Current Level 3	Name         Peak 15.000           Type         Ordinary         ✓           Is ISTD         None         ✓
Identification	Quantification
Identification Window       Search Window       Left Window       0.2       min       Right Window       0.2       min       Peak Selection       Nearest       Veak Selection       Nearest       Peak From Standard       15.000 min	Amount 0 mg Response Base Area Current From Standard Resulting Response [mV.s] - + 6207.99 > + 6207.99
Compound Current 15.000 min Update On	Calibration - adding a new level
< <less< td=""><td>OK Skip Cancel Help</td></less<>	OK Skip Cancel Help

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

#### 8.2 Adding a new calibration level

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

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

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							Ca	libration Sur	nmary Table (	ISTD - PA	H_EPA - S	ignal 1)						
		, Compound	Reten.	Left	Right	Peak	Named			Peak			Response	Resp.		🕘 Le	vel 5	
	Use	d Name	Time	Window	Window	Type	Groups	Is ISTD	Use ISTD	Color	LOD	LOQ	Base	Factor	Response	Amount	Resp. Fact	Rec No.
L	~	NAP	14.917	0.300 min	0.200 min	Ordnr		None			0.000	0.000	A	0.0000	24054.7871	800.000	0.0333	1
	~	ANA	19.750	0.300 min	0.300 min	Ordnr		None			0.000	0.000	A	0.0000	7831.3516	800.000	0.1022	1
	~	FLU	20.333	0.300 min	0.300 min	Ordnr		None			0.000	0.000	A	0.0000	21066.2227	800.000	0.0380	1
	-	PHE	22.217	0.300 min	0.300 min	Ordnr		None			0.000	0.000	A	0.0000	9159.0459	800.000	0.0873	1
	-	ANT	24.000	0.350 min	0.350 min	Ordnr		None			0.000	0.000	A	0.0000	31726.8965	800.000	0.0252	1
	-	FLT	25.900	0.300 min	0.300 min	Ordnr		None			0.000	0.000	A	0.0000	4024.9478	800.000	0.1988	1
	~	PYR	27.467	0.300 min	0.300 min	Ordnr		None			0.000	0.000	A	0.0000	10419.6768	800.000	0.0768	1
	~	BAA	31.800	0.300 min	0.300 min	Ordnr		None			0.000	0.000	A	0.0000	21665.9277	800.000	0.0369	1
	~	CHR	32.833	0.600 min	0.600 min	Ordnr		None			0.000	0.000	A	0.0000	10711.2725	800.000	0.0747	1
D	~	BBF	36.350	0.350 min	0.350 min	Ordnr		None			0.000	0.000	A	0.0000	9686.0918	800.000	0.0826	1
1	-	BKF	37.867	0.350 min	0.350 min	Ordnr		None			0.000	0.000	A	0.0000	0.0000	0.000	0.0000	0
2	-	BAP	40.050	0.500 min	0.500 min	Ordnr		None			0.000	0.000	A	0.0000	35500.3281	800.000	0.0225	1
3	-	DBA	42.733	0.500 min	0.500 min	Ordnr		None			0.000	0.000	A	0.0000	20966.0938	800.000	0.0382	1
4	-	BPE	45.933	0.500 min	0.500 min	Ordnr		None			0.000	0.000	A	0.0000	12994,4248	800.000	0.0616	1
5	~	IPY	47,400	0.700 min	0.700 min	Ordnr		None			0.000	0.000	A	0.0000	2113.2046	800.000	0.3786	1
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User Guide

- 2. Open the calibration file: choose File Open... or click on a.
- Open calibration standard: select File Open Standard... or click on (b).
   More Info:

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

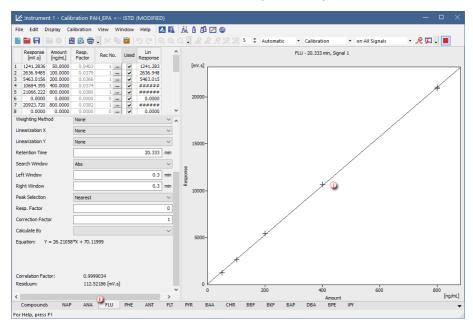
8 Calibration

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

In case more peaks than expected emerge in the calibration, the surplus peaks can be deleted by selecting them in the *Calibration Summary Table* and deleting them from *Calibration - Delete Compound* or clicking on  $\mathcal{R}$ .

- 7. Set the amounts of the particular compounds into the Calibration Summary Table, into the *Amount* column (g) of the respective calibration level.
- 8. Save the calibration file: choose *File Save* or click on  $\overline{\Box}$  (h)

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



#### 8.3 Applying a calibration to a chromatogram

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

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

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Re	esult Table (Und	al - D:\clarity\	(DataFiles (DEM	101\Data\Sam	ole_Vial_8-1)	Ô	College Star Elle (Deale Table)		n for All Signals		
Reten. Time	Area	Height	Area	Height	W05	Compound Name	<ul> <li>Calibration File (Peak Table)</li> </ul>			Calculation	
	• •		• •	• •			(None)			Uncal	
							Open with stored calibra	tion		Integration	Algorithm
							d set	Nono	View	_	~
3.650	56.395	8.050	2.3	2.5	0.09		Sec	NOTIC	VIEW	0.0	
		20,719	6.8	6.4	0.13		Report in Result Table		Unidenti	fied peaks	
3,980	168,916				0.14					e Base:	Area
	168.916 615.509	72.408	24.8	22.5	0.14		All Peaks				
3.980 4.300 5.887	615.509 61.429	7.528	2.5	2.3	0.13				Respons		
3.980 4.300 5.887 6.790	615.509 61.429 338.621	7.528 44.742	2.5 13.6	2.3 13.9	0.13		All Identified Peaks		Respons		Height
3.980 4.300 5.887 6.790 7.040	615.509 61.429 338.621 575.336	7.528 44.742 71.065	2.5 13.6 23.1	2.3 13.9 22.1	0.13 0.12 0.12		All Identified Peaks     All Peaks in Calibration				
3.980 4.300 5.887 6.790 7.040 9.500	615.509 61.429 338.621 575.336 314.014	7.528 44.742 71.065 44.872	2.5 13.6 23.1 12.6	2.3 13.9 22.1 13.9	0.13 0.12 0.12 0.11		All Identified Peaks		Respons		Height
3.980 4.300 5.887 6.790 7.040	615.509 61.429 338.621 575.336 314.014 290.385	7.528 44.742 71.065 44.872 43.461	2.5 13.6 23.1 12.6 11.7	2.3 13.9 22.1 13.9 13.5	0.13 0.12 0.12		All Identified Peaks     All Peaks in Calibration			æ Factor	Height
3.980 4.300 5.887 6.790 7.040 9.500 9.860	615.509 61.429 338.621 575.336 314.014	7.528 44.742 71.065 44.872	2.5 13.6 23.1 12.6	2.3 13.9 22.1 13.9	0.13 0.12 0.12 0.11		All Identified Peaks All Peaks in Calibration Hide ISTD Peaks		Respons	æ Factor	Height
3.980 4.300 5.887 6.790 7.040 9.500 9.860	615.509 61.429 338.621 575.336 314.014 290.385	7.528 44.742 71.065 44.872 43.461	2.5 13.6 23.1 12.6 11.7	2.3 13.9 22.1 13.9 13.5	0.13 0.12 0.12 0.11		All Identified Peaks All Peaks in Calbration Hide ISTD Peaks Scale	1	Respons	æ Factor	Height 0 1 Amount 2
				received the control of the con	r, m         g           g         g           g         g           g         g           g         g           g         g           g         g           g         g           g         g           g         g           g         g           g         g           g         g           g         g           g         g           g         g           g         g           g         g           g         g           g         g           g         g           g         g           g         g           g         g           g         g           g         g           g         g           g         g           g         g           g         g           g         g           g         g           g         g           g         g           g         g           g         g	r, r	r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r	Result Table (Jrcsl - Dr)dsr/lsc (2EMD 1) Data (Sample _ Idd (8-1))         Compound Name         Calibration File (Pesk Table)           0         2         4         6         8           Time           Result Table (Jrcsl - Dr)dsr/lsc (2EMD 1) Data (Sample _ Idd (8-1))           Calibration File (Pesk Table)           0         2         4         6         8           Time           Result Table (Jrcsl - Dr)dsr/lsc (2EMD 1) Data (Sample _ Idd (8-1))         Oc           Calibration File (Pesk Table)           (Mone)         0.020         0.021         0.020           IDen with stored calibra           IDen with stored calibra	r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r         r	Image: Second	

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

16		-				Window Help		🖸 🖥 🚳 🔄 🔄				
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	Reten. Time	D	Amount	Amount%	Peak Type	Compound Name		Calibration File (Peak Tabl	le)		Calculation	,
	[min]	Response	[u]	[%]	Реак Туре	Compound Name		Demo 1			ISTD	
	0.580	3.217 32.441	0.000	0.0				Open with stored calib	ration		Integration Alg	orithm
1	1.380	30,590	0.000	0.0				Set	None	View	8.0	
2	3.650	56.395	1.251		Ordnr (by IST	Chloroform						
2 3		168.916	1.222	14.1	Ordnr (by IST	Trichloroethane		Report in Result Table		Unidenti	fied peaks	
2 3 4	3.980	615,509	1.268			Tetrachlormethan		All Peaks		Respons	se Base: 💿 A	Area
2 3 4 5 6	4.300		1.234			Trichloroethylene		<ul> <li>All Identified Peaks</li> </ul>			0	leight
2 3 4 5 6 7	4.300 5.887	61.429				Bromodichloroeth ISTD		All Peaks in Calibration	1		_	-
2 3 4 5 6 7 8	4.300 5.887 6.790	61.429 338.621	1.202 ISTD	ISTO				Hide ISTD Peaks		Respons	se Factor	0
2 3 4 5 6 7 8 9	4.300 5.887 6.790 7.040	61.429 338.621 575.336	ISTD	ISTD 14.6								
2 3 4 5 6 7 8 9 10	4.300 5.887 6.790	61.429 338.621		14.6	Ordnr (by IST	Tetrachloroethyle Dibromochloromet						
2 3 4 5 6 7 8 9 10	4.300 5.887 6.790 7.040 9.500	61.429 338.621 575.336 314.014	ISTD 1.261	14.6	Ordnr (by IST	Tetrachloroethyle		Scale		Amount [ul]	ISTD1 Am	
2 3 4 5 6 7 8 9 10	4.300 5.887 6.790 7.040 9.500 9.860	61.429 338.621 575.336 314.014	ISTD 1.261 1.210	14.6 14.0	Ordnr (by IST	Tetrachloroethyle		Scale		Amount [ul] 0	ISTD1 Am	
1 2 3 4 5 6 7 8 9 10 11	4.300 5.887 6.790 7.040 9.500 9.860	61.429 338.621 575.336 314.014	ISTD 1.261 1.210	14.6 14.0	Ordnr (by IST	Tetrachloroethyle		Scale	1		ISTD 1 Am	

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

## 8.4 Setting the calibration in the template method

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

- 1. **Open the template method** from the Instrument window by using the *File Open Method...* command.
- 2. Open the Method Setup Calculation dialog: select Method Calculation

on the *Instrument* window.

Method Setup N	oname (M	ODIFIED)										_		×
New Open	Save	Save as	Report setup	Ro Audit trail	Send	method by mail	? Help							
Common for all de	etectors													
Calibration File (Peak Table)		D:\clarity\Data	aFiles\DEMO1\Calib	¢ View		Scale	ale Factor							
a Set	b	New	Clone	None		Scale Fact	or	1						
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- 3. Click the Set... button (a) to select a calibration file for the template method, or create a new calibration file by clicking the New... button (b).
- 4. Change the default calibration type in the Calculations field ©.
- 5. Click *OK* (d) to apply the changes to the template method and then save the changes to the opened method from *File Save Method*.
- 6. You can **modify the calibration file after acquisition**. For more info go to Apply the calibration to a Chromatogram.

#### 8.5 Calibrating with manually entered Response Factors

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

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

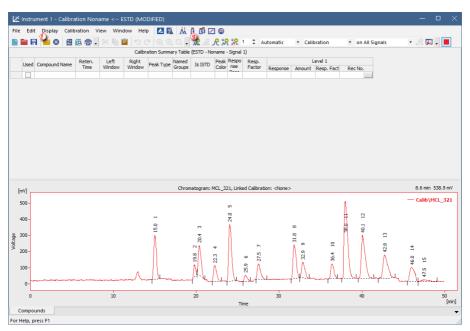
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					Cali	bration Su	ummary Tab	ole (ESTD - N	loname	- Signal	1)						
Used Compour Name	d Reten. Time	Left Window	Right Window	Peak	Named Groups	Is ISTD	Use ISTD	Peak Color	LOD	LOO	Response Base	Resp.		Lev			
Name	Time	Window	Window	Type	Groups						Base	Factor	Response	Amount	Resp. Fact	Rec	No.
Compounds																	•
For Help, press F1																	//

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

alibration Options Defaults				C	
Calibration Description:				Display Mode	
				ESTD	
Number of Signals	1	~		Recalibration	
Calibration	Mode			Replace	
Automatic	Calibrate			Average	
() Manual	Recalibrate			No. of Points	
				10	
Apply on	Curve Check			○ <u>W</u> eight	
On All Signals	Deviation			Weighting Factor	
On Active Signal	0		%	0.25	
Units					
Compound:	Correlation			Search Criteria	_
mg	0			0	%
Enable Response Value (	Change				
Update Retention Time					
Default Injected Volume	0			μL	
Retention Indexes use L	og. Interpolation	with Unr	etaine	d Peak	
Response Factor as Resp	oonse / Amount				

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

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



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

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

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

Ľ	Instr	ument 1 - Calibra	ation resp	onze facto	ors < ES	TD												_		$\times$
File	Ed	it Display Calib	ration V	iew Wind	dow Hel	P 🔼 🎋	Å.	0 Ø 🖸	0											
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						Calibratio	n Summ	ary Table (E	STD - Nor	name - Sigr	nal 1)		<u>_</u>							^
		Compound Name	Reten.	Left	Right		Named	Is ISTD	Peak	Respon	Resp.	Curve Fit		Le	evel 1					
			Time	Window	Window		Groups	15 1510	Color	se Base	Factor	Type	Response		Resp. Fact	Rec No.				
1	~	Peak 15.000		0.200 min				None		A		Free Ca	6207.993	0.000	0.0000	1				
2	-	Peak 19.800		0.200 min				None		A		Free Ca	1320.158	0.000	0.0000	1				
3	~	Peak 20.367		0.200 min				None		A		Free Ca	4266.108	0.000	0.0000	1				
4	~	Peak 22.250 Peak 24.033		0.200 min				None		A		Free Ca Free Ca	2415.335	0.000	0.0000	1				
6	-	Peak 24.033 Peak 25.950		0.200 min 0.200 min				None		A		Free Ca	9089.145 956.3875	0.000	0.0000	1				
7	-	Peak 25.950 Peak 27.500		0.200 min				None		A			2767.424	0.000	0.0000	1				~
		Peak 27.300	27.300	0.200 1111	0.200 1111	orun		INDIAC		^	0.0000	precion_	2/07.424	0.000	0.0000	1				
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For H	elp	press F1																		
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Since **Clarity** 8.0 when constructing calibration curve there is check that calibration curve could be constructed, that means all amounts have nonzero value. In case calibration curve could not be constructed for any compound, no results are calculated (as the total amount could be wrong]. If you do not want to calculate amounts for all identified compounds, you could use free calibration with zero response factor.

#### 8.6 Recalibrating a calibration

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

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

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1									arity\DataFile				30 C5-C15-	RI - Signal	1)			
Τ.		Compound	Reten.	Left	Right	Peak	Named			Peak			Response	Resp.		Lev	vel 1	
ľ	Jsed	Name	Time	Window	Window	Type	Groups	Is ISTD	Use ISTD	Color	LOD	LOQ	Base	Factor	Response	Amount	Resp. Fact	Rec No.
	-	n-Pentane		0.200 min				None			0.000	0.000	A	0.0000	4724.4275	0.000	0.0000	1.
	-	n-Hexane	20.500	0.200 min	0.200 min	Ordnr		None			0.000	0.000	A	0.0000	4384.6177	0.000	0.0000	1.
	-	n-Heptane	28.880	0.200 min	0.200 min	Ordnr		None			0.000	0.000	A	0.0000	8713.0309	0.000	0.0000	1 .
	~	n-Octane	38.693	0.200 min	0.200 min	Ordnr		None			0.000	0.000	A	0.0000	10596.7032	0.000	0.0000	1 .
		n-Nonane	49.687	0.200 min	0.200 min	Ordnr		None			0.000	0.000	A	0.0000	11577.5428	0.000	0.0000	1.
	-	n-Decane	61.063	0.200 min	0.200 min	Ordnr		None			0.000	0.000	A	0.0000	6271.1765	0.000	0.0000	1.
	-	n-Undecan	72.393	0.200 min	0.200 min	Ordnr		None			0.000	0.000	A	0.0000	12734.3308	0.000	0.0000	1.
	-	n-Dodecan	83.017	0.200 min	0.200 min	Ordnr		None			0.000	0.000	A	0.0000	6416.3005	0.000	0.0000	1 .
	~	n-Tridecan	93.273	0.200 min	0.200 min	Ordnr		None			0.000	0.000	A	0.0000	13119.1941	0.000	0.0000	1.
				0.000 min	0.200 min	Ordor		None			0.000	0.000	A	0.0000	6801.6947	0.000	0.0000	1.
	-	n-Tetra	102.720															
F		n-Tetra n-Penta		0.200 min				None			0.000	0.000	A		14341.0531	0.000	0.0000	
													A					
	<b>&gt;</b>						chu	None	Control o Viola		0.000	0.000						
nV]							Chro	None	Sample_Vial_	6-1, Linked	0.000	0.000	ne>	0.0000	14341.0531	0.000	0.0000	1
							Chro	None	Sample_Vial_1	6-1, Linked	0.000 d Calbratio	0.000	ne>	0.0000	14341.0531	0.000	0.0000	1
80							Chro	None	Sample_Vial_	6-1, Linked	0.000 d Calbratio	0.000	ne>	0.0000	14341.0531	0.000	0.0000	1
80								None matogram:	Sample_Vial_	6-1, Linked	0.000	0.000	ne>	0.0000	14341.0531	0.000	0.0000	1
80 60				0.200 min			ú	None	Sample_Vial_	6-1, Linkec	0.000 d Calbratio	0.000	ne>	0.0000	14341.0531	0.000	0.0000	1
80 60				0.200 min			4 66 N	None matogram:	Sample_Vial_	7	0.000 d Calbratio	0.000	ne>	0.0000	14341.0531	0.000	0.0000	1
80 60 40		n-Penta	111.883	ი.200 min ო ყვ			4 66 N	None matogram:	Sample_Vial_	7	0.000 d Calbratio	0.000	ne>	0.0000	14341.0531	0.000	0.0000	1
80 60 40		n-Penta	111.883	0.200 min			4 99 S	None matogram:	Sample_Vial_	6-1, Linked	0.000 d Calbratio	0.000	ne>	0.0000	14341.0531	0.000	0.0000	1
nV]			111.883	ი.200 min ო ყვ			4 66 N	None matogram:	Sample_Vial_	7	0.000 d Calbratio	0.000	ne>	0.0000	14341.0531	0.000	0.0000	1
60 40		n-Penta	111.883	0.200 min 9 9			4 66 N	None matogram:	Sample_Vial_	2:30 7	0.000 d Calbratio	0.000	ne>	0.0000	14341.0531	0.000	0.0000	1 •
80 60 40		n-Penta	111.883	ი.200 min ო ყვ			4 66 N	None matogram:	Sample_Vial_	7	0.000 d Calbratio	0.000	ne>	0.0000	14341.0531	0.000	0.0000	1

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

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

- 4. Select the Level you wish to recalibrate. ⓒ
- Open the Calibration Options dialog: choose Calibration Options... or click on (a).

Calibration Options (D:\clari	ty\DataFiles\DI	EMO_DH	A\Cali	ib\ASTM67 ?	$\times$
Calibration Options Defaults					
Calibration Description:				Display Mode	
				ISTD	$\sim$
Number of Signals Calibration Automatic Manual Apply on O n All Signals	1 O Calibrate Recalibra Curve Ched	ate <sup>(9)</sup> k		Recalibration Replace (b) Average No. of Points 10 Weight	
On Active Signal	0	1	%	Weighting Factor	
Units Compound:	Correlatio	on		Search Criteria	
mg	0			0	%
Enable Response Value C      Update Retention Time     Default Injected Volume     Retention Indexes use L     Response Factor as Response F	og. Interpolation		retaine	µL d Peak	
		OK		Cancel	Help

- 6. Set the Calibration option to Automatic to add the peaks without modification or to Manual to modify them one by one f.
- 7. Set the Mode to Recalibrate (8).
- 8. Select how and whether the new values will be added (Replace, Average, Weighting Factor and Search Criteria) on the *Calibration Options* dialog (h).
- Add peaks to be recalibrated from the calibration standard to the calibration file on the Calibrationwindow using Calibration Add Existing or clicking on Rev.
- 10. If you selected *Manual* calibration:
  - Fill in any parameters related to the peak in the *Calibrate Peak* window. This window will open once for each one of the peaks processed.

ak 12.903	2 📮 R	ecalibration:	1	<b>_</b> ×		
ame	n-Pentane					
Old	New		Departure			
Value	Value	Units	Units	%		
2106.077	17.405	[mV.s]	-2088.672	-99.2		
666.255	5.727	[mV]	-660.528	-99.1		
0.000	0.000	mg				
	U Cold Value 2106.077 666.255	Old         New Value         New Value           2106.077         17.405           666.255         5.727	Image: Image in the second s	Image: Image of the state of the s		

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

# 8.7 Recalibrating a calibration automatically using a sequence

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

- 1. **Open the method file**: use *File Open Method...* on the Instrument window or click on **Sec.**
- 2. **Open the Method Setup Calculation dialog:**select *Method Calculation* **b** on the Instrument window.

Method Setup D:\clarity\DataFiles\DEMO1\Ethanol in blood (MODIFIED)		_		×
	d method by e-mail			
Common for all detectors				
Calibration File (Peak Table) Uiew View	Scale			
Set (a) New Clone None	Scale Factor 1			
Calculations ISTD V Integration Algorithm 8.0 V	Units g/kg			
Author				
Description	Unidentified Peaks			
	Response Base: Area ~			
Created Modified	Response Factor 0 [Am/Rsp]			
Report in Result Table	Calibration Cloning In Sequence			
Hide ISTD Peaks	[None]			
All Identified Peaks     All Peaks in Calibration	t and the second s			
All Peaks in Calibration				
Event Table Measurement Acquisition Integration Calculation Advanced				
Cancel		•	Send Met	thod

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

ile Edi	Sequence V	iew W	indow	Help 🚺 🔼	N A	l 🔀 🖸	0												
) 📄 F	1 🗟 🙆 👼 .	5	- 🗶 🖣	b 🖬 🛛 🛛 🖬	42 💌	- <b>&gt;&gt; 1</b>	) iii (i	6 7 1	0 🏄	7 🗟 8			(0						
	Status	Run	SV	EV	I/V	Sample ID	Sample	Sample Amount	ISTD1 Amount	Sample Dilut.	Inj.Vol. [µL]	File Name	Sample Type	LVI	Method Name	Report Style	Open	Open Calib.	Print
		~	1	1	1	blank		0.000	0.200	1.000	2.000	%q_%R	Unk		D:\darity\ 🖣	Analysis	~		
		-	2	2	1	std1	0.4	0.000	0.200	1.000		%q_%R	Sta	1	D:\darity\	Analysis	~		
		~	3	3	1	std2	0.8	0.000	0.200	1.000	2.000	%q_%R	Sta	2	D:\darity\	Analysis	-		
		~	4	4	1	std3	1.4	0.000	0.200	1.000	2.000	%q_%R	Sta	3	D:\darity\	Analysis	-		
		-	5	5	1	std4	1.9	0.000	0.200	1.000	2.000	%q_%R	Sta	- 4	D:\darity\	Analysis	-		
		-	6	6	1	std5	2.4	0.000	0.200	1.000	2.000	%q_%R	Sta	5	D:\darity\	Analysis	-		
		-	6	6	1	std5	2.6	0.000	0.200	1.000	2.000	%q_%R	Sta	6	D:\darity\	Analysis	-		
		-	7	7	1	0442		0.000	0.200	1.000	2.000	%q_%R	Unk		D:\darity\	Analysis	-		
		-	8	8	1	0445		0.000	0.200	1.000	2.000	%q_%R	Unk		D:\darity\	Analysis	-		

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

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

8. Save the sequence file: select File - Save or click on 😿 . 🕢

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

#### 8.8 Calibrating using clone at first recalibration

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

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

Method Setup STI	DADD (MODIFIED)									×
New Open	Save Save as	Report setup	Audit trail	Send m	ethod by nail	? Help				
Common for all det	ectors									
Calibration File (Peak Table)	(a) test		View		Scale	ale Factor				
Set	New	Clone	None		Scale Facto	or	1			
Calculations	ESTD V Alg	egration brithm 8.0		$\sim$	Units		ul			
Author Description	Administrator				Unidentifier Response I		Area			~
	Created 8/13/2018 12:01:42 PM	8/13/20	Modified 18 1:20:04 PM		Response	Factor	0	[Am/R	sp]	
Report in Resu	ilt Table				Calibration	Cloning In S	Sequence			
Hide ISTD F	C	All Peaks All Identified Peaks All Peaks in Calibra		Þ	%s %L %	iR.				•
Event Table A	IS GC Measureme	nt Acquisition I	ntegration Ca	lculation	Advanced					
<b>П</b> ОК (	Cancel							2:	S <u>e</u> nd Met	hod

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

- Set the row/s for the standard/s. C
- Add a row for a blank, if you wish to.
- Set the row/s for the unknown samples.
- Repeat the row/s for the standard/s after the unknown sample/s.
- Repeat the previous three steps for every unknown sample you wish to add.
- Before running the sequence, go to the following step.

🔂 In	strum	ient 1	1 - Se	quenc	e te	st (MODIFIE	D)												—	
<u>F</u> ile	<u>E</u> dit	Sequ	uence	Viev	v <u>v</u>	<u>N</u> indow <u>H</u> e	ip 🔼	M 14	ć 🔝 @	)			<b>d</b>							
	H	1	<u>0</u>	<b>.</b>	5	୯ ⊁ 🕒	<b>e</b>	E - E -	<b>▶</b>  ▶ i			0	2	🔣 😸 🗸						
C St	atus	Run	sv	EV	I/V	Sample ID	Sample	Comments	Sample Amount	ISTD1 Amount	Sample Dilut.	Inj.Vol. [µL]	File Name	Sample Type	Lvl	Method Name	Report Style	Open	Open Calib.	Print
1		•	1	1	1	1 std1			0,000	0,000	1,000	0,000	%q_%R	Stan	1	std 1	Full 💌	~		
2		-	2	2	1	1 std2			0,000	0,000	1,000	0,000	%q_%R	Stan	2	std2	Full	~		
8		-	3	3	1	1 std3			0,000	0,000	1,000	0,000	%q_%R	Stan	3	std2	Full	-		
•		-	6	6	1	1 BLK			0,000	0,000	1,000	0,000	%q_%R	Blan		BLK	Full	-		
5		-	- 4	- 4	1	1 unkl			0,000	0,000	1,000	0,000	%q_%R	Blan		unkl 1	Full	-		
5		-	7	7		1 std1			0,000	0,000	1,000	0,000	%q_%R	Stan		std 1	Full	-		
		-	8	8		1 std2			0,000	0,000	1,000	0,000	%q_%R	Stan		std2	Full	-		
8		-	9	9		1 std3			0,000	0,000	1,000	0,000	%q_%R	Stan		std2	Full	-		
		-	15	15		1 BLK			0,000	0,000	1,000		%q_%R	Blan		BLK	Full	-		
0		<b>&gt;</b>	14	14	1	1 unkl			0,000	0,000	1,000		%q_%R	Blan		unkl 1	Full	-		
1		-	16	16	1	1 std1			0,000	0,000	1,000		%q_%R	Stan		std 1	Full	-		
2		•	17	17	1	1 std2			0,000	0,000	1,000		%q_%R	Stan	2	std2	Full	-		
.3		-	18	18	1	1 std3			0,000	0,000	1,000	0,000	%q_%R	Stan	3	std2	Full	-		
.4																				
For Hel	p, pre	ss F1									Sing	jie Analys	is: No metho	d sent - Re	eady t	o send met	hod or start s	equence	Vial: 1	/ Inj.: 1

6. Click on 差 to open the Options Dialog. d

٠	Select	Clone	on first	recalibration	<b>e</b>	and click	OK.
---	--------	-------	----------	---------------	----------	-----------	-----

Sequence Option	5		>
Sequence Mode			
Active $\checkmark$			
Ide Time be	fore First Injection		
Idle Time	0 [min]		
Idle Time	U [min]		
Run Lines			
1-13			
Counter (%n)		Format	
Start at:	00	O Automatically	
	① 1     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①     ①      ①     ①     ①     ①     ①     ①      ①     ①     ①     ①     ①     ①      ①     ①     ①     ①     ①      ①     ①     ①     ①     ①     ①     ①      ①     ①     ①     ①      ①     ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①      ①	Manually	
	-		
Reset when:	Run Sequence		
	Open Instrument		
	Onever		
Current Value	1		
Calibration and Se	quence Usage		
O Calibration use	d as specified by user		
Clone on first r	ecalibration (safe calibration usage)		
O Standard Addit			
O Calibration Bra	cketing		
Description:			
	OK	Cancel	Help
	UK	Cancer	пер

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

## 8.9 Compensating for response drift using bracketing

Bracketing is a simplified direct calibration method used to compensate for the variation on instrument response with time. Typical use is for detector response deteriorating or for sample containing compounds staining the column or interacting with it. Bracketing is not useful for random variations. Bracketing may be in place when 2 calibration curves measured on same series of standards have a stable trend and good correlation but they are not the same. In bracketing sequence contains standards, then unknowns, then standards again. Usually two standards are used, more standards could be used if the measuring instrument has a non-linear response. Samples are evaluated on average of both calibrations after both calibrations are measured. As every unknown sample series is demarcated by calibration standards and as such uses a single calibration file, calibration will be cloned from the previous calibration clone whenever an unknown sample or blank follows the calibration standard. Newly cloned calibration file has all responses cleared - apart from the responses from the last series (immediately preceding the current unknown samples) of calibration standards.



#### File Edit Sequence View Window 山玐 Å 🗠 Help 🖹 🔭 🏷 0- ----- 🕨 🕨 🔞 \* 🕒 🖬 Sample Sample Status Run SV Sample L vI TD Type 1 Sta... Sta ~ Standards 2 ~ 2 Sta... Sta 2 3 Sta... 3 ~ Sta 3 4 ~ 4 Unk... Unk Calibration -Unknowns 5 ~ 5 Unk... Unk 6 ~ 6 Unk... Unk ~ 7 Sta... 7 Sta 1 Standards 8 ~ 8 Sta... Sta 9 Sta... 9 ~ Sta 3 ~ 10 10 Unk... Unk Calibration · Unknowns 11 Unk... 11 ~ Unk 12 ~ 12 Unk... Unk 13 13 Sta... ~ Sta Standards 14 ~ 14 Sta... Sta 15 15 Sta... Sta 3 ~ 16 For Help, press F1

- 1. **Open the method that will be used in the sequence**: click *File Open Method*... from the *Instrument* window.
- 2. Open the Method Setup Calculation dialog: click Method Calculation or

from Instrument Window click on Method - Calculation 📾

3. Set the template calibration as Calibration File: click Set... (a) and select the calibration.

Note that this calibration will remain unchanged, newly created clone of the calibration will be used with new responses.

4. Set the name of the cloned calibration (b): you can use predefined parameters (refer to Creating customized file names automatically).

Bracketing in Clarity

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

Method Setup pda_test			$\times$
New Open Save Save as Report setup Audit trail Send method by email			
Common for all detectors			
Calibration File (Peak Table) bracketing_template View Scale Use Scale Factor			
Set Olone None Scale Factor 1			
Calculations ESTD V Integration Algorithm 8.0 V Units UL			
Author Abraham			
Description Unidentified Peaks			
Response Base: Area V			
Created         Modified         Response Factor         0         [Am/Rsp]           8/14/2018         11:51:52 AM         8/14/2018         11:51:52 AM         0         [Am/Rsp]			
Report in Result Table Calibration Cloning In Sequence			
Hide ISTD Peaks			
All Identified Peaks			
All Peaks in Caloration			
Event Table Measurement Acquisition Integration Calculation Advanced			
Cancel	2	Send Me	thod

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

🖄 Inst	trument 1 -	Calibratio	on bracket	ing_temp	late < E	STD (MO	DIFIED)										— (	⊐ >
File E	dit Display	Calibrat	tion View	Window	v Help	山戸	Å Ö	🗗 🗹 🎯										
	🔚 📄 🛛	🔣 🔯	ā. 🤋	< 🕒 🖹	<b>D</b> C		QR		였 1	2 Aut	omatic	• Ca	libration	+ on	All Signals	-	Л. 🗖 🛛	•
	C	(d)				Calbrati	on Summar	y Table (ESTD	- bracket	ing_templa	te - Sigr	al 1)						
Use	Peak A	Time 0.090	Left Window 0.200 min 0.200 min			Named Groups	Is ISTD None None	Use ISTD	Peak Color	LOD 0.000 0.000	LOQ 0.000 0.000		Resp. Factor 0.0000 0.0000	Response 0.0000 0.0000		vel 1 Resp. Fact 0.0000 0.0000	Rec No.	
3 🗸	Peak C	0.423	0.200 min	0.200 min	Ordnr		None			0.000	0.000	A	0.0000	0.0000	3.000	0.0000	0	
Comp For Help,	oounds , press F1	Peak A	Peak B	Peak C	- 104 41	Ontine	(han alaati	ng templat	->				?	×				
						Options		ng_templat	e)									
					Calibrati	on Descrip	tion:				Disp ES	lay Mode ID		~				
					Number Calibrat	omatic		1 Mode O Calibra @ Recalib	-	~		alibration Replace Average of Points	<b></b>					
					Apply o	n All Signals		Curve Ch			0	Neight						

Weighting Facto

Search Criteria

μL

Cancel

%

Help

0.25

0

7. Open Sequence window and create a new sequence: click Analysis - Sequence and then on □ icon.

0

0

Retention Indexes use Log. Interpolation with Unretained Peak

Correlation

0

OK

- 8. Set the sequence according to the following steps (for more details about creating the sequence refer to Creating and running a sequence):
  - Set the row/s for the standard/s. k

On Active Signal

Enable Response Value Change
 Update Retention Time

Response Factor as Response / Amount

Default Injected Volume

Units

Compound: mg

- Add a row for a blank, if you wish to.
- Set the row/s for the unknown samples.
- Repeat the row/s for the standard/s. Note that the sequence must start and end with a row containing calibration.
- Repeat the previous four steps for every "bracket" of unknown samples you wish to add.

ile E	Edit	Sequer	nce Vier	w Windo	w Help	🔺 🕅 📈	12 🗹 (	3											
	H	恁 🛍	ā 🖶 🗸	<b>୬</b> ୧ 🎖	< 🗈 🖹	oz 🖅 🖅 🗸	▶ ▶	iii O = 4	b 🗃 II 🧕	1 2	2 🗄 🛙	3E -							
Sta	atus	Run	SV	EV	I/V	Sample ID	Sample	Sample Amount	ISTD 1 Amount	Sample Dilut.	Inj.Vol. [ul.]	File Name	Sample Type	Lvl	Method Name	Report Style	Open		
		~	1	1		1 std1		0.000	0.000	1.000	0.000	%q_%R	Sta	1	bracketin		~		
		~	2	2		1 unknown1		0.000	0.000	1.000	0.000	%q_%R	Unk		bracketin		-		
		~	3	3		1 unknown2		0.000	0.000	1.000	0.000	%q_%R	Unk		bracketin		~		
		~	4	4		1 blank		0.000	0.000	1.000	0.000	%q_%R	Blan		bracketin		~		
		~	5	5		1 std2		0.000	0.000	1.000	0.000	%q_%R	Sta	1	bracketin		~		
																		•	

#### 9. Set the sequence to operate in the calibration bracketing mode:

- Click on Ficon to open the Sequence Options dialog.
- Check Calibration Bracketing.
- Click OK.

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

Sequence Options			×
Sequence Mode			
Idle Time bet	fore First Injection		
Idle Time	0 [min]		
Run Lines			
1-5			
Counter (%n)		Format	
Start at:	00	O Automatically	
	1	Manually	
Reset when:	Run Sequence     Open Instrument     Never		
Current Value	1		
Calibration and Sec	uence Usage		
O Calibration used	l as specified by user		
	calibration (safe calibration usage)		
O Standard Additi	<u> </u>		
Calibration Brac	keting 🤠		
Description:			
	ОК	Cancel Help	þ

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

More Info:

The results shown while the sequence is running are recalculated at the end of each bracket, when the standard after the unknown sample is acquired. The calibration used is an average of the two calibrations, before and after the unknown.

#### 8.10 Creating a Multisignal Calibration

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

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

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

#### **Prerequisites:**

- [µS/cm] — Calib\10000ppm - Anions - Calib\10000ppm - Cations 150 ---- Calib\15000ppm - Anions - Calib\15000ppm - Cations - Calib\2000ppm - Anions - Calib\20000ppm - Cations 100 Voltage 50 10 9 R 2
- Integrated chromatograms of standards.

Integrated chromatogram of sample.

2

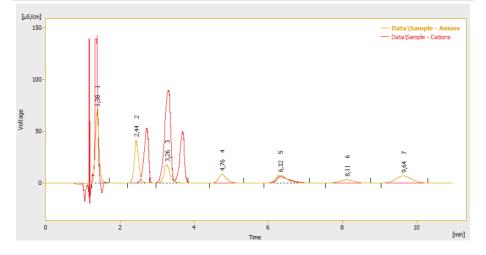
4

6

Time

8

10 [min]



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

If all peaks in the standard chromatogram are unique across all signals it is viable to change the option to *on All Signals*.

7. Set section *Units* to *ppm* field (f) and click *OK* button then.

Edit	Display Calibr	ation Vie	w Winde	ow Help	ムダ						7	
<b>-</b> 6		Q 🖶 🗸	× 🗈 🖹	19 C		Calibration Options (Nonam	e)		?	×	als 🔹 尺 🌉 🗸 🔳	1
)	<b>W</b>					Calbration Options Defaults					<b>(b)</b>	
Used	Compound Name	Reten. Time	Left Window	Right Window	Peak Type	Calibration Description:			Display Mode		Level 1 nse Amount Resp. Fact	Rec No.
						Example of Multisignal Calibre	ration in Clarity 🧿		ESTD	$\sim$		
						Number of Signals	2	~	Recalibration			
						Calibration	Mode		OReplace			
						Automatic	Calibrate		Average No. of Points			
						OManual	ORecalibrate		10	1		
						Apply on O On All Signals	Curve Check		⊖ Weight	1		
						On All Signals     On Active Signal (0)	Deviation		Weighting Factor			
						Units		%	0,25			
						Compound:	Correlation		Search Criteria			
						ppm 🕦	0		0	%		
						Enable Response Value (	Change					
						Update Retention Time						
						Default Injected Volume	0		μL			
						Retention Indexes use L		Inretaine	d Peak			
L						Response Factor as Response Fact	oonse / Amount					
ompou	ndr											
Help, pro							C	к	Cancel H	Help		

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

File			ation Vie															_	
	6	1 🗎 🛛 🖾 🕯	Q 🖶 🗸	* 🖷 🖿	0 C		Q . R.M					Calibration		▼ on A	ctive Signal	•	Л 🗖 -		
							Calibi Wion	Summary Ta	able (ESTD -	Noname - Si	gnal 1)								
	Used	Compound Name	Reten. Time	Left Window	Right Window	Peak Type	Named Groups	Is ISTD	Use ISTD	Peak Color	LOD	LOQ		Resp. Factor			evel 1		
													0		Response		Resp. Fact	Rec No	
		Peak 1,382		0,200 min				None			0,000	0,000		0,0000	295,0630	0,000			
		Peak 2,442		0,200 min				None			0,000	0,000		0,0000	204,9183	0,000			
		Peak 3,260 Peak 4,757		0,200 min 0,200 min				None			0,000	0,000		0,0000	121,1077 77,8398	0,000			
		Peak 6,318		0,200 min				None			0,000	0,000		0,0000	97,3427	0,000			
		Peak 6,318 Peak 8,113		0,200 min				None			0,000	0,000		0,0000	97,3427 50,4286	0,000			
		Peak 9,643		0,200 min				None			0,000	0,000				0,000			
	-	Peak 9,045	9,045	0,200 mm	0,200 mm	Oruni		None			0,000	0,000	•	0,0000	110,0919	0,000	0,0000		
IS/	cm] _						Chromato	gram: 1000	Oppm, Linke	d Calibration	: <none></none>								
ıS/	cm] 80- 60- 40-				4 2	A	Chromato	gram: 1000	Oppm, Linke	d Calibration						_	Calib \1000 Calib \1000p		
	80- 60- 40- 20- 0-				244 2	C QUE	Chromato	gram: 1000	Oppm, Linke		,	1		8,11 6			Calib\10000p		
	80- 60- 40- 20-					ARE	Chromato	4	Oppm, Linke	6	,	1	1			-	Calib\10000p		

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

```
      Instrument 1 - Calibration Noname <-- ESTD (MODIFIED)</td>
      -- □ ×

      File
      Edit Display
      Calibration View Window Help
      Image: A gradient of the state of the state
```

13. Fill the Calibration Summary Table with peaks from the currently selected

(second) signal in chromatogram using  $Add All \Re$  icon. After clicking  $Add All \Re$  icon there will be invoked dialog with question if reuse an already used chromatogram for this calibration. It is necessary to confirm the reuse by clicking Yes button.

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

Clarity		$\times$
?	Chromatogram \Calib\10000ppm.prm has been already used in this calibration. Reuse this chromatogram?	
	Yes No	
Dono	ot warn before reusing a Standard Chromatogram in Calibration.	

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

More Info:

Be noticed the that for resolution what signal of chromatogram is active and is being worked with is given by the *Calibration Summary Table* title's color and displayed number of currently active signal.

	Edit		ration Vie				∆iā 6ā ⊲ , <u>∧</u> € ∧€		R 1 ÷	Automatic	-	Calibration	▼ on A	ctive Signal	-	.R 🗖 🗸		
			_							Noname - Sig				-				
	Used	Compound Name	Reten.	Left	Right	Deals Trees	Named Groups	Is ISTD	Une ICTO	Peak Color	LOD	LOO Respo	Resp.		L	evel 1		
	Useu	Compound Name	Time	Window	Window	Реак туре	Nameu Groups	151510	USE ISTD	Peak Color	LOD	LOQ nse	Factor	Response	Amount	Resp. Fact	Rec No	
1		Peak 1,382	1,382	0,200 min	0,200 min	Ordnr		None			0,000	0,000 A	0,0000	0,0000	0,000	0,0000	0	
2		Peak 2,442	2,442	0,200 min	0,200 min	Ordnr		None			0,000	0,000 A	0,0000	0,0000	0,000	0,0000	0	
3	-	Peak 2,730	2,730	0,200 min	0,200 min	Ordnr		None			0,000	0,000 A	0,0000	279,5434	0,000	0,0000	1	
		Peak 3,260	3,260	0,200 min	0,200 min	Ordnr		None			0,000	0,000 A	0,0000	0,0000	0,000	0,0000	0	
	~	Peak 3,308	3,308	0,200 min	0,200 min	Ordnr		None			0,000	0,000 A	0,0000	627,0532	0,000	0,0000	1	
	-	Peak 3,692	3,692	0,200 min	0,200 min	Ordnr		None			0,000	0,000 A	0,0000	265,0761	0,000	0,0000	1	
'		Peak 4,757	4,757	0,200 min	0,200 min	Ordnr		None			0,000	0,000 A	0,0000	0,0000	0,000	0,0000	0	
		Peak 6,318	6,318	0,200 min	0,200 min	Ordnr		None			0,000	0,000 A	0,0000	0,0000	0,000	0,0000	0	
	-	Peak 6,322	6,322	0,200 min	0,200 min	Ordnr		None			0,000	0,000 A	0,0000	90,3431	0,000	0,0000	1	
)		Peak 8, 113	8,113	0,200 min	0,200 min	Ordnr		None			0,000	0,000 A	0,0000	0,0000	0,000	0,0000	0	
1		Peak 9,643	9,643	0,200 min	0,200 min	Ordnr		None			0,000	0.000 A	0,0000	0,0000	0,000	0,0000	0	
s/	cm] 80- 60-				2,73 1	3,31 2	Chromato m 69	gram: 1000	Oppm, Linke	d Calibration:						alb\10000pp Calib\10000		
	40 20 0		$\mathcal{N}$	,	μĄ	Ą	Λ	$\sim$		6.32		1						-
	20-	V	$\mathcal{N}$	2	ĻΛ	Ą	<u>∧</u>		Tir	6			8			10		-

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

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

	Edit		ation Vie			_	0		0			Calibration			II Signals		R 🗖 🗸		
				~ <u>-</u>			Calibration :					Calibration		• on A	ii Signais	•	JC (41) -		
1		a 10	Reten.	Left	Right								Respo	Resp.		U	evel 1		
	Used	Compound Name	Time	Window	Window	Peak Type	Named Groups	Is ISTD	Use ISTD	Peak Color	LOD	LOQ	nse	Factor	Response	Amount	Resp. Fact	Rec No	
1		Flourides (-)	1.382	0,200 min	0,200 min	Ordnr		None			0.000	0.000	A	0.0000	295.0630	10000.00	33,8911	1	
1		Chlorides (-)	2,442	0,200 min	0,200 min	Ordnr		None			0,000	0,000	λ	0,0000	204,9183	10000,00	48,7999	1	
1	T	Lithium (+)	2,730	0,200 min	0,200 min	Ordnr		None			0,000	0,000	A	0,0000	0,0000	10000,00	0,0000	0	
1	-	Nitrites (-)	3,260	0,200 min	0,200 min	Ordnr		None			0,000	0,000	λ	0,0000	121,1077	10000,00	82,5711	1	
Ì		Natrium (+)	3,308	0,200 min	0,200 min	Ordnr		None			0,000	0,000	λ	0,0000	0,0000	10000,00	0,0000	0	
	<b></b>	Ammonium (+)	3,692	0,200 min	0,200 min	Ordnr		None			0,000	0,000	A	0,0000	0,0000	10000,00	0,0000	0	
Î	-	Bromides (-)	4,757	0,200 min	0,200 min	Ordnr		None			0,000	0,000	λ	0,0000	77,8398	10000,00	128,4690	1	
	-	Nitrates (-)	6,318	0,200 min	0,200 min	Ordnr		None			0,000	0,000	A	0,0000	97,3427	10000,00	102,7299	1	
		Kalium (+)	6,322	0,200 min	0,200 min	Ordnr		None			0,000	0,000	A	0,0000	0,0000	10000,00	0,0000	0	
İ	-	Phosphates (-)	8,113	0,200 min	0,200 min	Ordnr		None			0,000	0,000	λ	0,0000	50,4286	10000,00	198,3001	1	
ſ	-	Sulphates (-)		0,200 min				None			0,000	0,000		0,0000	118,0919		84,6798	1	
;/·	m] 80- 60-				0		Chromato	gram: 1000	Oppm, Linke	d Calibration	: <none></none>						Calib\1000 Calib\10000p		
5/0	80-		1 81		2,44 2	A	Chromato	gram: 1000 	Oppm, Linke	d Calibration				9			Calib\10000p		
5/0	80- 60- 40- 20-		I.			238		gram: 1000	Oppm, Linke		5			8,11 6	_	-0	Calib\10000p		
	80- 60- 40-			/ <i>*</i>		2,26		*	Oppm, Linke	U	5	1	1	-		-0	Calib\10000p		

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

区 Instrument 1 - Calibration Noname < ESTD (MODIFIED)	— 🗆 ×
File Edit Display Calibration View Window Help 🔼 🖾 🖞 🚺 🔀 🕼 🕜	
📔 🖿 🖬 🚞 🛯 🖉 🌆 🗓 🛠 🖷 🖹 り C 🔍 Q Q 🔍 💭 🥀 沢 沢 2 💠 Automatic 🔹 Calibration 🔹 on All Signals 🔹	R 🗖 - 🔳 🔳

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

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

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

	Edit			w Winde		_	≦000 0		<b>R</b> 2 🛟	Automatic	•	Calibration	1	▼ on A	II Signals		R 🗖 🖡	
										Noname - Si								
			Reten.	Left	Right								Respo	Resp.		L	evel 2	
	Used	Compound Name	Time	Window	Window	Peak Type	Named Groups	Is ISTD	Use ISTD	Peak Color	LOD	LOQ	nse	Factor	Response	Amount	Resp. Fact	Rec No.
L		Flourides (-)	1.382	0,200 min	0,200 min	Ordnr		None			0.000	0.000		0.0000		20000.00	0.0000	0
		Chlorides (-)	2,442	0,200 min	0,200 min	Ordnr		None			0,000	0,000	A	0,0000	0,0000	20000,00	0,0000	0
	-	Lithium (+)	2,730	0,200 min	0,200 min	Ordnr		None			0,000	0.000	A	0.0000	419,3152	20000.00	47,6968	1
		Nitrites (-)	3,260	0,200 min	0,200 min	Ordnr		None			0,000	0,000	A	0,0000	0,0000	20000,00	0,0000	0
		Natrium (+)	3,308	0,200 min	0,200 min	Ordnr		None			0,000	0,000	A	0,0000	940,5798	20000,00	21,2635	1
		Ammonium (+)		0,200 min				None			0,000	0,000		0,0000	397,6141	20000,00	50,3000	1
		Bromides (-)	4,757	0,200 min	0,200 min	Ordnr		None			0,000	0,000	A	0,0000	0,0000	20000,00	0,0000	0
	Π	Nitrates (-)		0,200 min				None			0,000	0,000	A	0,0000	0,0000	20000,00	0,0000	0
	-	Kalium (+)	6,322	0,200 min	0,200 min	Ordnr		None			0,000	0.000	A	0.0000	135,5146	20000.00	147,5855	1
		Phosphates (-)	8,113	0.200 min	0,200 min	Ordnr		None			0,000	0.000	A	0.0000	0.0000	20000.00	0,0000	0
	Π	Sulphates (-)	9,643	0,200 min	0.200 min	Ordnr		None			0,000	0,000	A	0.0000	0,0000	20000,00	0,0000	0
	cm]		1.0			1	Chromato	gram: 1500	Oppm, Linke	d Calibration	: <none></none>						alib\15000pp alib\15000	m - Anions ppm - Catio
	100- 50- 0-	v	A	,	- <sup>22</sup> 2	15,5	3,69	~				I						

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

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

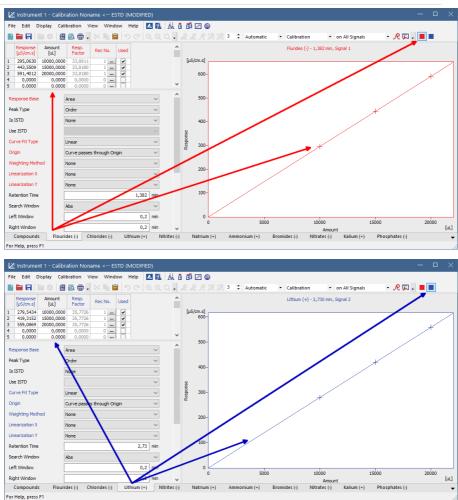
22. Enter value into *Amount* column. As in this guidance this chromatogram to concentration 20 000 ppm of each ion there will be filled in all rows with this value. The last concentration level is finished now.

e	Edit		ation Vie				100 0 10 10 0 - 10 10		R 3 0	Automatic	-	Calibratio	n	+ on A	ll Signals	-	<u>R</u> 🗖 .		
							Calibration	Summary Ta	ible (ESTD -	Noname - Sig	nal 1)								
	Used	Compound Name	Reten.	Left Window	Right Window	Peak Type	Named Groups	Is ISTD	Use ISTD	Peak Color	LOD	LOQ	Respo nse	Resp. Factor			evel 3		
	~	Flourides (-)		0.200 min		Order		None			0.000	0.000	0		Response 591,4012		Resp. Fact 33.8180	Rec No	
	~	Chlorides (-)		0,200 min				None			0,000	0,000		0.0000		20000,00	48,7999		
	-	Lithium (+)		0,200 min				None			0,000	0,000		0.0000		20000,00	0,0000		
	-	Nitrites (-)		0,200 min				None			0,000	0,000		0.0000		20000,00			
	-	Natrium (+)		0,200 min				None			0,000	0,000		0,0000	0,0000	20000,00	0,0000		
	H	Ammonium (+)		0,200 min				None			0.000	0.000		0.0000		20000.00	0,0000		
	-	Bromides (-)		0.200 min				None			0.000	0.000				20000.00			
	~	Nitrates (-)		0.200 min				None			0.000	0.000		0,0000		20000,00		1	
	÷	Kalium (+)		0,200 min				None			0.000	0.000		0.0000		20000.00	0.0000		
	-	Phosphates (-)		0,200 min				None			0,000	0,000		0,0000		20000.00			
	-	Sulphates (-)		0,200 min				None			0,000	0,000			242,6884	20000.00		1	
	cm] 150- 100- 50- 0-	v	Į,		2,44 2	2,26		gram: 2000  ♥ 92.*♥	oppm, Linke	d Calibration:		I		8,11 6			Calib \2000		
	0	unds Flouride		2			4		Tin	6 1e				8		Phosp	10		[

#### More Info:

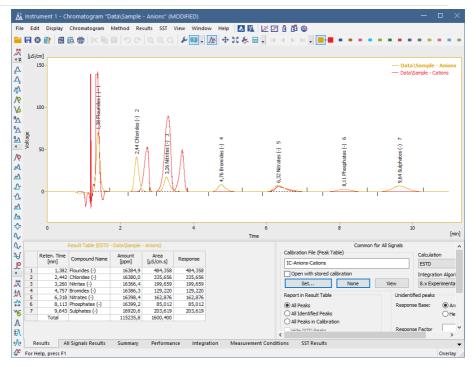
It is possible to review calibration curves for each ion on the respective tabs of individual ions. Be noticed that calibration curve are displayed only for valid signal.

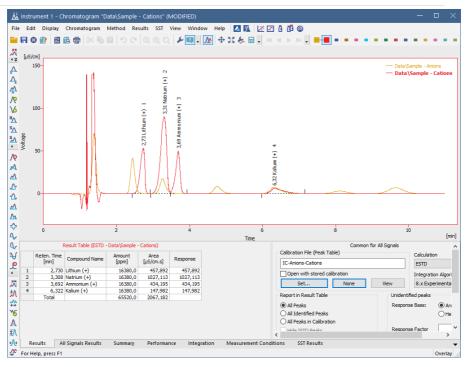
*Note:* If you want to review calibration curve of ion which is calibrated on second signal you need to select second signal within the tab. Signal selection is still located in right upper corner of the *Calibration Window*.

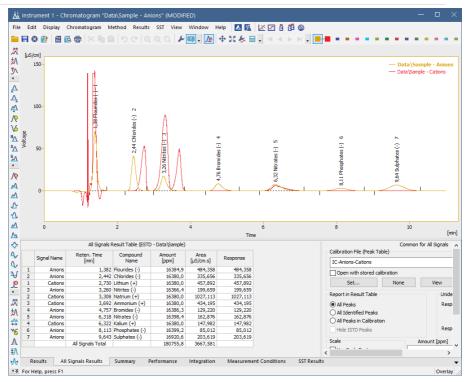


- 23. If calibration is finished do not forget to save it using select *File Save* or click on **a**.
- 24. For calculating result in sample open the **Chromatogram window** select *Window Chromatogram* on the *Instrument* window or click on A and open chromatogram of sample and link the calibration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

#### 8 Calibration

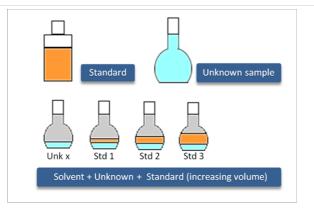






## 8.11 Improving quantification with the standard addition method

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



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

Aethod Setup Demo2 (MODIFIED)	—
New Open Save Save as Report setup Audit trail	Send method by Help e-mail
Common for all detectors	
Calibration File (Peak Table)         STDADD_calib         View           Set         (b)         New         (a)         Clone         None	Scale Use Scale Factor Scale Factor 1
Calculations STDADD C V Integration 8.0	Vinits ul
Author Administrator	Unidentified Peaks Response Base: Area ~
Created Modified 8/13/2018 12:01:42 PM 8/13/2018 12:01:42 PM	Response Factor 0 [Am/Rsp]
Report in Result Table Hide ISTD Peaks O All Identified Peaks All Peaks All Identified Peaks All Peaks All Peaks in Calibration	Calibration Cloning In Sequence
Event Table AS GC Measurement Acquisition Integration Calcul	lation Advanced
R OK Cancel	Send Method

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

- Note: Make sure that each of the samples measured will have a unique calibration name; good example might be using unique sample ID for each sample (duplicating it over the standard addition files) and using it as a name of new calibration by inputting the parameter %q.
- 6. **Open the Calibration window** by selecting *Window Calibration* in the *Instrument* window.
- Open the Calibration Options dialog: choose Calibration Options... or click on Select the STDADD in the Display Mode combobox and click OK.

Calibration Options Defau	lts			
Calibration Description:			Display Mode	
			STDADD	~
Number of Signals	1 ~		Recalibration Replace	
Calibration	Mode		0	
Automatic	Calibrate		Average	
() Manual	Recalibrate		No. of Points	
Apply on	Curve Check		10	
On All Signals			○ Weight	
On Active Signal			Weighting Factor	
O OT ACTVE Signal	0	%	0.25	
Units Compound:	Correlation		Search Criteria	
uL.			0	<b>-</b>
UL	U		U	%
Enable Response Valu	e Change			
Update Retention Tim	e			
Default Injected Volur	ne 0		μL	
Retention Indexes us	e Log. Interpolation with Un	etaine	ed Peak	
Response Factor as R	esponse / Amount			

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

L 📄 🖪	鼠	<u>í</u> 0, 1	a . '	୭ 🕑 🎖	< 🖹	0		. >>	<b>⊳</b> i≊i (	9 = 6	8 11	0 🔎	2 🗄 🖇	Ξ.							
Status	Run	SV	EV 1	I/V Sam	ole ID Si	ample	Sample Amount	ISTD1 Amount	Sample Dilut.	Inj.Vol. [µL]	Correction 1	Correction 2	Analysis UserVar3	File Name	Sample Type	Lvl	Method Name	Open	Open Calib.	Print	Stored Calib.
	-	1	1	1 Samp	e A		0.000	0.000	1.000	1.000	0.000	0.000	0.000	%q	Unknown		STDADD	~			
	~	2		1 stdA_			0.000	0.000	1.000	1.000	0.000	0.000		%q	Standard		STDADD	~			
	-	3		1 stdA_			0.000	0.000	1.000	1.000	0.000	0.000		%q	Standard		STDADD	~			
	-	4	4	1 stdA_			0.000	0.000	1.000	1.000	0.000	0.000		%q	Standard	3	STDADD	~			
	-	5		1 Samp			0.000	0.000	1.000	1.000	0.000	0.000		%q	Unknown		STDADD	~			
	-	6	6	1 stdB_			0.000	0.000	1.000	1.000	0.000	0.000		%q	Standard		STDADD	~			
	-	7	7	1 stdB	2		0.000	0.000	1.000	1.000	0.000	0.000	0.000	%q	Standard	2	STDADD	~			
																	1				

- *Note:* In case you want to use a blank sample too, such sample shall be always put in the sequence before the unknown sample.
- 10. Click on *F* to open the Sequence Options dialog. (e) and select *Standard Addition Measurement* and click *OK*.

Sequence Option	s		>
Sequence Mode			
Active 🗸			
Idle Time be	efore First Injection		
Idle Time	0 [min]		
Run Lines			
1-7			
Counter (%n)		Format	
Start at:	0	Automatically	
	1	Manually	
Reset when:	Run Sequence		
	Open Instrument		
	ONever		
Current Value			
Current value	1		
Calibration and Se	quence Usage		
O Calibration use	d as specified by user		
	ecalibration (safe calibration usage)		
	tion Measurement		
O Calibration Bra	cketing		
Description:			
	ОК	Cancel	Help

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

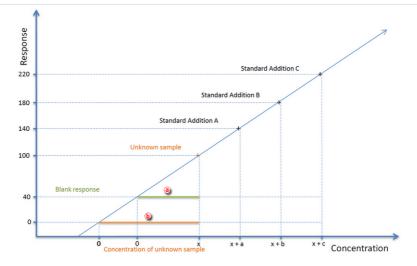
	Calibration View Window			
		<u>n</u> 0	0.0.0	🔍 👳 💬 💠 🖑 🔱 📜 Automatic 💽 Calibration 💿 on All Signals 💽 🦉 📕
Response [mV.s]         Amou [ul.]           4         4003,9735         Unkni 8826,3214         4,0           13693,0250         8,0         13693,0250         8,0           18581,4578         12,0         0,00000         0,0	Factor         Rec No.         Us           own         0,0000         1          ¥           000         0,0005         1          ¥           000         0,0006         1          ¥		[mV.s] 20000-	Sample A - 0, 170 min, Signal 1 Standard 3
0,0000 0,0	000 0,0000 0 0 000 0,0000 0 0	•	15000-	Standard 2 ,+
eak Type s ISTD Ise ISTD	Ordnr None	=	10000-	
Curve Fit Type Inknown Veighting Method	Linear Curve passes through Unknow None	Mn	ι <u>κ</u>	Standard 1 +
inearization X inearization Y Letention Time	None		5000-	+ Unknown
earch Window eft Window	Abs		0	0 5 10 Amount [ul

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

#### How the concentration is calculated

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

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



# 8.12 Using a reference peak to improve compound identification

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

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

				tion View					10 🖸 🎯										
	F	1 🖬 🕄	🔣 🔯	. 🖶 - 🤌	< 🗗 🔚			J 🕈 📲		R 🛠 1	Manual	•	Recal	bration	<ul> <li>on A</li> </ul>	II Signals	-	Л 🏹 -	
				C		đ		Calibrat	ion Summar	y Table (ISTD	- PAH_EPA -	Signal 1)							
		Compound	Reten.	Left	Right	Peak 🥯	Peak	Named	Is ISTD	Use ISTD	Peak Color	LOD	LOO	Response	Resp.		L	evel 1	
b	eu	Name	Time	Window	Window	Selection	Type	Groups	151510	Use 151D	Peak Color	LOD	LOQ	Base	Factor	Response	Amount	Resp. Fact	Rec No.
	1	NAP	14.955	0.300 min	0.200 min	Biggest	Refer		None			0.000	0.000	A	0.0000	1667.879	50.000	0.0300	1 .
	•	ANA	19.778	0.300 min	0.300 min	Nearest	Ordnr		None			0.000	0.000	A	0.0000	433.4798	50.000	0.1153	1 .
	•	FLU	20.342	0.300 min	0.300 min	Nearest	Ordnr		None			0.000	0.000	A	0.0000	1241.283	50.000	0.0403	1
	•	PHE	22.230	0.300 min	0.300 min	Nearest	Ordnr		None			0.000	0.000	A	0.0000	589.1113	50.000	0.0849	1 .
	•	ANT	24.012	0.350 min	0.350 min	Nearest	Ordnr		None			0.000	0.000	A	0.0000	2260.720	50.000	0.0221	1 .
	•	FLT	25.908	0.300 min	0.300 min	Nearest	Ordnr		None			0.000	0.000	A	0.0000	0.0000	0.000	0.0000	0.
		PYR	27.487	0.300 min	0.300 min	Nearest	Ordnr		None			0.000	0.000	A	0.0000	918.7693	50.000	0.0544	1 .
		BAA	31.803	0.300 min	0.300 min	Nearest	Ordnr		None			0.000	0.000	A	0.0000	1571.017	50.000	0.0318	1.
	•	CHR	32.855	0.600 min	0.600 min	Nearest	Ordnr		None			0.000	0.000	A	0.0000	825.6080	50.000	0.0606	1 .
		BBF	36.378	0.350 min	0.350 min	Nearest	Ordnr		None			0.000	0.000		0.0000	695.4784	50.000	0.0719	1 .
	•	BKF	38.000	0.350 min	0.350 min	Nearest	Ordnr		None			0.000	0.000	A	0.0000	3195.949	50.000	0.0156	1
		BAP	40.078	0.500 min	0.500 min	Nearest	Ordnr		None			0.000	0.000		0.0000	2074.632	50.000	0.0241	1 .
		DBA	42.763				Ordnr		None			0.000	0.000		0.0000	1170.654	50.000	0.0427	1 .
		BPE		0.500 min			Ordnr		None			0.000	0.000		0.0000		50.000	0.0577	1 .
	•	IPY	47.473	0.700 min	0.700 min	Nearest	Ordnr		None			0.000	0.000	A	0.0000	0.0000	0.000	0.0000	0

- 2. Open the calibration file: choose File Open... or click on
- 3. Select Refer on the Peak Type column for an easily identifiable compound (i.e. main compound, ISTD standard, any well resolved peak of the matrix) that you will use as a reference (a). To apply the reference peak, *Used* checkbox must be checked (b). If not checked, ordinary peaks would not be recalculated.
- 4. Edit the Left and Right window values to define the range within which the peak should appear. ©

More Info:

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

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

More Info:

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

To add the Peak Selection column:

- Right click anywhere on the table
- Select Set Up Columns to open the relevant window.
- Select Peak Type on the right and click on Show and then Ok.
- 6. Repeat steps 3 to 5 to add more reference peaks.

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

#### More Info:

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

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

Collaboration Summary Table (557) - 0:1(darty/DataFleet/DetO1(Cable )550(#F41 - Signet 1)           Used         Compared Name         Return Res         Right Number         Peakt Type         Oracle Oracle         15170 None         Les 1517         De (D) Peak Color         Color         Regoring Resconse         Resconse Resconse         Resconse Resconse         Resconse Resconse         Resconse Resconse         Resconse Resconse         Resconse Resconse         Resconse         Rescon		l	1 🖿 O	盘 🔯	ā - 🖇	< 🗈 🖻	<b>D</b> C <sup>4</sup>		0.		R 였 1	C Automat	ic •	Recali	bration	• on A	II Signals	-	R 🗖 -	
Unce         Time         Time         Window         Window         Selection         Type         Groups         Is 100         Use Is 10         Peel Coor         COO         Dog         Peer         Percore         Reporter         Repor							Cal	ibration Su	mmary Tabl	e (ESTD - D:	\clarity\Data	Files \DEMO 1 \	Calib\250x	(8HR 1 - 5	ignal 1)					
1         j poslič         4.551         0.100 min         0.000 News	l	Jsed								Is ISTD	Use ISTD	Peak Color	LOD	LOQ	Response					Rec No.
2         orbit         5.333         0.000 min         0.000 min         0.000 k         0.0000         56.2510         0.210         0.0058           0         Instruction         5.433         0.000 min         0.000 min         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000<		-							Groups	None			0.000	0.000						Rec No.
v         Intrain:         5.423         0.000 m         0.000																				1
Image: space         6.053         0.100 min         0.100 min         Neme         0.000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000         0.0000 <t< td=""><td></td><td></td><td></td><td>5,423</td><td>0.100 min</td><td>0,100 min</td><td>Nearest</td><td>Ordnr</td><td></td><td>None</td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td>0.0045</td><td>1</td></t<>				5,423	0.100 min	0,100 min	Nearest	Ordnr		None									0.0045	1
Image: Texture         6.577         0.100 min         0.000 No	T	-	ducose	6.053	0.100 min	0.100 min	Nearest	Ordnr		None			0.000	0.000	A	0.0000	0.0000	0.600	0.0000	1
Image: science         8.127         0.100 min         0.500 min         None         0.000         A         0.000         S1.550         0.239         0.075           Image: black         8.550         0.100 min         0.500 min         None         0.000         A         0.0000         S1.3500         0.239         0.075           Image: black         8.550         0.100 min         0.500 min         None         0.000         A         0.0000         S1.3560         0.600         0.117           Image: black         8.550         0.100 min         0.550 min         None         0.000         0.000         A         0.000         1.233         0.000           Image: black         10.337         0.00 min         None         0.000         A         0.000         2.4850         0.222         0.001           Image: methandist         Codim         None         0.000         A         0.0000         2.4350         0.002         A.0000         0.000         A.0000         A.000		-	malic	6.303	0.100 min	0.100 min	Nearest	Ordnr		None			0.000	0.000	A	0.0000	217.4548	1.003	0.0046	1
w         lssct         8.550         0.100 min         0.000 min <td></td> <td>-</td> <td>fructose</td> <td>6.577</td> <td>0.100 min</td> <td>0.100 min</td> <td>Nearest</td> <td>Ordnr</td> <td></td> <td>None</td> <td></td> <td></td> <td>0.000</td> <td>0.000</td> <td>A</td> <td>0.0000</td> <td>0.0000</td> <td>0.600</td> <td>0.0000</td> <td>1</td>		-	fructose	6.577	0.100 min	0.100 min	Nearest	Ordnr		None			0.000	0.000	A	0.0000	0.0000	0.600	0.0000	1
glyceral         8.900         0.100 min         0.050 min         Nearest         Order         None         0.000         A         0.0000         2.223         0.0000           Concetic         10.337         0.100 min         0.000 min         Nearest         0.000         A         0.0000         24.385         0.202         0.0001           Concetic         10.337         0.100 min         0.000 min         Nearest         0.0001         A         0.0000         24.385         0.202         0.0001           Concetic         10.337         0.100 min         0.000 min         None         0.0001         0.000         0.0000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000         0.000<		-	succinic	8.177	0.100 min	0.100 min	Nearest	Ordnr		None			0.000	0.000	A	0.0000	31.5600	0.239	0.0076	1
acetic 10.337 0.100 min 0.100 min Nearest (h 2ndr None 0.000 A 0.0000 A 0.0000 24.9350 0.202 0.0081 methanol 12.710 0.100 min 0.100 min Biggest Refer None 0.000 0.000 A 0.0000 A 0.0000 0.104 0.0000		~	lactic	8.550	0.100 min	0.100 min	Nearest	Ordnr		None			0.000	0.000	A	0.0000	51.3650	0.600	0.0117	1
rethanol 12.710 0.100 min 0.100 min Biggest Refer None 0.000 0.000 A 0.0000 0.0000 0.104 0.0000		•	glycerol							None			0.000	0.000	A	0.0000	0.0000	1.223	0.0000	1
	æ	~	acetic	10.337	0.100 mig	0.100 min	Nearest (	Ordnr		None			0.000	0.000	A	0.0000	24.9850	0.202	0.0081	1
ethanol 🕘 14.833 0.100 min 0.100 min Last 💌 Refer None 0.000 0.000 A 0.0000 0.0000 10.847 0.0000	٣	V	methanol	12.710	0.100 min	0.100 min	Biggest	Refer		None			0.000	0.000	A	0.0000	0.0000	0.104	0.0000	1
		•	ethanol 🧿	14.833	0.100 min	0.100 min	Last 💌	Refer		None			0.000	0.000	A	0.0000	0.0000	10.847	0.0000	1
		_																		

• Check Used check-box () for reference peak with Peak Selection criteria corresponding to displayed signal (k).

-				·B· • 0							Automat		Recali		• on A	II Signals	•	Я 📮 -	
		Compound	Reten.	Left	Right	Peak	Peak	Named						Response	Resp.			evel 1	
Us	sed	Name	Time	Window	Window	Selection	Type	Groups	Is ISTD	Use ISTD	Peak Color	LOD	LOQ	Base	Factor	Response		Resp. Fact	Rec No
I.	-	oxalic	4.561	0.100 min	0.100 min	Nearest	Ordnr		None			0.000	0.000	A	0.0000	49.0499	0.101	0.0021	1
	•	citric	5.203	0.100 min	0.100 min	Nearest	Ordnr		None			0.000	0.000	A	0.0000	44.8259	0.210	0.0047	1
	-	tartaric	5.423	0.100 min	0.100 min	Nearest	Ordnr		None			0.000	0.000	A	0.0000	65.4451	0.441	0.0067	1
	-	glucose	6.053	0.100 min	0.100 min	Nearest	Ordnr		None			0.000	0.000	A	0.0000	69.3691	0.600	0.0087	1
	-	malic	6.303	0.100 min	0.100 min	Nearest	Ordnr		None			0.000	0.000	A	0.0000	44.0495	1.003	0.0228	1
	•	fructose	6.577	0.100 min	0.100 min	Nearest	Ordnr		None			0.000	0.000	A	0.0000	83.3144	0.600	0.0072	1
	•	succinic	8.177	0.100 min	0.100 min	Nearest	Ordnr		None			0.000	0.000	A	0.0000	44.8535	0.239	0.0053	1
		lactic	8.550				Ordnr		None			0.000	0.000		0.0000	37.3782	0.600	0.0161	1
	•	glycerol	8.900	0.100 min	0.060 min	Nearest	Ordnr		None			0.000	0.000	A	0.0000	46.5463	1.223	0.0263	1
a.	-	acetic		0.100 min			Ordnr		None			0.000	0.000		0.0000	35.3775	0.202	0.0057	1
Ψſ		methanol		0.100 min					None			0.000	0.000		0.0000	4.0787	0.104	0.0255	1
	-	ethanol	14.833	0.100 min	0.100 min	Last 🧐	Refer		None			0.000	0.000	A	0.0000	118.3734	10.847	0.0916	1

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

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

Calibration Description:			Display Mode	
			ESTD	~
Number of Signals	2	,	Recalibration	
Calibration	Mode		Replace	
			Average	
Automatic	O Calibrate		No. of Points	
Manual	Recalibrate		10	
Apply on	Curve Check		0	
On All Signals	Deviation		○ Weight	
On Active Signal	0	%	Weighting Factor	
		70	0.25	
Units Compound:	Correlation		Search Criteria	
uL	0		0	%
			Ľ	^
Enable Response Valu	e Change			
Update Retention Tim	e 🕕			
Default Injected Volur	ne O		μί	
Retention Indexes us	e Log. Interpolation with U	nretaine	d Peak	
Response Factor as R	esponse / Amount			

## 8.13 Calibration adjustments

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

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

19	CI	Guiu	-															0 Gali	Diatio
Ľ	Instru	ıment 1 -	Calibratio	on Nonam	ie < EST	ID (MODI	IFIED)											-	
File	Edi	t Display	Calibrat	tion View	Windo	w Help	山外	Å 0 i	5ª 🛃 🎯										
•	e e	1 🖿 🛛		a. 🤋	< 📭 🗎	<b>D</b> C		Q . R	<b>R</b> R %	R 92 1 1	Autom	atic	• Calibr	ration	• on A	II Signals	•	R 🗖 - 📕	
							C	albration Su	immary Table	(ESTD - Non	ame - Sigr	al 1)							
	Used	Compound	Reten.	Left	Right	Peak	Named	Is ISTD	Use ISTD	Peak Color	LOD	100	Response	Resp.			Level 1		
	Used	Name	Time	Window	Window	Type	Groups	151510	Use ISTD	Peak Color	LOD	LOQ	Base	Factor	Response	Amount	Resp. Fact	Rec No.	
1		comp. 1		0.200 min				None			0.000	0.000		0.0000		0.400		1	
2		comp. 2		0.200 min				None			0.000	0.000		0.0000		0.400		1	
3		comp. 3		0.200 min				None			0.000	0.000			688.9561	0.400		1	
ł		comp. 4		0.200 min				None			0.000	0.000		0.0000		0.400		1	
5		comp. 5		0.200 min				None			0.000	0.000			378.2976	0.400		1	
		comp. 6		0.200 min				None			0.000	0.000			639.2591	0.400		1	
7		comp. 7		0.200 min 0.200 min				None		_	0.000	0.000			355.8900 239.1096	0.400		1	
8	-	comp.8	9.880	0.200 min	0.200 min	Uranr		None			0.000	0.000	A	0.0000	239.1096	0.400	0.0017	1	
								Chrome	togram: Sam	ple Vial 6-1.	Linked Ca	libration	<none></none>						
[m 	V] 30-							Chi Onic	nogram. Jam	pic_10i_0-1,	CHINCO CC		, shones		- D:\c	larity\Da	taFiles\DEM	01\Data\Sampl	e Vial 6-1
													۸		0110			or (outer (outing)	x
	50-							19				6.81	a			ŝ	8		
								5 Q				Ā	902			, i			
	40-							- 13				- 11 1	2			- ľ	1 //		
		-		n v			4	66		~		- 11 1	1			- 1	1 11		
	20-	N		52			3.66	ÄLL		5.90		-IM	1				1.11		
		0.57		17			m	$\Lambda I \Lambda$		ui.		- I V	1			J.	$\Lambda \Lambda$		
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	0			2				4		6				8			10		12 [mir
c	ompo	unds	comp. 1	comp. 2	acomp	. 3 co	mp. 4	comp. 5	comp. 6	comp. 7	ime comp	.8							
	dalo o	ress F1																	

8 Calibration

### Modifying Response Base

User Guide

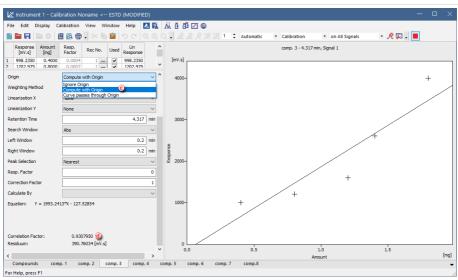
Set the *Response Base* (b) to modify whether the calibration curve will be calculated using *Area* or *Height* of the corresponding peak belonging to the specific compound. Changing the *Response Base* can help to create better fitting of the calibration to not well resolved peaks.

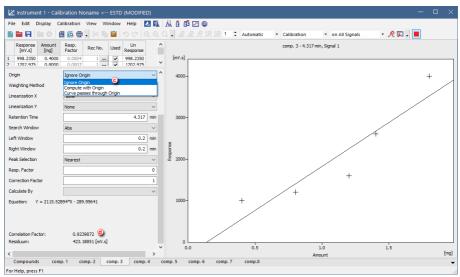
File Edit	Display C	alibration	View Wi	ndow		2 <u>1</u> 7	Á ũ ũ ⊠ ©					- □ >
		X 🙆 🖶	- * •				a. <u>RRR</u> R	Automatic	<ul> <li>Calibration</li> </ul>	<ul> <li>on All Signals</li> </ul>	• 🥂 🏹 • 📕	
Response [mV.s]	Amount [mg]	Resp. Factor	Rec No.	Used	Lin Response	î			comp. 3 - 4.317	'min, Signal 1		
998.2350		0.0004	1	~	998.2350		[mV.s]					
2 1202.975		0.0007	1	-	1202.975							
3 1596.741 4 2601.150		0.0008	1	~	1596.741 2601.150		4000-					+
3997.879		0.0005	1	~	3997.879							
6 0.0000		0.0000	0		0.0000							/
7 0.0000		0.0000	0		0.0000							
8 0.0000 9 0.0000		0.0000	0		0.0000	~					/	
0.0000	0.0000	0.00001			0.0000							
Response Bas	se	Area				~ ^	3000-					
Peak Type		Area Height										
Is ISTD		Area Pero	ent							/	4	
		None					2000-					
Use ISTD						$\sim$	8					
Curve Fit Typ	e	Linear				~	<i>≌</i> 2000−					
Origin		Curve pas	ses through	Origin		~			/	+		
Weighting Me	thod	None				~				Ţ		
Linearization 3		None				~		/	+			
Linearization '		None				~	1000-	+ /				
		None										
Retention Tim				_	4.317	1		/				
Search Windo	w	Abs				~						
Left Window					0.2	min						
Right Window	v				0.2	min 🗸	0.0	0.5		1.0	1.5	
						>				Amount		[r
Compound	ds com	пр. 1 со	mp. 2 c	omp. 3	comp.	4 0	comp. 5 comp. 6	comp. 7 comp.8				

## **Modifying Origin**

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

K Instrument 1 - Ca	libration Noname < ESTD (						_	
—	Calibration View Window							
🗎 🖬 🖬 🖿 🛛	🔣 🔞 👼 🔍 🗶 🐚 🖹 💌		2 . R. R. R 1	R 🔐 1 📫 Automatic	Calibration	on All Signals	• 🥂 🗖 • 🔳	
Response Amount [mV.s] [mg]	Resp. Factor Rec No. Used	Lin A			comp. 3 - 4.317 m	in, Signal 1		
998.2350 0.4000 1202.975 0.8000	0.0004 1 🗸	998.2350 1202.975	[mV.s]					
Origin	Curve passes through Origin	~ ^	4000-					+
Weighting Method Linearization X	Ignore Origin Compute with Origin Curve passes through Origin	0						/
inearization Y	None	~					/	
Retention Time		4.317 min	3000-					
earch Window	Abs	~						
eft Window		0.2 min	e)			/	4	
Right Window		0.2 min	2000-					
eak Selection	Nearest	$\sim$	2000-					
lesp. Factor		0				+		
Correction Factor		1				1		
Calculate By		~			/ +			
Equation: Y = 1897.2	5207*X		1000-	+				
Correlation Factor:	0.9508580 🔕			/				
Residuum:	400.30299 [mV.s]		0.0	0.5		1.0	1.5	
:		>	0.0	0.0		iount		[n
	mp. 1 comp. 2 comp. 3	comp. 4 co	mp. 5 comp. 6	comp. 7 comp.8				
r Help, press F1								





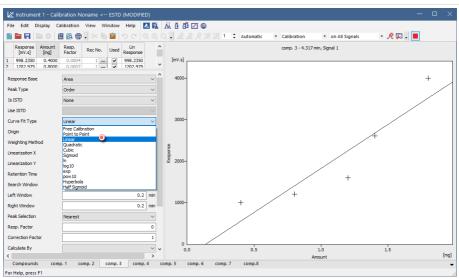
As you can see from the *Correlation factor* (d) values, changing the *Origin* setting from the *Curve Passes through Origin* to *Compute with Origin* improved the curve fit. However, the option *Ignore Origin* has proved to be the best match for the used detector.

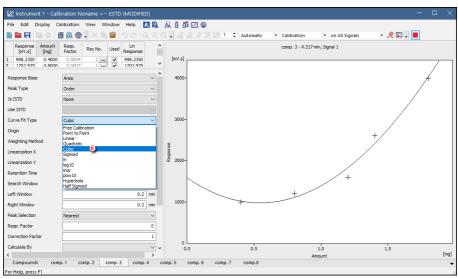
#### Modifying Curve Fit Type

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

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

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



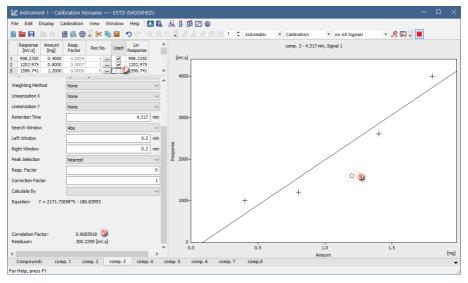


As you can see, changing the *Curve Fit Type* from *Linear* to *Cubic* increased the *Correlation Factor* from 0.951 to 0.999.

#### **Excluding of Measured Point from Calibration**

Clarity also allows excluding any point from calibration. This is helpful in case that the specific measurement went wrong. Following images

describe how to do that. Please keep in mind that the excluded point isn't deleted, the point is still part of the calibration, however, it is omitted from calculation of calibration curve. To exclude the selected measurement point from the calibration simply uncheck that measurement in the *Used* (f) column. The excluded point in the graph of calibration curve will be changed from cross to empty circle (g) and calibration curve *Equation* and Correlation Factor (h) will be recalculated.



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

## 8.14 Normalized Area % Calculation

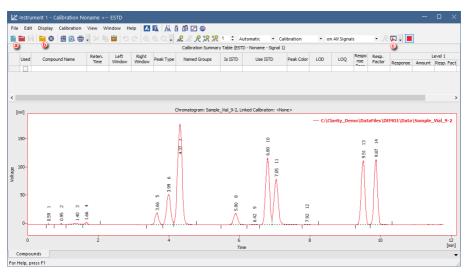
For Normalized Area% calculation no specific settings are necessary, the calculation results are always present in the *Area*% column in the Result table.

## 8.15 Normalized Amount % Calculation

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

A) Application of specific Response Factors

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



- 2. Create a new calibration file: select *File New* or click on (a) and insert name for this calibration.
- Open calibration standard: select *File Open Standard...* or click on 
   More Info:

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

4. **Open the Calibration Options dialog:** select *Calibration - Options...* or click on **S** (c).

Calibration Options (Nona			?	×
Calibration Options Defaul Calibration Description:	0		Display Mode	(b)
Example for normalized an	nount		NORM	<b>S</b>
Number of Signals Calibration	1 Mode Calibrate Recalibrate	~	Recalibration Replace Average No. of Points	
Apply on On All Signals On Active Signal Units	Curve Check Deviation 0	%	10 O Weight Weighting Factor 0.25	
Compound:	Correlation		Search Criteria	%
Enable Response Value     Update Retention Time     Default Injected Volum     Retention Indexes use     Response Factor as Re	e 0 Log. Interpolation with U	Inretaine	uL ed Peak	
	C	К	Cancel	Help

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

Calibration Options (Nona	ime)		?	$\times$
Calibration Options Defau	lts			
Response Base	Area	$\sim$		
Origin	Curve passes through Origin	$\sim$		
Curve Fit Type	Free Calibration 🚺	$\sim$		
Weighting Method	None	$\sim$		
Linearization X	None	$\sim$		
Linearization Y	None	$\sim$		
Identification Windows Search Window Left Window Right Window	Abs     Rel     .200 min 10.000 %     .200 min 10.000 %			
Peak Selection	Nearest	$\sim$		
Set All	Now For Current Signal 🧕			
	ОК	Cancel	Н	elp

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

#### More Info:

Select *Calibration - Add All* or click on  $\mathcal{R}$  to add all peaks or the Add Peak  $\mathcal{R}$  Add Group  $\mathcal{R}$  icons to add specific peaks.



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				Calibrati	ion Summar	y Table (NO	RM - nor	malized_am	ount_n	ormaliza	ation - Signa	al 1)								
			Reten.	Left	Right		Named		Peak	Respo	Resp.		Le	vel 1						
	Used	Compound Name	Time	Window	Window	Peak Type	Groups	Is ISTD	Color	nse		Response	Amount	Resp. Fact	Rec No	<b>.</b>				
1	~	Compound A	3.660	0.200 min	0.200 min	Ordnr		None		A	1.5000	148.2831	0.000	0.0000	1					
2	~	Compound B	3.990	0.200 min	0.200 min	Ordnr		None		A	1.4000	442.6730	0.000	0.0000	1					
3	~	Compound C	4.320	0.200 min	0.200 min	Ordnr		None		A	1.3000	1611.800	0.000	0.0000	1					
ł		Compound D		0.200 min				None		A			0.000	0.0000	1					
5		Compound E		0.200 min				None		A	1.1000	5.5150	0.000	0.0000	1					
5		Compound F		0.200 min				None		A		913.3987	0.000	0.0000						
		Compound G		0.200 min				None		A		674.6443	0.000	0.0000						
		Compound H		0.200 min				None		A		827.9039	0.000	0.0000						
	~	Compound I	9.870	0.200 min	0.200 min	Ordnr		None		A	0.6000	800.3847	0.000	0.0000	1					
(n	v]				Chro	omatogram:	Sample_	Vial_9-2, Lir	iked Ca	alibration	n: normalize	ed_amount_			DataFiles	s\DEM01	\Data\	Sample	e Via	1 9-1
1	50-				Chro	2	A	Vial_9-2, Lir	iked Ca		n: normalize	~		n Cy_Demo\[	DataFiles	s\DEMO1	\Data \	\Sample	e_Via	ıl_9-;
1					Chro	1 ound B 2	A	Vial_9-2, Lin	iked Ca	4	2	-			λ	1	\Data\	\Sample	e_Via	ıl_9-;
1	50-				Chro		Sample_ Combined C	Vial_9-2, Lir	ked Cz		2	~			λ	DEMO1	\Data \	\Sample	e_Via	i]_9-;
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1	50- 50- 0	unds Comp		Compour	1	3.66 Compound A 1 3.99 Compound B 2	4.32 Compared C 3	Vial_9-2, Lin	Τ-4	o 5:90 Compound D 4	6.42 Compound E 5	~	- C:\Clarif		951 Compound H B	9.87 Compound 1-9	1	\Sample		:- <b>9_14</b>

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

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

Report       Response       Anountity       Description       Compand 4	🕂 Inst	trum	ent 1 - Cl	nromatogram "C:\۱	Clarity_Demo	\DataFiles\(	DEMO1\Dat	a\Sample_Via	al_9-2" (MOC	IFIED)								-	
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3       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9       9	^	150-						1			- Pi								
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Note         Provide         Provide         Office         Provide         Office           1         3         4         3         4         3         4         3         4         3         4         3         4         3         6         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         <			Re	sult Table (NORM - C:	Clarity_Demo	DataFiles\DEM	01\Data\Sam	ple_Vial_9-2)					Comm	on for All	Signals				
Immo         Response         D         (%)         Peer type         Name         Correction         (Clothy, Demo Date)         (Demonstrate Calibration         (Meering)         (Demonstrate Calibration         (Demonstrate Calibration         (Demonstrate Calibration         (Demonstrate Calibration         (Demonstrate Calibration         (Demonstrate Calibration         (Demonstrate Calibration)         (Demonstrate Calibration) <td>9</td> <td>Re</td> <td>ten Time</td> <td></td> <td>Amount</td> <td>Amount%</td> <td></td> <td>Compound</td> <td>Total</td> <td>C</td> <td>alibration File (Peak</td> <td>k Table)</td> <td></td> <td></td> <td></td> <td>Calculat</td> <td>ion</td> <td></td> <td></td>	9	Re	ten Time		Amount	Amount%		Compound	Total	C	alibration File (Peak	k Table)				Calculat	ion		
1       3.660       148.283       222.425       4.0       Order Free       Compand A       0.000         2       3.590       49.27       Order Free       Compand B       0.000         3       4.320       161.1800       2005.30       3.7       Order Free       Compand B       0.000         3       4.320       161.1800       2005.30       3.7       Order Free       Compand B       0.000         4       2.877       164.835       177.2       Order Free       Compand B       0.000         6       5.500       91.2583       821.527       1.45.1       Order Free       Compand B       0.000         7       7.474       67.2683       533.127       -7.7       Order Free       Compand B       0.000         8       5.510       827.904       575.533       10.4       Order Free       Compand B       0.000         9       5.570       800.35       500.0       Order Free       Compand B       0.000         1       Total       800.35       500.0       Order Free       Compand B       0.000         9       5.700       800.35       500.0       Order Free       Compand B       0.000         1 <td>4</td> <td></td> <td></td> <td>Response</td> <td></td> <td>[%]</td> <td>Peak Type</td> <td></td> <td></td> <td></td> <td>C:\Clarity Demo\Dr</td> <td>ataFiles</td> <td>DEMO2\C</td> <td>alib \norma</td> <td>alized am</td> <td>NORM</td> <td></td> <td>~</td> <td></td>	4			Response		[%]	Peak Type				C:\Clarity Demo\Dr	ataFiles	DEMO2\C	alib \norma	alized am	NORM		~	
1       3-390       #44.660       2634.42       11.10       Odor Frie       Compound 0       0.100         3       6.509       55.10       Odor Frie       Compound 0       0.000         5       6.400       5.099       5.099       5.090       1.10       Odor Frie       Compound 0       0.000         6       6.500       9.2638       538.127       9.7       Odor Frie       Compound 0       0.000         8       5.130       827.592       1.13       Odor Frie       Compound 0       0.000         8       5.130       827.592       1.13       Odor Frie       Compound 0       0.000         8       5.130       827.592       1.13       Odor Frie       Compound 1       0.000         8       5.130       827.592       1.10       Odor Frie       Compound 1       0.000         9       5.870       800.355       460.211       6.000       1       Packis in Cabrination       Respone Factor       0         1       Total       70.00       1       0       1       1       0       1         1       Cole State Factor       1       1       Notice Factor       0       1       1       1						4.0					Onen with stored	d callbrat					teres all second large		
4       5.897       164-435       197.292       1.51       Oddr Free       Compand 0       0.000         5       6.400       5.099       1.0047       Free       Compand 1       0.000         6       6.500       91.2858       621.572       1.48       Ordr Free       Compand 1       0.000         7       70.477       67.268       53.91.27       3.73       1.04       Ordr Free       Compand 1       0.000         8       6.510       67.5764       57.533       1.04       Ordr Free       Compand 1       0.000         7       Total       0.003       5559.699       100.0       Ordr Free       Compand 1       0.000         8       6.510       27.564       57559.699       100.0       Ordr Free       Compand 1       0.000         0       1000       0.000       0.000       Ordr Free       Compand 1       0.000       0       2												_				_	ion Algorithm	-	
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6       5.500       912.538       252.572       14.6       Order Free       Compound F       0.000         7       7.074       672.658       5531.27       0.077       Free       Compound F       0.000         8       9.510       827.904       579.533       10.4       Order Free       Compound H       0.000         9       5.510       827.904       579.533       10.4       Order Free       Compound H       0.000         9       5.510       827.904       579.533       10.4       Order Free       Compound H       0.000         9       5.510       827.904       5555.609       800.05       Order Free       Compound H       0.000         9       6.87.90       8.00.05       Order Free       Compound H       0.000       Amount I       Heals in Calibration         9       0.00.0       0       0       1       Istroit Amount I										R	eport in Result Tabl	de			Unidentit	fied peaks			
8         9.510         827.904         579.533         10.4 Order Free         Compound H         0.000           9         9.5.00         800.3251         8.6 Order Free         Compound H         0.000           1         Total         5559.899         100.0         Image: Compound H         0.000           Scale         Amount I         Distance         Image: Compound H         0         Image: Compound H           Image: Compound H         0.000         Image: Compound H         0.000         Image: Compound H			6.800	912.858	821.572	14.8	Ordnr Free		0.000	(	All Peaks				Respons	e Base:	Area		
8       5.30       62/394       5/4.33       10.4       Gordy Free       Compound T       0.000         7       Tobal       60.335       5550.899       1000       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       1       Intel® in Calibration       Intel® in Calibration       Intel® in Calibration       0       0       0       0       0       0       0       1       0       0       1       Intel® in Calibration       Inte										Ċ	All Identified Peal	ks					Height		
Total       S559.899       100.0       Impact of the state of th										C	All Peaks in Calibr	ration							
Scale     Amount ]     ISTD 1 Amount ]       Scale Scale Factor     0     2       Scale Factor     1     Duton       Units     0     1       O     0     1       O     1     Duton       O     1     Duton       O     1     Name       Value     1     Analysis Variables       Name     Value     1       1     Analysis Variables       1     Analysis Variables       Name     1       1     Analysis Variables       2     Analysis Variables	vĽ			000.303			Unun mee	Compound 1	0.000	E E	Hide ISTD Peaks				Respons	e Factor	0		
Use Scale Factor       0       2          Scale Factor       1       Inj. Volume [J4]       Diution         Units       ul       0       1         Auber Vanibles       Name       Value       1         Name       Value       1       Method/ser/vr1       0         2       Analysis/JoerVar1       0       2       Method/ser/vr2       0	ī.										cala.								
Scale Factor     1     Urits     Urits     Diuton       Units     ui     0     1       Of User Variables     All Signals Results     Method UserVariables       Name     Value     0     1       1     AnalysisticerVaria     0     1       2     AnalysisticerVaria     0     2       2     Method UserVariables     0     2	J													Amo		15			
Inits     ull     0     1       Units     0     1       Quest Valueles     Analysis Vanables     Method Variables       Name     Value     1       1     Analysis Vanables/varia     0       2     Analysis Vanables/varia     0	0												1						
All Signals Results     Summary     Performance     Integration     Measurement Conditions     SST Results	2									5	ale Factor			Inj. Volu		Di	lution		
Analysis Variables         Method Variables         Method Variables           Name         Value         1         Name         Value           1         Analysis/LerVir1         0         1         Method.serVir1         0           2         Analysis/LerVir2         0         2         Method.serVir2         0	×									U	nits		ul		0		1		
Analysis Variables         Method Variables         Method Variables           Name         Value         1         Name         Value           1         Analysis/LerVir1         0         1         Method.serVir1         0           2         Analysis/LerVir2         0         2         Method.serVir2         0	A									0	User Variables								
Name         Value         Value         Value           1         AnalysistuerVari         0         1         Method.tserVari         0           2         AnalysistuerVari         0         2         Method.tserVari         0           Results         All Signals Results         Summary         Performance         Integration         Messurement Conditions         SST Results															والمراجع المرجعا				
1     AnalysisiserVar1     0     1     Method.iserVar1     0       2     AnalysisiserVar2     0     2     Method.iserVar2     0	¥.									~			(alua	14		162	Value		
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Results All Signals Results Summary Performance Integration Measurement Conditions SST Results	1													_					
	λ									2	AnalysisUserVar	r2		2	MethodUs	erVar2			
		Resu	Its Al	I Signals Results	Summary	Performance	e Integra	ition Mea:	surement Con	ditions	SST Results			-					
	•																		Overlay

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

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

#### User Guide

	Display Ca						00⊡ ⊡ © "R. R. P. R. %	R 1 ≑ Au	omatic + Ci	alibration	• or	All Signal	s	- <i>R</i>	<b>F</b> .	1	
0	ю								- Noname - Signal 1						C	-	
Used	Compound	Name	Reten. Time	Left Window	Right Window	Peak Type	Named Groups	Is ISTD	Use ISTD	Peak Color	LOD	LOQ	Respo	Resp. Factor	Response		Level 1 Resp. Fa
imV]						c	Chromatogram: Samp	ole_Vial_9-2, Lini	ed Calibration: <n< td=""><td>one&gt;</td><td>— c:\d</td><td>arity_Der</td><td>no\Data</td><td>aFiles\Di</td><td>MO1\Data</td><td>\Sample_</td><td>_Vial_9-;</td></n<>	one>	— c:\d	arity_Der	no\Data	aFiles\Di	MO1\Data	\Sample_	_Vial_9-;
nV] 150- 100- 50-						3.66 5 3.39 6 0	Chromatogram: Samp	ole_Vial_9-2, Lini	01 02 00 00 00 00 00 00 00 00 00 00 00 00	ne>	— c\d	arity_Der	no\Data 81 196	aFiles \DI	:MO1\Data	\Sample_	_Vial_9-;

- 2. Create a new calibration file: select *File New* or click on **(a)** and insert name for this calibration.
- Open calibration standard: select File Open Standard... or click on b.
   More Info: Select a measured and qualitatively evaluated chromatogram where all peaks are available.
- 4. **Open the Calibration Options dialog:** select *Calibration Options...* or click on **S**(**c**).

Calibration Options (Nonar	ne)		?	×
Calibration Options Default	a			
Calibration Description:			Display Mode	a
Example for normalized am	ount		NORM	<b>9</b>
Number of Signals Calibration Automatic Manual Apply on On All Signals On Active Signal	1 Mode © Calibrate ○ Recalibrate Curve Check □ Deviation 0	%	Recalibration Recolar Content of Points Recolar Content of Points Recola	
Units Compound: mg	Correlation		Search Criteria	%
Enable Response Value     Update Retention Time     Default Injected Volume     Retention Indexes use     Response Factor as Ret	e 0 Log. Interpolation with U		μL 2d Peak Cancel	Help

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

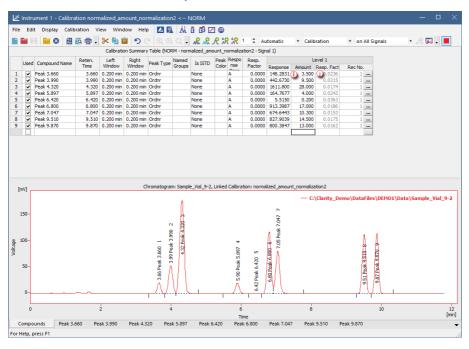
Calibration Options (Nonam	e)		?	×
Calibration Options Defaults				
Response Base	Area	$\sim$		
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Curve Fit Type	Linear 🚺	$\sim$		
Weighting Method	None	$\sim$		
Linearization X	None	$\sim$		
Linearization Y	None	$\sim$		
Identification Windows				
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Right Window	0.200 min 10.000 %			
Peak Selection	Nearest	$\sim$		
Set All No	w For Current Signal 🛛 🧕			
	ОК	Cancel	Help	,

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

#### More Info:

Select *Calibration* - *Add All* or click on  $\mathcal{R}$  to add all peaks or the Add Peak  $\mathcal{R}$  / Add Group  $\mathcal{R}$  icons to add specific peaks.

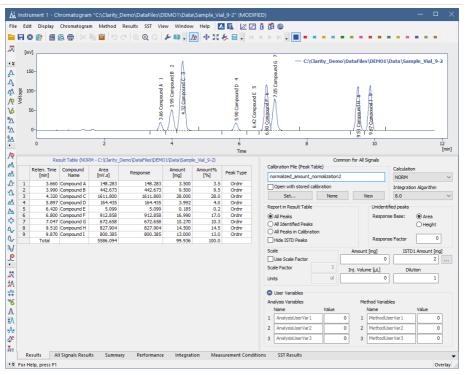
10. Insert values in *Amount* column (i). These values represent actual fraction composition of the standard sample. Note that *Response Factor* (j) values are calculated immediately.



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

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

#### 8 Calibration



## 9 Results and Calculations

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

## 9.1 User Columns

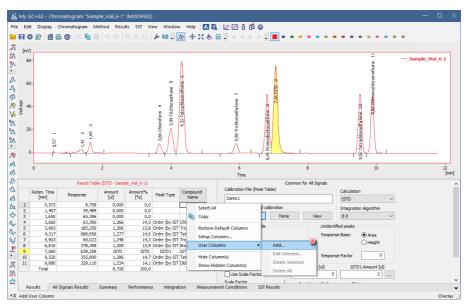
This article describes how to append a new column with user-defined calculation to the *Chromatogram* - *Result Table*. For more details about User Columns refer **Reference Guide Manual**.

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

1. Open Chromatogram window: select Window - Chromatogram from the

*Instrument* window or click on *M* icon.

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



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

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

I Add User	Column				×	<	
Title	Ratio Chlorof	orm/ISTD	Units		ок	]	
			alculate Total		Cancel	Select Compound	×
Expression:		(i)			Help	Select compound	$\sim$
[Chloroform	n\$Area]/[ISTD\$Are					Bromodichloroethane (9)	
Opers: () + - * != <= > >	abs acos asin atg cos exp ln log max min round	Columns: Capacity Eff/I Symmetry/Talling Resolution Response Area Height Area [%] Height [%] W05	^	Variables: Sample Amount Sample Dilution Injection Volume ISTD 1 Amount ISTD2 Amount ISTD3 Amount ISTD5 Amount ISTD5 Amount ISTD6 Amount ISTD7 Amount ISTD7 Amount	^	Chivoform ISTD Tetrachiornethane Tetrachioroethylene Trichioroethylene Trichioroethylene	
	sin v	Reten. Index Despense Easter Special Va	alues 🕦 👻	ISTD9 Amount	~	OK Cancel Help	

- 8. Click OK (i) in Add User Column dialog.
- 9. New User Column is added in the end of Result Table ().

				Method Resi				\$ ■ • • •						
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								Time						
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	Reten.		Response	Amount	Amount%	Peak Type	Compound	Ratio			rable)		Calculation	
	[min]			[u]	[%]		Name	Chloroform/ISTD		Demo1			ISTD	`
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2		.650	65,3					0,099		Set	None	View	8.0	
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7 8		,903	69,0 378,2				Bromodichloro	0,099		All Identified Peak			⊖ Height	
9		,060	639,2		ISTD		ISTD	0,099		All Peaks in Calibra	tion			_
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										Scale Factor	1		2	

## 9.2 User Variables

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

## A) Setting of Analysis User Variables in Single Analysis window

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

- 2. Unroll the Analysis User Variables section, click on the chevron button (a).
- 3. Define **Name** of the variable **b**.

More Info:

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

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

	(b)Name			Value		
Variable 1	AnalysisUserV	/ar1			0	
Variable 2	AnalysisUser	/ar2			0	
Variable 3	AnalysisUserV	/ar3			0	
		٩				
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nalysis Post Rui	n Settings User Vari	(a) iables				
		a) ables	<u>S</u> top	S Abort	5gapsho	it
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ontrol S <u>e</u> nd meth	iod <u>R</u> pler Via	un 🔳	Ştop	S Abort	illi Sgapsho	t.

### B) Setting of Analysis User Variables in Sequence window

1. Open Sequence window: select Analysis - Sequence from the Instrument window or click on 🛄 icon.

2. Show the User Variable columns: Click Edit - Setup Columns...

More Info:

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

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

Setup Columns			×
Table Properties			
Hide Columns		Show Columns	
ISTD9 Amount ISTD9 Amount ISTD9 Amount ISTD9 Amount AnalysisLeerVer2 AnalysisLeerVer2 AnalysisLeerVer2 Print to PDF Export Data Export Data Export AIA Export AIA Export AIA Export AIA Export AIA Program Program Program Program Colore AII	<ul> <li>Show All</li> <li>Show</li> <li>Hide</li> <li>Hide All</li> </ul>	Status           Rin           SV           SV           EV           IV           Sample ID           Sample Admunt           Sample Jult           Sample ID           Sample ID      <	
Selected Column(s) Properties			
Use Default Font		O Places     O Decimal P     Preview	laces 3 123,457
	OK Cancel	Default	Help

6. Define **Name** of the variable: type the value directly in the appropriate row  $\mathbf{b}$ .

sv	EV	I٨	Sample ID	Sample	Sample															
				Sample	Amount	ISTD1 Amount	Sample Dilut.	Inj.Vol. [µL]	Correction	Correction 2	Analysis UserVar3	File Name	Sample Type	Lvl	Method Name	Report Style	Open	Open Calib.	Print	Stored Calib.
1		1	1 Haloc	Std_1	0,400	2,000	1,000	5,000	1,000	2,000	0,000	%Q	Sta	1	Demo1	Calibration				
2		2	1 Haloc	Std_2	1,000	2,000	1,000	5,000	10,000	-3,000	-1,000	%Q	Sta	2	Demo1	Calbration				
3				Std_3	3,000	2,000	1,000	5,000	0,000	0,000			Sta	3	Demo1	Calibration				
4		4	1 Haloc	Std_4	5,000	2,000	1,000	5,000	5,000	5,000	0,000	%Q	Sta	- 4	Demo1	Calbration		~		
5		8	2 Haloc	Sample	5,000	2,000	1,000	5,000	0,000	0,000	100	%Q	Unk		Demo1	Analysis	-			
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#### C) Setting of Method User Variables in Method Setup window

- 1. Open **Method Setup window**: select *Method Advanced...* from the *Instrument* window.
- Define Name of the variable (i).
   More Info: Note If the field is left empty, default name MethodUserVar1-MethodUserVar3 would remain filled in.
- 3. Define numerical **Value** of the variable (j).

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	Value -0,8								
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Cancel	Send Method								

#### D) Setting of User Columns with User Variables

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

1. Open **Chromatogram window**: select *Window - Chromatogram* from the

*Instrument* window or click on <u>M</u> icon.

- 2. Unroll the *User Variables* section in the right side of the window, click on the chevron button **(***k*).
- 3. Define / re-type the Name or Value () of the variable.
- 4. Add User Column m as described in User Columns using User Variables.

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## 9.3 Signal to Noise Ratio Calculation

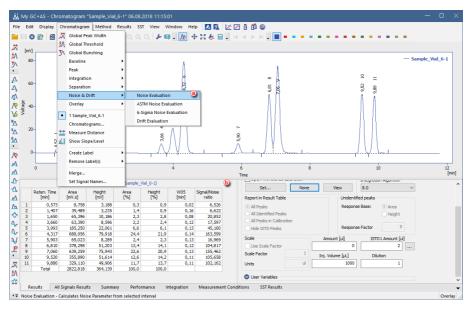
This article describes how to calculate Signal to Noise Ratio using User Columns calculations with Variables.

#### 9.3.1 Noise Parameter Evaluation

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

- 1. Open measured chromatogram in the Chromatogram window
- After selecting Chromatogram Noise & Drift Noise Evaluation (a) the interval for Noise calculation can be selected. The same result can be obtained from the Integration Table after selecting the Evaluation - Noise operation and inputting the desired interval manually.

- 3. The value of the evaluated Noise Parameter is shown in the *Result Table* header (b).
- 4. For the same chromatogram such value is stored as a *Noise* variable in the *Edit User Columns Variables* (e).



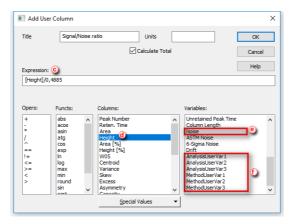
## 9.3.2 Calculating Signal to Noise Ratio

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

Two possible approaches exist:

- The Noise is determined from the same chromatogram within area with no peaks. The Noise variable (e) can be used directly in the formula entered in the Expression (c) edit box. In that case the resulting formula will be for example [Height]/[Noise].
- The Noise is determined from other chromatograms (e.g by measuring blanks and evaluating the Noise in the area of expected peak). In the Edit User Column dialog in the Expression © edit box use the [Height] ⓓ from the Columns section for peak height and enter the calculated Noise value as a constant. The resulting formula will be then e.g. [Height]/0,4885, where the number 0,4885 is the calculated Noise parameter. Alternatively, the calculated Noise parameter could be stored as a Method User Variable or as

an *Analysis User Variable* (f) to simplify changes of the value - this variable can be then used instead of entering the numerical value in the *Expression* edit box.



- *Note:* In the *Expression* edit box, variables are treated as numbers, therefore operators and numbers can be used to modify the formula. The resulting formula can be e. g. 2\*[Height]/0,4885 or 2\*[Height]/([Noise] + 3,141).
- *Note:* Setting the *Analysis User Variable* or the *Method User Variable* is described in the section **User Variables on pg 134**.

# 9.4 How to Display Older Results when Linked Calibration is Modified

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

- chromatogram with linked calibration. To avoid this, two approaches are possible:
- Make a copy of the calibration file so each series of measured chromatograms will be linked to a separate calibration file. This has advantage in case some amendments to the calibration will be necessary later, as the amendments will affect only the related chromatograms. Such

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

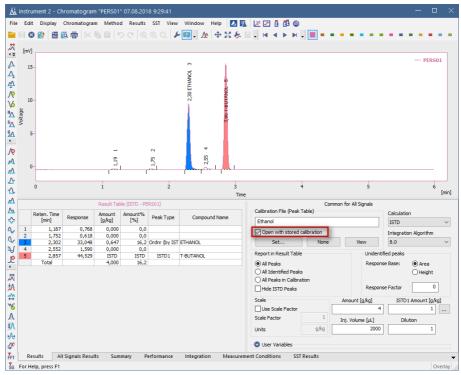
- 2. Using the *Open with stored calibration* option. Such option is accessible from multiple dialogs, depending on whether Single Analysis or Sequence is measured (automated approach) or this option can be selected upon opening the chromatogram.
  - In the Single Analysis dialog Post Run Settings tab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

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

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5																			

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



# 9.5 Calculating percentage content of a compound in a solid sample

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

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

More Info:

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

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

More Info:

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

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

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For Help	o, press F1																	

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

More Info:

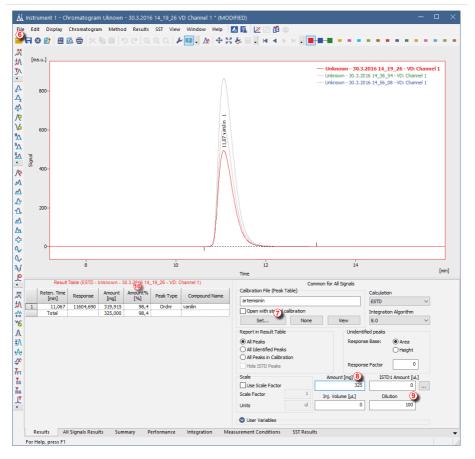
**Amount** refers to the mass of the sample used. Units are automatically copied from the Calibration Options (see step 3). In our example: *325 mg* sample had been used.

9. Fill the dilution that had been used 9.

More Info:

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

10. Column *Amount%* in the *Result Table* now displays the percentage amount of the compound in the sample (1).



## 9.6 Comparing the results from several chromatograms

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

General       Graph       Axes Appearance       Signals & Curves       Gradent & Auxilary Signals       Directories         Show windows on the taskbar.       Image: Signals & Curves       Zoom Button         Play sounds assigned to selected events.       Image: Signals & Curves       Image: Signals & Curves         Request confirmation when opening old file formats.       Image: Signals & Curves       Image: Signals & Curves         Warm when maximum zoom reached.       Image: Signals & Curves       Image: Signals & Curves       Image: Signals & Curves         Warm when reusing a Standard Chromatogram in Calibration       Set Signal to Active       Show Properties Dialog         Recent Files       Image: Curves       Curves (%n)       Image: Curves         S       Image: Curves       Only Vertical Line         Nouse Wheel Step       Start at:       0	er Options (Administrator -	tor - Clarity)			?	$\times$
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- 1. Open the Instrument and then the Chromatogram window.
- 2. Disable the Overlay Mode, click on M or un-check it from File Overlay Mode and open the first chromatogram selecting File Open chromatogram....
- 3. Enable now the Overlay Mode (same as above).
- 4. Open the rest of the chromatograms.
  - You can also use *File Open Chromatograms From Sequence...* command which opens all chromatograms from sequence including Standards.
- 5. Click on the Summary tab in the lower part of the window to display the Summary table.
  - In the rows you can see chromatograms and signals with measured values and in the columns there are identified peaks from all calibrated chromatograms.

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- 6. **Right click on the Summary Table**, if you want to change the visualization of the table or add a custom column, etc.
- To see all signals, click on the Show All Signals checkbox in the Summary Table Options dialog accessible from the pop-up menu of the Summary Table. By default, only signals containing calibrated peaks are visible in the Summary Table.

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Table Inverted	Chromatogram Header Ochromatogram / Signal Signal / Chromatogram
Report in Summary Table	Parameter Header Ompound / Parameter Parameter / Compound
OK Ca	ancel Help

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

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

The identity of a compound can be confirmed by using a dual wavelength detector in conjunction with the *Virtual Detector* and checking if the signals ratio is constant with the following procedure.

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

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

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

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$\begin{array}{c c c c c c c c c c c c c c c c c c c $				
HW Status <b>76.874 a.u.</b> Event Table Measurement Acquisiton Integration Ca	lculation Advanced	Det Status		
Cancel		ſ	Send Met	thod

9. Send the Method (i) and click OK.

## **10 Data Reports**

How to create a report, adjust it and print.

## 10.1 Setting up a report style for printing

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

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

#### More Info:

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

For example, the *Chromatogram* tab in the *Chromatogram Report Setup* refers to the chromatograms opened in that specific window and the one in the *Calibration Report Setup* refers to the calibration standard opened in the *Calibration* window if any. In the *Instrument* window it will refer to the chromatograms produced after the last run or analysis.

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

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

- 1. From the *Instrument, Calibration, Chromatogram* or *Sequence* windows, **select** *File Report Setup*. From the *Method Setup* window **click** on the *Report* button.
- Click on the New button if you wish to create a new report style or on the Open button © to use one created previously. Otherwise the current style will be the last used.
- 3. Select the tab corresponding to the section you wish to modify. (a)
- 4. Click and drag the tabs to a new position if you wish to change the order in which they will be printed in the report.

More Info:

Right click on the tabs to move them or to reset to their position by default from the context menu. The first and last tabs have a fixed position.

- 5. Select and configure the elements you would like to include in that section.
   (b)
- 6. Click *Preview* to see the result and repeat steps 3 and 4 if you wish to modify anything. ©
- 7. Click Save As to save a new report style or OK to accept the changes to the current style.

		(b)		
Page Setup	Black and White Print			🔚 ок
🕗 Lab. Header	Print Background Color of Gra	ohs	Header Font	Cancel
Report Header		[	Form Font	Help
Method		[	Value Font	
Calibration			value Font	New
Chromatogram	Margins [mm]	-		
Results		Top: 5		Open
Sequence	Left: 5 💂	Between: 2	Right: 5	Save As
SST SST				
🛿 PDA		Bottom: 5 🔹		Printer
🛿 MS	Orientation			
😢 Audit & Signatures	Use Printer Sett	ing		Preview
	Override Printer			Print
	Portrait	-		Print To PDF
	<ul> <li>Landscap</li> </ul>	e		Send PDF

## 10.2 Printing or previewing a report

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

#### More Info:

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

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

#### To print a Report:

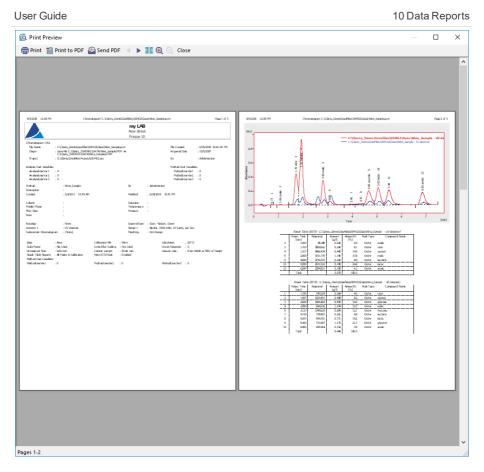
- 1. Select *File Print* on the *Instrument, Calibration, Chromatogram* or *Sequence* windows or **click on the** *Report* **button** on the *Method Setup* window and then **on the** *Print* **button** on the Report Setup window.
- A print dialog will open for you to setup your printing options and confirm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

### To Print to PDF:

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

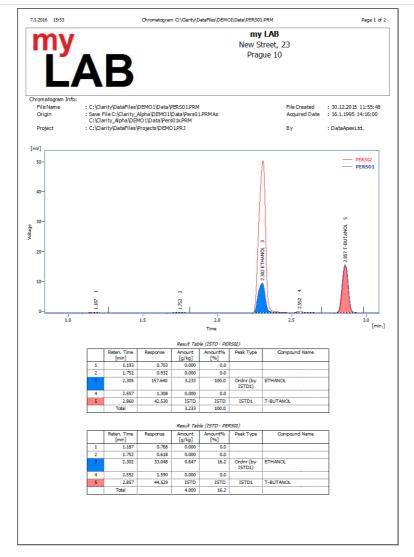
#### To get a *Print Preview*:

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



## **10.3 Creating a report style (example)**

This is an example on how to setup a new report style to obtain the results shown in the picture and in the attached **report**.



Description       10 EMO Example - 6C - Autosampler - Ethenol in blood         Dreated       130.31995       14:48       Modified       15.1.2016       16:50         Data       1 db 624-30m-3.0u-0.22 ld       Detection       FED         Data       1 db 624-30m-3.0u-0.22 ld       Detection       : FLD         Data       1 db 62       0 m/min       Temperature       : Ramped to 225         Data       is short linear velocity 50 cm/sec       column       : Starral Start       : Starr - Restart, Down         Value       0.000 min       External Start       : Starr - Restart, Down       Matching       : None         Detection 1       :       10.00 min       External Start       : Starnal Start       : Starnal Start         Value       Idobal Filter - Bunching       0.000       Imin       0.020 min       0.020 min         Detection 1       :       0.000       0.000       Imin       0.000 min       Imi	Description       : DEMO Example - 6C - Autosampler - Entend         Dreated       : 30.31995       14-48       Modified       : 5.1.2016       16:50         Solumn       : db 624-30m-3.0u-0,22 id       Detection       : FID         Solumn       : db 624-30m-3.0u-0,22 id       Detection       : FID         Solumn       : db 624-30m-3.0u-0,22 id       Detection       : FID         Solumn       :: db 624-30m-3.0u-0,22 id       Detection       : FID         Solumn       :: db 624-30m-3.0u-0,22 id       Detection       : FID         Solum Rate       :: 00 m/min       Temperature       : Ramped to 225         Nor Rate       :: 00 m/min       Temperature       : Starred to 225         Nor Rate       :: 00 m/min       Temperature       : Starred to 225         Nor Rate       :: 00 m/min       External Start       : Starr - Restart, Down         Solutaction Chromatogram       : (Nore)       Matching       : No Change         Solutaction Chromatogram       : (Nore)       Matching       : No Change         Solutaction :: Ethanol       : By       : None       : None         DetectNegative       : 0.000       0.000       0.000       Yes         Solutation :: ISTD       Mode       : Cali	7.1.2016 15:53		Chromato	ogram C:\C	arity∖DataFile	s\DEMO1\0	Data\PE	RS01.PF	им			F	age 2 of 2
Ethanol in blood       Detected     13.0.3195     14.48     Modified     : 5.1.2016     16:50       Column     : db 624-30m-3.00,32 id     Detection     : FID       Note The image of the	Ethanol in blood       Detected     13.0.3195     14.48     Modified     15.1.2016     16:50       Column     : db 624-30m-3.00,32 id     Detection     : FID       Note the set in hydrogen     : for more at respective     Ramped to 225       Nave Rate     : 90 m/min     Pressure     : 5.57 pil       Note the set in hydrogen     : short linear velocity 50 cm/sec     : column initial 45 deg       Nutostop     : 10.00 min     External Start     : Start - Restart, Down       Nutostop     : 10.00 min     External Start     : Start - Restart, Down       Nutostop     : 10.00 min     External Start     : Start - Restart, Down       Nutostop     : 10.00 min     External Start     : Start - Restart, Down       Nutostop     : 10.00 min     External Start     : Start - Restart, Down       Nutostop     : 10.00 min     External Start     : Start - Restart, Down       Nutostop     : 10.00 min     External Start     : Start - Restart, Down       Nutostop     : 10.00 min     External Start     : Start - Restart, Down       Nutostop     : 10.00 min     : Start - Restart, Down     : Down       Started     : 30.3195 14:20:18     Modified     : 30.122015       Started     : 30.3.1995 14:20:18     Modified     : 30.025 <t< td=""><td>Method</td><td></td><td></td><td></td><td></td><td>у</td><td></td><td>Admin</td><td>istrator</td><td></td><td></td><td></td><td></td></t<>	Method					у		Admin	istrator				
Created       : 30.31995       14-48       Modified       : 5.1.2016       16:50         Column       : db 624-30m-3.0u-0,22 id       Detection       : FID         Now Rate       :: 0 m/min       Temperature       : Ranged to 225         Now Rate       :: 0 on m/min       Temperature       : 5.57 pi         Note       :: short linear velocity 50 cm/sec       : column initial 45 deg         Nutostop       :: 10.00 min       External Start       : Start - Restart, Down         Velocitor 1       :       Range 1       :: Bipolar, 1250 mV, 10 Samp. per Sec.         Nutostop       :: 10.00 min       External Start       : Start - Restart, Down         Velocitor 1       :       Range 1       :: Bipolar, 1250 mV, 10 Samp. per Sec.         Nutostop       :: 10.00 min       External Start       : Start - Restart, Down         Global Peak Width       0.000       0.000 v       : Start - Restart, Down         Global Treehold       0.000       0.000 v       : Start - Restart, Down         Sciubrator       :: Bunching       0.000 0.000 v       : Start - Restart, Down         Sciubrator       :: Bunching       0.000 0.000 v       : Start - Restart, Down         Sciubrator       :: Bunching       0.000 0.000 v       : Start - Restart	Created     : 30.31995     14.48     Modified     : 5.1.2016     16:50       Column     : db 624-30m-3.0u-0,22 id     Detaction     : FID       Now Rate     :: 00 m/min     Temperature     : Ramped to 225       Now Rate     :: 00 m/min     Temperature     : S.57 psi       Note     :: short linear velocity 50 cm/sec     : S.57 psi       Note     :: short linear velocity 50 cm/sec     : S.57 psi       Nutostop     :: 1.000 min     External Start     : Start - Restart, Down       Velocitor 1     :< Modified	Description	: DEMO Exam	ple - GC - A	Autosample	r -								
Column       ::::::::::::::::::::::::::::::::::::	Column       ::db 624-30m-3.0u-0,32 id       Detection       ::FD         Nobile Phase       ::sb 0m/min       Pressure       ::S.57 psi         Nove Rate       ::sb 0m/min       Pressure       :S.57 psi         Note       ::sb minital 45 deg       Pressure       :S.57 psi         Nutostop       ::sb 0m nin       External Start       :Start - Restart, Down         Nutostop       ::sb 0m nin       External Start       :Start - Restart, Down         Nutostop       ::sb 0m nin       External Start       :Start - Restart, Down         Nutostop       ::sb 0m nin       External Start       ::sb 0m ni, 10 Samp. per Sec.         Nutostop       ::sb 0m nin       :sb 0m nin       :sb 0m nin       :sb 0m nin         Sidba Treshold       :mini       !mini       0.020 min       :sb 0m nin         Global Threshold       :sb 0m nin       :sb 0m nin       :sb 0m nin         Global Threshold       :sb 0m nin       :sb 0m nin       :sb 0m nin         Global Threshold       :sb 0m nin       :sb 0m nin       :sb 0m nin         Global Threshold       :sb 0m nin       :sb 0m nin       :sb 0m nin         Sidba Threshold       :sb 0m nin       :sb 0m nin       :sb 0m nin         Global Threshold													
toble Phase       : hydrogen       Temperature       : Ramped to 225         is rank take       : 9 om min       Pressure       : 5.57 psi         is too time velocity 50 cm/sec       : column initial 45 deg       Pressure       : 5.57 psi         vulostop       : 10.00 min       External Start       : Start - Restart, Down         wutostop       : 10.00 min       External Start       : Start - Restart, Down         wutostop       : (Nore)       Matching       : No Change          : (Nore)       : None       : (Nore)          : (Nore)       : None       : (Nore)          : (None)       : (None)       : (None)         ::::::::::::::::::::::::::::::::::::	Idolle Phase       : hydrogen       Temperature       : Ramped to 225         isore Rate       : 90 m/min       Pressure       : 5.57 pil         isote       : short linear velocity 50 cm/sec       column initial 45 deg         vulostop       : 10.00 min       External Start       : Start - Restart, Down         velocitor 1       :	reated	: 30.3.1995	14:48		м	oainea		5.1.20	10 16:50				
toble Phase       : hydrogen       Temperature       : Ramped to 225         is rank take       : 9 om min       Pressure       : 5.57 psi         is too time velocity 50 cm/sec       : column initial 45 deg       Pressure       : 5.57 psi         vulostop       : 10.00 min       External Start       : Start - Restart, Down         wutostop       : 10.00 min       External Start       : Start - Restart, Down         wutostop       : (Nore)       Matching       : No Change          : (Nore)       : None       : (Nore)          : (Nore)       : None       : (Nore)          : (None)       : (None)       : (None)         ::::::::::::::::::::::::::::::::::::	Idolle Phase       : hydrogen       Temperature       : Ramped to 225         isore Rate       : 90 m/min       Pressure       : 5.57 pil         isote       : short linear velocity 50 cm/sec       column initial 45 deg         vulostop       : 10.00 min       External Start       : Start - Restart, Down         velocitor 1       :	Column	: db 624-30m	-3.0u-0.32 i	d	D	etection		FID					
Iow Rate       : 90 m/min       Pressure       : 5.57 psi         Iobe       : short linear velocity 50 cm /acc column initial 45 deg       External Start : Start - Restart, Down         Vetector 1       :       :       Range 1       : Bipolar, 1250 mV, 10 Samp, per Sec.         Vetector 1       :       :       Range 1       : Bipolar, 1250 mV, 10 Samp, per Sec.         Vetector 1       :       :       Range 1       : Bipolar, 1250 mV, 10 Samp, per Sec.         Vetector 1       :       :       Range 1       : Bipolar, 1250 mV, 10 Samp, per Sec.         Vetector 1       :       :       Range 1       : Bipolar, 1250 mV, 10 Samp, per Sec.         Vetector 1       :       :       : Range 1       : Bipolar, 1250 mV, 10 Samp, per Sec.         Vetector 2       :       :       : Bipolar, 1250 mV, 10 Samp, per Sec.       :         Vetector 3       :       :       : Bipolar, 1250 mV, 10 Samp, per Sec.       :         Chromatogram       :       :       :       :       :       :         Chromatogram       :       :       :       :       :       :       :       :         Chromatogram       :       :       :       :       :       :       :       :       : <td>Iow Rate       : S0 m/min       Pressure       : S.S7 psi         Iobe       : short linear velocity S0 m/sec column initial 45 deg       External Start       : Start - Restart, Down         Veloctor 1       :       .       Range 1       : Bjolar, 1250 m/, 10 Samp, per Sec.         Veloctor 1       :       .       Range 1       : Bjolar, 1250 m/, 10 Samp, per Sec.         Veloctor 1       :       .       Range 1       : Bjolar, 1250 m/, 10 Samp, per Sec.         Veloctor 1       :       .       .       Range 1       : Bjolar, 1250 m/, 10 Samp, per Sec.         Veloctor 1       :       .       .       .       .       .         Veloctor 1       :       .       .       .       .       .         Veloctor 1       :       .       .       .       .       .       .         Veloctor 1       :       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .</td> <td>Mobile Phase</td> <td></td> <td></td> <td>-</td> <td></td> <td></td> <td></td> <td></td> <td>ed to 225</td> <td></td> <td></td> <td></td> <td></td>	Iow Rate       : S0 m/min       Pressure       : S.S7 psi         Iobe       : short linear velocity S0 m/sec column initial 45 deg       External Start       : Start - Restart, Down         Veloctor 1       :       .       Range 1       : Bjolar, 1250 m/, 10 Samp, per Sec.         Veloctor 1       :       .       Range 1       : Bjolar, 1250 m/, 10 Samp, per Sec.         Veloctor 1       :       .       Range 1       : Bjolar, 1250 m/, 10 Samp, per Sec.         Veloctor 1       :       .       .       Range 1       : Bjolar, 1250 m/, 10 Samp, per Sec.         Veloctor 1       :       .       .       .       .       .         Veloctor 1       :       .       .       .       .       .         Veloctor 1       :       .       .       .       .       .       .         Veloctor 1       :       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .       .	Mobile Phase			-					ed to 225				
Jobe       : short linesr velocity 50 cm/sec column initial 45 deg         Jutostop       : 10.00 min       External Start: : Start - Restart, Down         Vetector 1       : 10.00 min       Range 1       : Bipolar, 1250 mV, 10 Samp, per Sec.         Jubraction Chromatogram       : (None)       Matching       : No Change         Image: Start - Restart, Down	Jobe       : short linesr velocity 50 m/sec column initial 45 deg         Jutostop       : 10.00 min       External Start :: Start - Restart, Down         Vetector 1       : 10.00 min       Range 1       : Stort - Restart, Down         Vetector 1       : 0.00 min       Range 1       : Bipolar, 1250 mV, 10 Samp, per Sec.         wbtraction Chromatogram       (None)       Matching       : No Change         Image 1       : Stort - Restart, Down       0.020 min         Global Peek Width       0.020 min       0.000 mV         Global Filter - Bunching       0.000 0.000 Yes         Calchal Triter - Bunching       0.020 10.000 Yes         Calchal Filter - Bunching       0.020 10.000 Yes         Calchal Triter - Bunching       0.020 10.000 Yes         Calchal Triter - Bunching       0.020 10.000 Yes         Calchal Triter - Bunching       By : None         Screated       : 30.3.1995 14:20:18       Modified : 30.12.2015 11:55:48         Calculation       : ISTD       Mode       : Callbrate         Calculation       : ISTD       Mode       : Callbrate         Calculation       : ISTD       Mode       : Callbrate         Calculation       : ISTD       Search Criteria       : 0.00%         Pangre Reponce       <	Flow Rate												
column initial 45 deg Nutostop : 10.00 min External Start : Start - Restart, Down Netchor 1 : Bipplar, 1250 mV, 10 Samp. per Sec. Abbraction Chromatogram : (None) Matching : No Change	column initial 45 deg Nutostop : 10.00 min External Start : Start - Restart, Down Pector 1 : Range 1 : Bipolar, 1250 mV, 10 Samp, per Sec. Matching : No Change Image: Comparison of the second start is start - Restart, Down, 10 Samp, per Sec.           Image: Comparison of the second start is start - Restart, Down, 10 Samp, per Sec.           Image: Comparison of the second start is start - Restart, Down, 10 Samp, per Sec.           Image: Comparison of the second start is start - Restart, Down, 10 Samp, per Sec.           Image: Comparison of the second start is start - Restart, Down, 10 Samp, per Sec.           Image: Comparison of the second start is start - Restart, Down, 10 Samp, per Sec.           Image: Comparison of the second start is start - Restart, Down, 10 Samp, per Sec.           Image: Comparison of the second start is start - Restart, Down, 10 Samp, 10 Sam	Note		elocity 50 c	cm/sec				1					
Vetector 1       :       Range 1       : Elipolar, 1250 mV, 10 Samp. per Sec.         ubbraction Chromatogram       :(None)       Matching       : No Change         Indication Chromatogram       :(None)       Time A       Time B       Value         Global Peak Width       [min]       0.000 min       0.000 min         Global Peak Width       0.000       0.000 Ves       1         Detect Negative       Node       : Calibrate       20.000 Negative         Scalubation       : ISTD       Mode       : Calibrate       20.000 Negative         Calculation       : ISTD       Mode       : Calibrate       20.000 Negative         Detator Duration       : Search Criteria       : 0.00%       20.00%       20.00%         Detator Summary Table (ISTO - Ethand - Signal 1)       : Not Used       2.000 Negative	Vetector 1       :       Range 1       ::       Bipolar, 1220 mV, 10 Samp, per Sec.         ubbraction Chromatogram       :       Nochange         Image: 1       ::       Bipolar, 1220 mV, 10 Samp, per Sec.         Matching       ::       No Change         Image: 1       ::       Bipolar, 1220 mV, 10 Samp, per Sec.         Image: 1       ::       Matching       ::         Image: 1       ::       No Change         Image: 1       ::       Image: 1       ::         Image: 1       ::       No Change         Image: 1       ::       Image: 1       ::         Image: 1       ::       Image: 1       ::         Image: 1       ::       No Change       ::         Image: 1       ::       :       No Change         Image: 1       ::       :       No Change       :         Image: 1       ::       :       No Change       :       :         Image: 1       ::       :       :       :       :       :         Image: 1       ::       :       :       :       :       :       :       :       :       :       :       :       :       :		column initia	al 45 deg										
Vetector 1       :       Range 1       : Elipolar, 1250 mV, 10 Samp. per Sec.         ubbraction Chromatogram       :(None)       Matching       : No Change         Indication Chromatogram       :(None)       Time A       Time B       Value         Global Peak Width       [min]       0.000 min       0.000 min         Global Peak Width       0.000       0.000 Ves       1         Detect Negative       Node       : Calibrate       20.000 Negative         Scalubation       : ISTD       Mode       : Calibrate       20.000 Negative         Calculation       : ISTD       Mode       : Calibrate       20.000 Negative         Detator Duration       : Search Criteria       : 0.00%       20.00%       20.00%         Detator Summary Table (ISTO - Ethand - Signal 1)       : Not Used       2.000 Negative	Vetector 1       :       Range 1       ::       Bipolar, 1220 mV, 10 Samp, per Sec.         ubbraction Chromatogram       :       Nochange         Image: 1       ::       Bipolar, 1220 mV, 10 Samp, per Sec.         Matching       ::       No Change         Image: 1       ::       Bipolar, 1220 mV, 10 Samp, per Sec.         Image: 1       ::       Matching       ::         Image: 1       ::       No Change         Image: 1       ::       Image: 1       ::         Image: 1       ::       No Change         Image: 1       ::       Image: 1       ::         Image: 1       ::       Image: 1       ::         Image: 1       ::       No Change       ::         Image: 1       ::       :       No Change         Image: 1       ::       :       No Change       :         Image: 1       ::       :       No Change       :       :         Image: 1       ::       :       :       :       :       :         Image: 1       ::       :       :       :       :       :       :       :       :       :       :       :       :       :	Autosten	10.00 min			5	dama Ch		Chart	Destart D				
Libtraction Chromatogram : (None)       Matching : No Change         Image: Chromatogram : Comparison : Comparison : Chromatogram : Comparison : Comp	Libtraction Chromatogram : (None)       Matching : No Change         Image: Chromatogram : (None)       Chromatogram : (None)         Image: Chromatogram : (None)       By : None         Description : DEMO Example - Ethanol In Blood       By : None         Description : DEMO Example - Ethanol In Blood       By : None         Description : DEMO Example - Ethanol In Blood       Educator : Calibrator         Description : DEMO Example - Ethanol In Blood       Educator : Recalibrator : Structure : Note : Calibrate         Calibrator : ISTD : Mode : Calibrate : Search Criteria : 0.00%       Educator : Search : Search : Note : Note : Search : Search : Search : Note : Note : Search : Search : Search : Search : Structure : Note : Search : Structure : Note : Note : Note: : Note: : Note: : Note: : Note: : : : : : : : : : : : : : : : : : :											ner Sei		
Chromatogram       Grp.       Time A       Time B       Value         Global Presk Width       [min]       [min]       0.020 min         Global Titler - Bunching       0       0.000 NV       0.000 NV         Global Titler - Bunching       0       0.000 NV       0.000 NV         DetectNegative       0.000       0.000 Ves       1         DetectNegative       Modified : 30.12.2015 11:55:48       1         DetectNegative       Realibrator Type : Average       Average         Dialbrate       : Automatic       Realibrator Type : Average         Dialbrate       : Search Criteria       : 0.00%         DetatonLimit       : NotUsed       CorrelationLimit : NotUsed         DefaultInjected Volume : NotUsed       Collorator Summary Table (ISTO - Ethand - Signal 1)         Med       Compound Name       Realibrator Table Type         Veridov       Collorator Summary Table (IS	Chromatogram       Grp.       Time A       Time B       Value         Global Presk Width       [min]       0.020 min         Global Treshold       0.090 nV       0.090 nV         Global Filter - Bunching       0       0.000 nV         DetectNegative       0.000 0.000 Ves         Scalabraton :: Ethanol       By :: None         Description :: DEMO Example - Ethanol in blood       By :: None         Dreated :: 30.3.1995 14:20:18       Modified :: 30.12.2015 11:55:48         Calubrate :: Automatic       RecalibratonType :: Average         DiagRe Response :: Enable       Weight :: 0.25         Detaton Utuged       Search Criteria :: 0.00%         Detator Summary Table (ISTD - Ethanol :: Not Used         Verlaton Limit :: Not Used       CorrelationLimit :: Not Used         Cultorator Summary Table (ISTD - Ethanol :: 0.00%)         Used Compound Name         Detect Volume : Not Used	Subtraction Chromatogram									20 0000	, per se		
Operation         [min]         [min]         [min]         0.020 min           Global Threshold         0.400 mV         0.8900 mV         0.8900 mV           Global Threshold         0.000         0.8900 mV         1           DetectNegative         0.000         0.000         Yes           Calubration         : Ethanol         By         : None           DetectNegative         0.000         0.000         Yes           Calubration         : DTD         Modified         : 30.12.2015         11:55:48           Calubration         : ISTD         Mode         : Calibrate         : Automatic         RecalibrationType         : Average           Calculation         : ISTD         Mode         : Calibrate         : Search Criteria         : 0.00%           Detaton Unit         : NotUsed         Search Criteria         : 0.00%         : Search Criteria         : 0.00%           Defaultingeted Volume         : NotUsed         CorrelationLimit         : NotUsed         CorrelationLimit         : NotUsed	Operation         [min]         [min]         [min]         0.020 min           Global Threshold         0.0900 mV         0.0900 mV         0.0900 mV         0.0900 mV           Global Threshold         0.000         0.000         1         0.020 min         0.0900 mV           DetectNegative         0.000         0.000         Yes         1         0.000         0.000           Scalar Threshold         By         : None         1         0.000         1         1           DetectNegative         0.000         0.000         Yes         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1         1									-				
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- 1. Open one *Instrument* selecting the project DEMO1.
- 2. Open the Chromatogram window.
- 3. Open the chromatograms PERS01 and PERS02 in (C:\CLARITY\DataFiles\DEMO1\Data).
- 4. Select the Overlay mode from File Overlay Mode or click on M.
- 5. Select the area you want to print: click and drag the mouse pointer on the chromatogram graph.

6. Create a new report style.

#### More Info:

- Select the File Report Setup.
- Click on the New button to create a new report style.
- Click on the Save As... button and save the style under the name Myreport. (b)

<u>c</u> )				
age Setup	Black and White Print			🛃 ОК
3 Lab. Header	Print Background Color of Gra	phs	Header Font	Cancel
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2 Audit & Signatures	Use Printer Set	ing		Preview
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	O Landscap	e		Send PDF

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

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

#### 8. Set the Lab Header.

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

#### User Guide 10 Data Reports Report Setup myReport H OK Page Setup Print Number of Lines: 3 🕂 Line 1: 📄 🚊 🗐 Α 🛛 Lab. Header 🔞 Cancel 3 Report Header my LAB On First Page Only Help New street 3 Chromatogram Border Prague 10 8 Results Gray Background New 8 Method Calibration Open.. Image on the Left: Sequence Save As. Options... O SST O PDA Printer... 🙆 MS Image on the Right: Audit & Signatures Preview Options...

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Print... Print To PDF... Send PDF

9. Set the Report Header.

More Info:

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

Page Setup	Chromatogram Info	🔚 ок
2 Lab. Header On New Page	Printed Version Info	Cancel
Report Header 🙂	Sample Description	Help
3 Chromatogram	Sample Parameters	
8 Results	User Variables	New
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Audit & Signatures	GLP Information	Preview
	GCP_Information	Print
		Print To PDF
		Send PDF

10. Set the Chromatogram section.

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

#### User Guide

#### 10 Data Reports

Report Setup myReport			×
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			Send PDF

- 11. Set the Results section.
  - More Info:
    - Click on the *Results* tab. (g)
    - Check the boxes *Print* and *Result Table*.

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Audit & Signatures		Print Options	Preview
		Print User Column Formulas	Print
			Print To PDF
			Send PDF

12. Set the Method section.

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

#### User Guide

#### 10 Data Reports

Page Setup	✓ Print	☑ Info Header	🔚 ок
🕗 Lab. Header	On New Page	Instrument Parameters	Cancel
Report Header	Signals	Acquisition Parameters	Help
Chromatogram		GLP Info	
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O PDA		PDA Method	Printer
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Audit & Signatures			Preview
			Print
			Print To PDF.
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13. Set the Calibration section.

#### More Info:

- Click on the Calibration tab. ()
- Check the boxes Print, Info, Parameters and Summary.

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				Print
				Print To PDF
				Send PDF

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

## **10.4 Printing the summary table**

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

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

Page Setup	✓ Print	Result Table	🔚 ОК
3 Lab. Header	On New Page	All Signals Result Table	Cancel
Report Header	Signals	Special Results	Help
Method	() All	Performance Table	
3 Calibration	Active Chromatogram	Chromatogram Comments	New
3 Chromatogram	Only Active Signal	Summary Table	IVEV
Results		Word Wrap Long Texts	Open
3 Sequence		Table Layout	Save As
SST 3		As on Screen	
3 Audit & Signatures		Force Inverted	Printer
		Print Options	Preview
		Print User Column Formulas	Print
			Print To PDF
			Send PDF

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

🔯 Print F	review							×
Print	📸 Print to PDF	垫 Send PDF	< ▶ II ⊕ Q CI	ose				
								^
	08/03/2019	10:12	Chromatog	ram C:\Clarity\DataFiles	DEMO1\Data\PERS02.pd	m	Page 1 of 1	
				Summ	ary Table			
					C:\Carity8.2.00.52\Dat aFiles\DEMO1\Data\PE R501	C:\Clarity8.2.00.52\Da taFiles\DEMO1\Data\P ER502		
					Signal 1	Signal 1		
			Sam	nple ID	Mr. X.Y.	Mr. X.X.		
			Sa	imple	DEMO Example - ethanol in blood	DEMO Example - ethanol in blood		
			Sample	e Amount	4.000	0.000		
				Reten. Time [min]	2.302	2.305		
				Response	33.048	157.640		
			ETHANOL	Amount [g/kg]	0.647	3.233		
			E THRUGE	Amount% [%]	16.2	100.0		
				Peak Type	Ordnr (by ISTD1)	Ordnr (by ISTD1)		
				Compound Name	ETHANOL	ETHANOL		
				Reten. Time [min]	2.857	2.860		
				Response	44.529	42.530		
			T-BUTANOL	Amount [g/kg]	ISTD	ISTD		
				Amount% [%]	ISTD	ISTD		
				Peak Type	ISTD1	ISTD1		
				Compound Name	T-BUTANOL	T-BUTANOL	]	

## 11 File Management

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

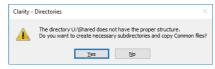
## 11.1 Setting up project directories

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

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

Instrument 1	U:\Shared	
Insuument I	0: phared	••
Instrument 2	U:\Shared	
Instrument 3	U:\Shared	
Instrument 4	U:\Shared	
	All As Instrument 1	
Existing projects you copy/move th	(e.g. DEMO projects) will not be visible from changed location unles hem manually	s

- 3. Set the desired directory E.g. U:\Shared
- 4. If desired change the Audit Trail directory
- 5. When saving the changes, the following dialog may occur



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

## 11.2 Creating a new project

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

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

Project Setup		×
Project Name (Directory):	WORK1	OK
		Cancel
		Help
Description:		
Default project for Instru	ument 1	Open
Analysis Subdir:	Calibration Subdir:	Save
Data	Calib	Save as
		New

#### More Info:

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

Login Dialog	×
Choose User Name and Enter Password	
Tom	$\sim$
Select Project:	
<new project=""></new>	$\sim$
All Possible Instruments	
OK Cancel Help	

2. Click the New button (a) to create a new project.

Create Project or Save a	5	$\times$
DEMO_EA DEMO_GCxGC DEMO_GCxGC DEMO_MS DEMO_PDA DEMO1 DEMO2 DEMO3 DEMO3 DEMO3 DEMO4 WORK1 WORK2 WORK3	Elemental Analysis DEMO data GCXGC Extension DEMO Data DEMO data GPC module MS Extension DEMO Data Natural Gas Analysis DEMO data DEMO data for PDA Demo project with GC examples Demo project with HPLC examples Demo project Demo project for Instrument 1 Default project for Instrument 3 Default project for Instrument 3 Default project for Instrument 4	<b>^</b>
MyProject	OK Cancel Help	>

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

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

Project Setup		:
Project Name (Directory):	MyProject	ОК
		Cancel
		Help
Description: 🕘		_
This is my new project		Open
Analysis Subdir:	Calibration Subdir:	Save
Data	Calib	Save as
		New

4. Fill in the project description in the *Description* field (d) and click *OK* (e). More Info:

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

## 11.3 Creating customized file names automatically

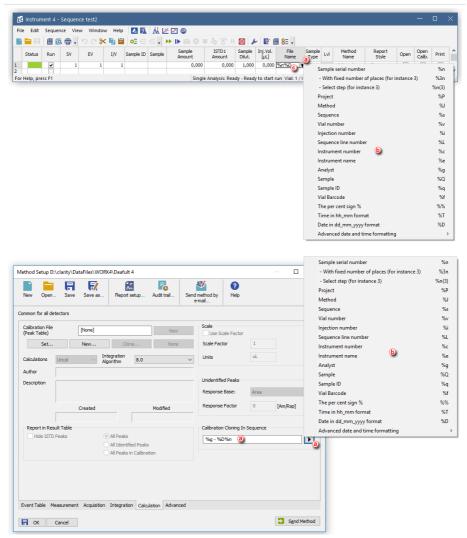
You can create customized file names automatically by appending variables to them.

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

- 1. Click on the respective icons **(**, **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**), **(**)
- 2. Click on b to open the variable list. (a)
- 3. Select the variable you want to include in the file name. (b)
- 4. Repeat the previous two steps to add more variables.
- 5. **Insert any allowed characters** between the variables to create your file name. ©

- Variables are preceded by the "%" character and they are substituted by their value upon file creation. For example "%g %Q -- %D" will create a file name with the name of the *Analyst*, the *Sample ID* and the *date* it was created: "*AdministratorEthanol29-07-2016.prm*".
- To prevent an Unresolved File Name error you can append the Sample Serial Number "%n" or the date and time "%R".

Single Analysis				×	
Sample ID					
Sample	Ethanol				
Comments					
Amount	0	ISTD1 Amount	0		
Dilution	1	Inj. Volume [µL]	0		
Sample Type	Unknown	Level	1	Sample serial number	%n
				- With fixed number of places (for instance 3)	%3n
Method	Ethanol in blood		Edit Meth	- Select step (for instance 3)	%n(3)
Report Style	Analysis		Edit Report	Project Method	%P %J
					%J %c
				Instrument number	%е
					%e %q
				Analyst Sample	%g %O
Analysis Post Run Se	ttings User Variables			Sample ID	%Q %q
				Vial Barcode	%q %f
Control				The per cent sign %	%%
Send method	🕨 <u>R</u> un 🔳	Stop 🛞 Abort	illii Sr	Time in hh_mm format	%T
				Date in dd_mm_yyyy format	%D
Chromatogram File N	ame (AdministrátorEthanol08 08 201	3)		Advanced date and time formatting	>
%g%Q%D (C)			@		
Enable File Overv	rite	Counter 1	Data Recovery		
		OK Cancel	H	ielp	



## 11.4 Storing files into project subfolders

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

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

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

	) 🖿 🖪	1	<u>6</u> .			Help 🔼			⊙ ■		4	😿 🔝 8E 🛛							
	Status	Run	sv	EV	I/V	Sample ID	Sample	Sample Amount	ISTD1 Amount	Sample Dilut.	Inj.Vol. [µL]	File Name	Sample Type	Lvl	Method Name	Report Style	Open	Open Calib.	Print
1		~	1	1	1	blank		0.000	0.200	1.000	2.000	%s\%q_%Q_%R	<b>₹</b> Unkn		Ethanol in	Analysis	~		
2		>>>	2	2		std1	0.4	0.000	0.200	1.000		%s\%q_%Q_%R	Stan	1	Ethanol in	Analysis			
3		-	3	3	1	std2	0.8	0.000	0.200	1.000		%s\%q_%Q_%R	Data\Ethanol in	bloc	d\blank 02.0	5 2010 11 30 4	7		
4		>>>>>	4	4	1	std3	1.4	0.000	0.200	1.000	2.000	%s\%q_%Q_%R	Stati		CUISION IN	Analysis			
5		-	5	5	1	std4	1.9	0.000	0.200	1.000	2.000	%s\%q_%Q_%R	Stan	4	Ethanol in	Analysis			
5		-	6	6	1	std5	2.4	0.000	0.200	1.000	2.000	%s\%q_%Q_%R	Stan	5	Ethanol in	Analysis			
7		-	6	6	1	std5	2.6	0.000	0.200	1.000	2.000	%s\%q_%Q_%R	Stan	6	Ethanol in	Analysis			
3		-	7	7	1	0442		0.000	0.200	1.000	2.000	%s\%q_%Q_%R	Unkn		Ethanol in	Analysis			
9			8	8	1	0445		0.000	0.200	1.000	2.000	%s\%q_%Q_%R	Unkn		Ethanol in	Analysis			
10																			

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

Look In:	Ethanol in blood		v 🕈 🛃 🛤	10 14 Ro 👗	C D	L L	Look In:	Ethanol in blood		v 🕈 🛃 🗄	e ini të të 👗	C D	
Å 0445_	02_05_019 11_24_46 02_05_019 11_24_58 02_05_0019 11_23_17	280 kB 280 kB			Last Change 02/05/2019 11:24 02/05/2019 11:24 02/05/2019 11:23		std2_0 std3_1 std4_1 std5_2	4.02.05.2019 11.23.3 8.02.05.2019 11.23.4 4.02.05.2019 11.23.5 9.02.05.2019 11.24.5 4.02.05.2019 11.24.0 4.02.05.2019 11.24.3	280 k8 280 k8 280 k8 280 k8 280 k8	PRM Chromatog PRM Chromatog PRM Chromatog PRM Chromatog	Created 02/05/2019 13:00 02/05/2019 13:00 02/05/2019 13:00 02/05/2019 13:00 02/05/2019 13:00 02/05/2019 13:00	02/05/2019 11:23 02/05/2019 11:24 02/05/2019 11:24	
File Name File Type	Chromatogram files (*	.prm)	s	gnals:	OK		ile Name ile Type	Chromatogram files (*.	prm)	;	Signals:	Canc	
Method			~		Overlay	Mode	4ethod			~		Overlay	Mod
Analyst: SampleID: Sample: Signature: GLP Mode			Version: Range/Ra Time: Has PDA I GCxGC:			s	Analyst: SampleID: Sample: Signature: SLP Mode			Version: Range/R Time: Has PDA GCxGC:			

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

## **12 Import and Export Data**

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

## 12.1 Importing a chromatogram into Clarity

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

1. **Open the Chromatogram window:** select Window - Chromatogram on the

*Instrument* window or click on <u>M</u>.

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

Data		v 🕈 💆			
b	Size	Туре	Created	Last Change	
01.CDF	1 k8	CDF File	07.08.2018 13:57	07.08.2018 13:57	
SIGNAL01.CDF				ОК	
	01.CDF	(b)	(D)	(b)	

- 5. Set the different parameters in the subsequent dialogs depending on the file format.
  - Import AIA File when importing AIA file (\*.CDF suffix).
  - Import Text File when importing Text, Multidetector or EZChrom ASCII file (\*.TXT, \*.CHR, \*.ASC and \*.CSV suffixes).
  - Save As when importing \*.RAW file, as there is no need to set other parameters.

# 12.2 Exporting a chromatogram from Clarity to a different chromatography data station

It is possible to export chromatograms to other formats used by chromatography data stations. The supported formats are : *AIA* (\*.CDF suffix), *EZChrom ASCII* (\*.ASC suffix), *Text format* (\*.TXT), or *Multi-detector format* (\*.CHR).

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

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

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

More Info:

You can choose individual signals, *All Detectors*, *3D Data* or *All Detectors* + *3D Data* (3D Data variants in EZChrom ASCII only).

- 5. Select the field separator character ⓒ .
- 6. Select the decimal separator character **d**.
- Select the character encoding for the exported file (ANSI or Unicode (UTF-8)) f.
- 9. Click OK to finish the export.

Export Chromatogram		×
Chromatogram	D:\clarity\DataFiles\DEMO1\Data\EXAMPLE.prm	
File Format	AIA Format (*.cdf)	~ (a)
Detector	- All Detectors -	~ b
Field Separator	<table by="" se<="" second="" th="" the=""><th>୍ତ</th></table>	୍ତ
Decimal Separator	, <window's locale=""></window's>	~ 🎱
Export to File	D:\Clarity\DataFiles\DEMO2\Data\EXAMPLE.cdf	
Character Encoding	ANSI	ି 🕐
	OK Cancel Help	

## 12.3 Exporting data for LIMS

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

#### **Export settings**

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

🅂 Instrumer	nt 1		- ×
Instrument Meth	od Analysis Evaluation	Setting Window Help 📐	
Ready	44	Export Data User Options Toolbars	
• ···,		*	
Status:	Ready to start run		
Sent method:	Demo1		📑 DEMO1  💄 Ben
Setting export data	parameters		

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

More Info:

- Otherwise the content will change according to changes on screen.
- 3. Select Export to Text File C.
- 4. Select Full Format option.

More Info:

- This will precede each result table row with a file name, date and time, thus allowing easy sorting after import.
- 5. Set File Name (d) and check the Append option, in this way all results will be exported to a single file which can then be simply imported directly to your LIMS.

More Info:

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

Export Content Result Table In Fixed Format Special Results	Chromatogram All Data Displayed Data	Text Format Fixed Width Delimited by:	
Summary Table Column Moments Calculation Parameters	X Axis Time Step: 0 min	<tab> Decimal Separator: <window's locale=""></window's></tab>	~
Chromatogram Chromatogram Header NGA Amounts NGA Summary DHA Results DHA Group Results	Append Character Encoding:	Export to Clipboard Text File © Excel dBase File (Result table only)	
☑ Table Headers ☑ Full Format ile Name: (path and name by chroma	atogram).txt		<b>@</b>

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

ser Opt	ions (Ad	ministrátor - Clarit	y)				?	$\times$
General	Graph	Axes Appearance	Signals & Curves	Gradient & Auxiliar	y Signals	Directories		
Print to	PDF Dire	ctory:						
					Defa	ult		
Export	Directory				Defa	ult		
L					Jeiu			
Import	Directory	9						
					Defa	ult		
			porting files to the s	amo directorios as d	romator	rame		
Hint: Le	eave dire	ctories empty for exp		ane unectones as u	inomatog	i uma.		
Hint: Le	ave dire	ctories empty for exp		ane di ectories as d	nomatog	i unis.		

#### Locations to Export from

Three most common locations in exporting data to LIMS are:

#### Single Analysis

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

More Info:

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

Single Analysis X
Single Analysis          Image Analysis          Open Chromatogram Window          Open Caleration Window          Print Results          Open Chromatogram Window          Open Chromatogram with stored Caleration          Open Chromatogram in SST          Export Chromatogram in ST          Export Chromatogram in ST Format          Export Chromatogram in NLT Format          Export Chromatogram in Multidetector Format          Program to Run       Only with Export         Parameters
Analysis Post Run Settings User Variables
Control
🔁 Send method 🕨 Run 🔳 Stop 🔇 Abort 🛍 Stapshot
Chromatogram File Name (Instrument 1 - 07.08.2018 13_12_33) %e - %R  Enable File Overwrite  Data Recovery
OK Cancel Help

#### Sequence

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

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

ē	🕯 Instrum	nent 1 -	Sequen	ice Demo1	I (MODIF	IED)												-	- C	ı ×
Fi	ile Edit	Sequer	nce Vie	w Windo	ow Help	ムダ	Å k													
	) 🖿 🖪	氯 🔞	i 🖬 .	<b>୬</b> ୧ ୫	K 🕒 🖻	05 Æ	- 1	▶ ▶ @ 0		0 🖌	- 🗹 í	8 8E .								9
	Status	Run	SV	EV	I/V	Sample ID	Sample	Sample Amount	ISTD1 Amount	Sample Dilut.	Inj.Vol. [µL]	File Name	Sample Type	Lvl	Method Name	Report Style	Open	Open Calb.	Print	Export Data
1		~	1	1	1	Std	%q	0,000	0,000	1,000	0,000	%Q	Sta	1	Demo1	Calibration	~			
2		~	2	2	1	Unk1	%q	0,000	0,000	1,000	0,000	%Q	Unk		Demo1	Calbration	~			~
3 4		~	3	3	1	Unk2	%q	0,000	0,000	1,000	0,000	%Q	Unk		Demo 1	Calibration	-			~
<																				>
Fo	r Help, pre	ss F1						Single	Analysis: No	method s	ent - Read	iy to sen	d metho	d or	start sequence	Vial: 1 / Inj.: 1			File	Name:

### Batch

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

Batch			×
2505MULTI EXAMPLE Instrument 1-07.08.2018 12_11_24 PERS01 PERS02 Sample_Vial_6-1 Sample_Vial_6-2 Sample_Vial_6-2 Sample_Vial_6-1 Sample_Vial_6-1 Sample_Vial_6-1 Sample_Vial_6-1 Sample_Vial_9-1 Sample_Vial_9-1	File Type: Chromatograms ✓ Select All Unselect All Sort by: (a) Name (b) Time Order: (c) Normal (c) Badoward	Options Performs by Method Complete Processing Open Chromatogram W Preserve Integration Open Calibration Windc Print Results Print Results Print Results Print Results to PDF Export Data Include in SST Open with calibration Export Chromatogram Export Chromatogram Export Chromatogram Export Chromatogram Program to Run C:Program Ties (v86) M Parameters %e Proceed	W Show Alerts Unchanged Unchanged In ALA Format In TXT Format In TXT Format

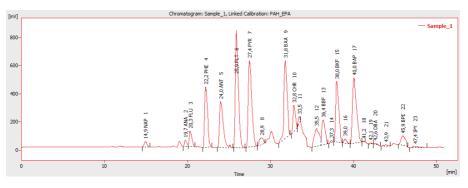
## 12.4 Exporting a chromatogram as a picture

You can export a chromatogram as a picture to the clipboard or as a file to a folder of your choice. The picture will include the labels and lines included in the chromatogram.

1. **Open the** *Chromatogram* window: select *Window - Chromatogram* from the

Instrument window or click on Mi

- 2. Open the chromatogram you want to export.
- Select File Export Export as picture to clipboard and paste the picture to MS Word, MS Powerpoint, Open Office Writer or any other suitable application of your choice.
- 4. Select *File Export Export as picture to file...* and then select the folder where you would like to save the file in Enhanced Metafile Format.



# **13 Mathematical Operations**

This functionality was implemented into Clarity to give users a powerful tool to manipulate already measured data without modifying original raw data. Mathematical operations present a very convenient approach to perform various actions such as extraction of a selected signal/s from multiple signal chromatogram or subtraction of various chromatograms from each other. You can display three examples of applications of Mathematical Operation in our web based User Guide to Clarity. Many other applications may be developed by Clarity users on their own.

# 13.1 Extract chromatogram's signal using Mathematical Operations

You can save a particular signal from a chromatogram that contains several of them. This results in a stand-alone chromatogram file containing only the individual signal of choice, not all of the signals from the original chromatogram which might be confusing when working with a larger number of signals.

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

Open Chromatogram - D:\clarity\DataFiles\DEMO2\Data							
Look In:	Data		- v 🕈 🛃 🔽	199 <b>189</b> 199 Ref	7 C D		
Name 🔺		Size	Туре	Created	Last Change		
ACopy.prr	n	447 kB	PRM Chromatog	8/7/2018 9:47 AM	8/7/2018 9:50 AM	· 1	
	t 1 - 8_9_2018 2_41	226 kB	PRM Chromatog		8/9/2018 2:41 PM		
Sample_1.	.prm	1171 kB	PRM Chromatog	6/30/2018 10:4	8/7/2018 1:35 PM		
Sample_2.	.prm	1186 kB	PRM Chromatog	6/30/2018 10:4	6/30/2018 10:41 PM		
Wine_Sam	ple.prm	1110 kB	PRM Chromatog	6/30/2018 10:4	6/30/2018 10:41 PM		
File Name File Type	Wine_Sample.prm Chromatogram files (	*.prm)	<b></b>	gnals: UV detector RI detector	OK		
Method	6/6/2018 2:34:03 PM	, IA: 8.0 Re	v.0 Recent (Li 🗸		Overlay Mc	de	
Analyst:	Administrator		Version:	Clarity			
SampleID:	Wine		Range/Ra	te: <varies></varies>			
Sample:	Sample		Time:	7.50 min			
Signature:	Not signed		Has PDA [	Data: No			
GLP Mode	Off		GCxGC:	No			
	M	Aa		~~~			

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

Mathematical Operations			×
Operand A		Operation	Operand B
The Whole Chromatogram		Copy Invert Differentiate A + B A - B	The Whole Chromatogram
Apply Method 0	C:\darity\DataFiles\\ ACopy OK	NORK4 Default4	

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

# **13.2 Subtraction of various chromatograms using Mathematical Operations**

If you would like to use one of your chromatograms as a baseline for another chromatogram (s) there is a way to subtract the desired chromatogram from any other chromatogram. This subtraction of chromatograms may be performed using Mathematical Operations.

1. **Open the** *Chromatogram* window: select *Window - Chromatogram* from the

*Instrument* window or click on <u>M</u>.

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

Look In:	Data		~ *	ካ 🤌 👩		54 Roll	m C	D	
Name 🔺		Size	Type		Created		Lact C	hange	-
1 2506MUL									
A EXAMPLE		1156 kB		hromatog		018 22:41		.2018 22:41	
A PERSO1.		812 kB 610 k8		hromatog hromatog		018 22:41		.2018 22:41	
M PERS02.		568 kB		hromatog		018 22:41		.2018 22:41	
A Sample		639 kB		hromatog		018 22:41		.2018 22:41	
A Sample_		509 kB		hromatog		018 22:41		.2018 11:46	
	Vial_0_2.prm	509 kB		hromatog		018 22:41		.2018 11:46	
A Sample_				hromatog		018 22:41		.2018 11:46	
A Sample				hromatog		018 22:41		.2018 11:46	
	Vial 8-2.prm	509 kB	PRM C	hromatog	30.06.2	018 22:41	02.08	.2018 11:46	
A Sample_		509 kB	PRM C	hromatog	30.06.2	018 22:41	02.08	.2018 11:46	
K Sample	Vial_9-2.prm	508 kB	PRM C	hromatog	30.06.2	018 22:41	02.08	.2018 11:46	
ile Name	PERS01.prm			Si	anals:			ОК	_
	PERSOTIPHI				Signal 1			UK	
ile Type	Chromatogram files	(*.prm)		~	- orginal x			Cancel	
ethod	06.06.2018 14:24:2	24, IA: 8.0 Re	v.0 Rec	ent (L 🗸				🗹 Overlay M	lod
nalyst:	DataApex Ltd.			Version:	Cla	rity			
ampleID:	Mr. X.Y.			Range/Ra	te: 125	60 mV / 10 H	łz		
ample:	DEMO Example - ethan	ol in blood		Time:	6,0	0 min			
ignature:	Not signed			Has PDA D	Data: No				
LP Mode	Off			GCxGC:	No				
		Å							

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

Look In:	omatogram - D:\clarity	\DataFiles\[		8 1	8 14 Rol		D	>
Name	Data	Size	Type	Creat		Last Cha		_
1 2506MULT		1156 kB			2018 22:41		018 22:41	
A EXAMPLE.		812 kB			2018 22:41		018 22:41	
PERS01.pr			PRM Chromatog. PRM Chromatog.		.2018 22:41		018 22:41	
PERS02.pr		568 kB			.2018 22:41		018 22:41	í.
A Sample Via		507 kB	<b>j</b>		2018 22:41		018 22:41	
Sample_Via		508 kB			2018 22:41		018 22:41	
Sample_Via		508 kB	-		.2018 22:41	30.06.2	018 22:41	
Sample_Via		509 kB	PRM Chromatog.	30.06	.2018 22:41	30.06.2	018 22:41	
K Sample_Via	al_8-1.prm	506 kB	PRM Chromatog.	30.06	.2018 22:41	30.06.2	018 22:41	
Kample_Via	al_8-2.prm	508 kB	PRM Chromatog.	30.06	.2018 22:41	30.06.2	018 22:41	
Sample_Via	al_9-1.prm	508 kB	PRM Chromatog.	30.06	.2018 22:41	30.06.2	018 22:41	
Sample_Via	al_9-2.prm	507 kB	PRM Chromatog.	30.06	.2018 22:41	30.06.2	018 22:41	
File Name	PERS02.prm			Signals:			OK	
File Type	Chromatogram files (	*.prm)	$\sim$	Signal	1		Cancel	
Method	06.06.2018 14:25:34	1, IA: 8.0 Re	v.0 Recent (L $ \sim$				Overlay Mod	de
Analyst:	DataApex Ltd.		Version	: 0	Clarity			
SampleID:	Mr. X.X.		Range/	Rate: 1	L250 mV / 10 H	Ηz		
Sample:	DEMO Example - ethano	l in blood	Time:	6	5,00 min			
Signature:	Not signed		Has PD	A Data: N	ło			
GLP Mode	Off		GCxGC	: N	ło			
			_Λ					

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

Mathematical Operations		×
Operand A	Operation	Operand B
The Whole Chromatogram  PERS02	• Сору	The Whole Chromatogram
	◯ Invert	
	O Differentiate	
	○ A + B	
	ОА-В	
×		
Apply Method Demo 1		
Save As Chromatogram ACopy		
OK	Cancel	Help

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

Mathematical Operations		×
Operand A	Operation	Operand B
PERS02	ОСору	PERS01
	() Invert	
	ODifferentiate	
	○ A + B	
v	🖲 А - В 🕘	v
Apply Method Demo1		
Save As Chromatogram		
ОК	Cancel	Help

From the dropdown menu (an arrow next to the name) in the Operand B section, select the desired chromatogram you want to subtract <sup>©</sup>. Fill out a name <sup>d</sup> and click OK <sup>®</sup> to save new subtracted chromatogram.

Mathematical Operations			×
Operand A	Operation	Operand B	_
PERS02	Copy Invert	PERS01	î
	○ A + B		~
Apply Method  Demo 1 Save As Chromatogram A-B ON	Cancel	 (1) Hep	

# 13.3 Copying of chromatogram using Mathematical Operations

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

1. **Open the Chromatogram window:** by selecting Window - Chromatogram

from the Instrument window or click on M.

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

🧧 Open Chro	matogram - C:\Clarity	_Demo\Dat	aFiles\DEMO2\Data	а	>
Look In:	Data		- v 🕈 🛃 🔽	198 <mark>199</mark> 197 Ref	👬 C D
Name 🔺		Size	Туре	Created	Last Change
Sample_1.	xm	1170 kB	PRM Chromatog	30.06.2018 22:41	30.06.2018 22:41
Sample_2.p	orm	1186 kB	PRM Chromatog	30.06.2018 22:41	30.06.2018 22:41
Wine Samp	le_1.PRM	337 kB	PRM Chromatog	02.08.2018 10:45	02.08.2018 10:45
Wine_Samp	ole.prm	1110 kB	PRM Chromatog	30.06.2018 22:41	30.06.2018 22:41
File Name	Sample_1.prm		Si	gnals:	ОК
File Type	Chromatogram files (	*.prm)	~	Signal 1	Cancel
Method	06.06.2018 14:34:24	l, IA: 8.0 Re	v.0 Recent (L 🗸		🗹 Overlay Mode
Analyst:	DataApex		Version:	Clarity	
SampleID:	0541		Range/Ra	te: 10000 mV / 10	Hz
Sample:	DEMO Example - PAH		Time:	50,98 min	
Signature:	Not signed		Has PDA [	Data: No	
	Off		GCxGC:	No	
GLP Mode					

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

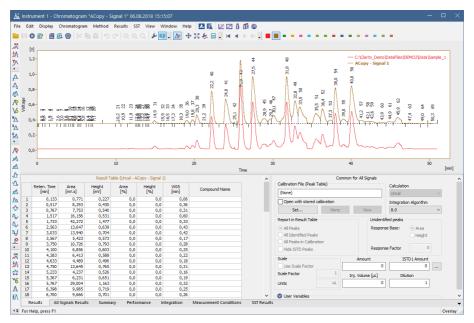
Graph Properties						?	×
Graph Axes Appearance Time Axis	Signal Axis	Signals	Gradient & Aux	diary Signals	Auxiliary Signal Details		
Use User Options		C:\	Clarity_Demo\Da	ataFiles\DEMO	2\Data\Sample_1	~	
Grey Out Inactive Signals		Show I	shele	Offset & S	icale	٦	
Scale Y Mode Preserve Signal Ratios Scale to All Signals Scale to Active Signal		_		X Offset X Scale	0,000000 [m	in]	
Scale Signals Separately		Line Width	1	Y Offset Y Scale	(a) 0 [m	v]	
Scale Maximum to: Maximum value	~	Color.			Original		
Scale Minimum to:		20101.			Orige tot		
Minimum value	$\sim$						
			OK	Can	cel Apply	Н	elp

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

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

Mathematical Operations				×
Operand A The Whole Chromatogram Sample_1		Operation © Copy O Invert O Ifferentiate O A + B O A - B	Operand B The Whole Chromatogram	
Apply Method 0	Demo2 ACopy OK	Cancel		

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



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

Graph Properties			?	×
Graph Axes Appearance Time Axis	Signal Axis Signals	Gradient & Auxiliary Signals	Auxiliary Signal Details	
Use User Options	AC	opy - Signal 1		$\sim$
Set Initial Colors				
Grey Out Inactive Signals	Show Show L	Offset & S	cale	
Scale Y Mode Preserve Signal Ratios		X Offset	0,000000 [min]	
<ul> <li>Scale to All Signals</li> <li>Scale to Active Signal</li> </ul>	Line Width		1	
○ Scale Signals Separately		1 Y Offset Y Scale	0 [V]	
Scale Maximum to:				
Maximum value	✓ Color.		Original	
Scale Minimum to:				
Minimum value	~			
		OK Can	cel Apply	Help

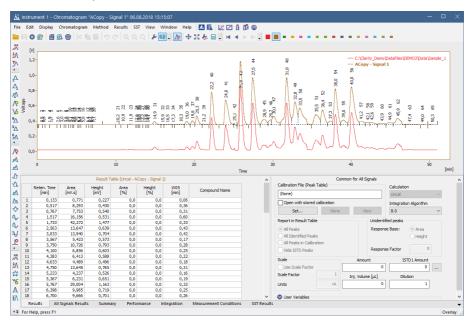
9. From the **Dropdown menu** select the original chromatogram.

Graph P	roperties						?	$\times$
Graph	Axes Appearance	Time Axis	Signal Axis	Signals	Gradient & Auxiliary Signals	Auxiliary Signal Details		
	Jse User Options			C	\Clarity_Demo\DataFiles\DEMC	2\Data\Sample_1	~	
	Set Initial Cold	ors			\Clarity_Demo\DataFiles\DEMC	2\Data\Sample_1	^	
Scal	Grey Out Inactive Sig e Y Mode Preserve Signal Ratio Scale to All Signals Scale to Active Sig	s		Sh #	2opy - Signal 1 3 <unassigned> 4 <unassigned> 5 <unassigned> 6 <unassigned> 3 <unassigned> 9 <unassigned> 10 <unassigned></unassigned></unassigned></unassigned></unassigned></unassigned></unassigned></unassigned>			
	Scale Signals Separat e Maximum to:	ely		##	11 <unassigned> 12 <unassigned> 13 <unassigned> 14 <unassigned> 15 <unassigned> 15 <unassigned> 15 <unassigned></unassigned></unassigned></unassigned></unassigned></unassigned></unassigned></unassigned>			
	ximum value		$\sim$	#	17 <unassigned> 18 <unassigned></unassigned></unassigned>			
	e Minimum to: imum value		~	#	19 <unassigned> 20 <unassigned> 21 <unassigned> 22 <unassigned> 23 <unassigned> 24 <unassigned></unassigned></unassigned></unassigned></unassigned></unassigned></unassigned>			
				#	25 <unassigned> 26 <unassigned> 27 <unassigned> 28 <unassigned> 29 <unassigned> 30 <unassigned></unassigned></unassigned></unassigned></unassigned></unassigned></unassigned>		Ŷ	lp

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

Graph Properties		? ×
Graph Axes Appearance Time Axis Sign Use User Options Set Initial Colors Grey Out Inactive Signals Scale Y Mode Preserve Signal Ratios © Scale to Al Signals O Scale for Active Signal O Scale Signals Separately Scale Maximum to:		illary Signals Auxiliary Signal Details taFiles/DEMO2/Data/Sample_1   Offset & Scale X Offset 0,000000 [min] X Scale 1 Y Offset 3331 [V] Y Scale 1
Skate Maximum UD: Maximum value Skate Minimum to: Minimum value	Color	Original Original

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



# 14 Back-up and Restore

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

# 14.1 Backing up a project (Creating an Archive)

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

- 1. **Open the Backup dialog** by selecting *Instrument- Archive...* on the *Instrument window*.
- 2. Select *Projects* on the *File Type* (a) option to archive a complete project directory.
- 3. Select the project or projects you wish to back up from the list. The Select All Files button (a) will select all projects.
- 4. Choose from the following options **b**:
  - Uncheck the *Without Compressing* option to archive all files into one compressed file.
  - Check the *Move to Archive* option to have the original files erased after backing them up.
  - Check the *Including Common* option to back up also the COMMON subdirectory.
- 5. Choose the output directory and name for the archive ©.

More Info:

Compressed files will have the .DGZ extension.

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

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

eate Archive Rest	ore Archive			
	ore Arctive			
ile List:			Selected Size:	560 1,72 kE
File Name	Date	Size Analyst	Description	
1 DEMO1	29.08.2006	1,41 kB Administrator	Demo project with GC examp	ples
2 DEMO2	29.08.2006	1,42 kB Administrator	Demo project with HPLC exa	mples
3 DEMO3	29.08.2006	1,10 kB Administrator	Demo project	
4 DEMO4	29.08.2006	1,09 kB Administrator	Demo project	
5 DEMO_DHA	04.10.2011	1,63 kB Administrator	Detailed Hydrocarbon Analys	
6 DEMO_EA	23.12.2004	1,25 kB Administrator	Elemental Analysis DEMO da	ta
7 DEMO_GPC	03.05.2004	1,28 kB dataapex	DEMO data GPC module	
8 DEMO_MS	11.11.2012	1,82 kB Administrator	MS Extension DEMO Data	
9 DEMO_NGA	11.06.2009	1,86 kB Administrator	Natural Gas Analysis DEMO o	data
10 DEMO_PDA	04.05.2004	1,22 kB kauf	DEMO data for PDA	
11 WORK1	25.10.1994	1,85 kB DataApex Ltd.	Default project for Instrume	nt 1
12 WORK2	25.10.1994	1,64 kB DataApex Ltd.	Default project for Instrume	
13 WORK3	25.10.1994	1,38 kB DataApex Ltd.	Default project for Instrume	
14 WORK4	25.10.1994	1,13 kB DataApex Ltd.	Default project for Instrume	nt 4
		a	Select All Files	Delete Selected Files
File Type:	Projects			
, ne type.	, rojecto		ation Standards 🛛 🗹 Witt	hout Compressing
		From	Common (b) May	ve to Archive
Target C:\		C		ic to Arctive
			ling Common	
			~	â

# 14.2 Restoring a project from an archive

- Open the Backup dialog by selecting *Instrument Restore...* on the *Instrument window*.
- Select Projects on the File Type (a) option to restore a complete project directory.
- Select the project or projects you wish to back up from the list. The Select All Files button (a) will select all projects.
- Choose from the following options (b):
  - Uncheck the *Without Compressing* option to restore all files from a compressed file.
  - Check the *Move from Archive* option to have the archived files erased after restoring them.
  - Check the *Including Common* option to restore also the COMMON subdirectory.
- 5. Choose the source directory and select the source file ⓒ. Compressed files will have the .DGZ extension.
- 6. Click on the Restore button (d) to restore the project or on the OK button (e) if you do not need to restore any more files.

ckup (DEMO	1)					-		>
reate Archive	Restore Archive							
File List:					Selected Size:			0 E
File	Name	Date	Size	Analyst	Description			
			(3)	Select All Files	Delete Sel	lected File	s	
File	Type Projects		~	Calibration Standards	Without Compre	uning.		
				To Common	Mariout Compression     Move From Arch			
	C:/		©	Including Common	<u> </u>			
Source								
Source [				e e		<b>d</b>		

# 14.3 Backing up specific files (Creating an Archive)

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

- 1. **Open the Backup dialog** by choosing *Instrument Archive...* on the *Instrument window*.
- 2. Select the *File Type* (a) option according to the files you wish to back up.
- Select the files you wish to back up from the list. The Select All Files button

   a will select them all.
- 4. Choose from the following options (b):
  - Uncheck the *Without Compressing* option to archive all files into one compressed file.
  - Check the *Move to Archive* option to have the original files erased after backing them up.
  - Check the Calibration Standards option when archiving chromatograms. The chromatogram files from the CALIB subdirectory (instead of the DATA subdirectory) should be listed.
  - Check the *From Common* checkbox for displaying the system files from the COMMON directory.
- 5. Choose the output directory and name for the archive ©.

More Info:

Compressed files will have the .DGZ extension.

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

ckup (DEMO	1)						
reate Archive	Restore Ar	chive					
File List:					Se	lected Size:	0 E
File	Name	Date	Size	Analyst	t Sar	nple ID	San
1 2506MUL	п	01.08.2003	1156,03 k D	DataApex	SN4616 wine	5 ul stand	lard wine mix 1
2 EXAMPLE		29.05.2003	812,28 kB E	DataApex			
3 PERS01		16.01.1995	610,89 kB E	DataApex Ltd.	Mr. X.Y.	DEMO Exa	ample - ethanol i
4 PERS02		05.01.1995	568,95 kB D	DataApex Ltd.	Mr. X.X.	DEMO Exa	ample - ethanol
5 SAMPLE	VIAL_6-1	07.08.2018	507,37 kB /	Administrator	Halocarbons	Sample	
6 SAMPLE	VIAL_6-2	07.08.2018	508,18 kB A	Administrator	Halocarbons	Sample	
7 SAMPLE	VIAL_7-1	07.08.2018	508,39 kB /	Administrator	Halocarbons	Sample	
8 SAMPLE	VIAL_7-2	07.08.2018	509,31 kB A	Administrator	Halocarbons	Sample	
9 SAMPLE	VIAL_8-1	07.08.2018	506,82 kB /	Administrator	Halocarbons	Sample	
10 SAMPLE	VIAL_8-2	07.08.2018	508,21 kB A	Administrator	Halocarbons	Sample	
11 SAMPLE	VIAL_9-1	07.08.2018	508,33 kB /	Administrator	Halocarbons	Sample	
12 SAMPLE	VIAL_9-2	07.08.2018	507,01 kB /	Administrator	Halocarbons	Sample	
<					_		>
				<u>a</u>	Select All Files	Delete Selected	Files
File 1		matograms			oration Standards	Without Compressing	
		natograms ence Files		^			
C Target		od Templates		Fron	n Common	Move to Archive	
		ation Files		Indu	uding Common		
		rt Styles			-		
		lethod Files					
		Calibration Files			OK	Cancel Archive	Help

### 14.4 Restoring a file from an archive

- 1. **Open the Backup dialog** by choosing *Instrument Restore...* on the *Instrument window*.
- 2. Select the File Type (a) option according to the files you wish to restore.
- Select the files you wish to restore from the list. The Select All Files button

   a will select them all.
- 4. Choose from the following options (b):
  - Uncheck the *Without Compressing* option to restore all files from a compressed file.
  - Check the *Move from Archive* option to have the original files erased after restoring them.
  - Check the Calibration Standards option when restoring chromatograms to the CALIB subdirectory (instead of the DATA subdirectory).
- 5. Choose the source directory and select the source file<sup>©</sup>.

#### More Info:

Compressed files will have the .DGZ extension.

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

									>
eate Archive Re	store Archive								
ile List:					Se	elected Size:			0 B
File Na	me	Date	Size	Analyst	De	scription			
				•					
					ct All Files	De	lete Selected Fi	les	
File Typ								les	
~	Chromator Sequence	rams Files		~	Standards	Without	lete Selected Fi Compressing om Archive	les	
File Typ	Chromatoc Sequence I Method Te	rams Files mplates		Calibration S	Standards	Without	Compressing	les	
~	Chromator Sequence I Method Te Calibration Report Sty	rams Files mplates Files fles		Calibration S	Standards	Without	Compressing	les	
~	Chromator Sequence I Method Te Calibration	rams Files mplates Files des d Files ation Files		Calibration S	Standards	Without (	Compressing	les Help	

# 15 Managing the Chromatography Station

Following chapters contains extended information how to set restrict access to various parts of Clarity to certain users or set up communication with a mobile application.

# 15.1 Enabling instruments to be used by Clarity2Go application

**Clarity** enables to send specific parameters over the internet to be monitored via **Clarity2Go** application available at Android (**Google Play** store) and iOS (**Apple** store) smartphones. In this way you can monitor your analyses while outside the laboratory.

The whole solution consists of three independent parts:

- **Clarity** station (at your side) sends information about state and running analyses to the server
- Server (at DataApex's side) dispatches the information from Clarity stations to Clarity2Go clients
- Client (at your side) device (smartphone or tablet) with installed Clarity2Go application processes information from the server

DataApex is providing a free public server for this use.

### How to set up Clarity:

- 1. In the Clarity main window, go to *System* menu and click on the command *Clarity2Go....*
- 2. In the opened Clarity2Go Configuration dialog, check the checkbox of Instrument 1 to 4, depending on the instruments you want to monitor. Every checked Instrument will get its unique *Instrument ID*.
- 3. Press the *OK* button to save the configuration and continue with steps described in **How to set up Clarity2Go** section.

Clarity2Go Configuration	on	×
	Instrument ID	
Instrument 1	54433046	
Instrument 2		
Instrument 3		
Instrument 4		
Advanced >>	OK Cancel Help	

Fig 1: Clarity2Go Configuration - Basic

Options described below are optional and are not obligatory for correct functionality. They are revealed by pressing the *Advanced* button.

- Unregister All Instruments disables the monitoring in the Clarity2Go application. Instruments that have been registered will no longer be available for monitoring. If you will later change your mind, you will have to generate new Instrument ID.
- Web Server Address do not change this field. It defines the address of Clarity2Go web server. Address other than default will result in the monitoring to be not functional! Press the *Default* button to set functional web address of the server.
- *Proxy Server Address* consult with your local administrator if a proxy server is applied in your local network and then provide the proxy server address.
- Protect by Password provided password will be valid for all Instruments. The same password needs to be provided in the Clarity2Go application to unlock the monitoring.
- Press the OK button to save the configuration and continue with steps described in **How to set up Clarity2Go**.

Clarity2Go Configuratio	on	×
	Instrument ID	
Instrument 1	54433046	
Instrument 2		
Instrument 3		
Instrument 4		
	Unregister All Instrume	ents
Web Server Address:	http://darity2go.dataapex.com:80/	Default
Proxy Server Address:		(optional)
Protect by Password:		(optional)
<< Basic	OK Cancel	Help

Fig 2: Clarity2Go Configuration - Advanced

### How to set up Clarity2Go:

Once you have configured instrument(s) in **Clarity**, it's time to monitor those instruments using **Clarity2Go** application. This part assumes that you have **Clarity2Go** for Android application installed and running.

- Make sure that you are not in the Clarity Demo mode, indicated by a gray stripe at the bottom of the application with the inscription DEMO mode. Tap on the TURN OFF DEMO.
  - **Clarity Demo** mode does not allow to add instruments. Stripe at the bottom serves as an information center. Changes in the

configuration or notifications are displayed here.

DEMO mode TURN OFF DEMO

Fig 3: Clarity Demo mode gray stripe

- 2. In the Settings, tap on *Demo Switch to demo mode* which turns the Clarity **Demo** mode *OFF*.
- 3. Return back. In case you are configuring **Clarity2Go** for the first time, you will see that there is no instrument.



Fig 4: No Instrument screen

- 4. Tap on the blue "plus" button at the bottom right corner to add a new instrument.
- 5. Enter *Instrument ID* that has been generated by **Clarity** and enter password (only if you have set it up in **Clarity**). Tap on the *OK* button to start monitoring this instrument.



Fig 5: New Instrument screen

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

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

# 15.2 Locking/Auto Locking a Clarity Instrument

You may lock a Clarity Instrument protected by password if you want to prevent unauthorized access to it, for example, when an analysis is running.

### Manual Lock

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

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

🔺 (	Clarity			- ×
System	Instruments View Help			
• '	Open Instrument 1			
-	Logout from Instrument 1	Instrument 2	Instrument 3	Instrument 4
۲	Lock Instrument 1	R.S.R.		E A E
<b>e</b>	🔑 Login to Instrument 2		litro.	
	Open Instrument 3		Locked	
	Unlock Instrument 3			
C	Login to Instrument 4			
0	💄 Abraham 🚺 Running		🚊 Abraham 🛛 📀 Ready	
I	Lock Instrument Instrument 1			

### Auto Lock

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

- 1. **Open the User Accounts window:** click on  $\stackrel{\bullet}{=}$  or choose System User Accounts.
- 2. Check the Auto Lock function (a).
- 3. Set the period of inactivity in minutes after which all opened *Instruments* will be locked. (b)

User List       Password Restrictions - Common for All         Min. Length       1 0 (Chars.)         John       LifeTime         John       1 0 (Days)         Degrete	User Accounts			×
User Name Abraham Description Other Users Can  Read & Write Cread & Crea	Abraham Anne John Tom		Min. Length	1         +         [Chars.]           1         +         [Days]           5         +         [Days]           1         +         [Days]
Other Users Can       Instrument 1	User Name Abraham Desktop File Abraham	User Details for: Abraham	Password: Password Changed:	07. srpen 2018
Open User Accounts     Edit Sequence     Open Configuration     Cettificate     Certificate     Certificate     Certificate     Certificate     Certificate For Exporting To PDF	Other Users Can	Instrument <u>1</u> Instrument <u>2</u> Instrument <u>3</u>	Change	e Password
	Open User Accounts Open Configuration Edit Method Edit Method Edit Chromatogram Edit Calibration Projects	Edit Report Style     Select Method     Open Audit Trail Settings     Archive / Restore     Post Run Settings		g To PDF

## 15.3 Unlocking a Clarity Instrument

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

#### User Guide

	Clarity n Instruments View Help			- ×
• © • • • • •	Instrument 1 P Unlock to Abraham	Instrument 2	Instrument 3	Instrument 4
	Unlock Instrument Instrument 1 (LC)			

# Unlocking Instrument after entering wrong password three or more times:

#### More Info:

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

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

### 15.4 Monitoring Events and Operations in Clarity

The *Audit Trail* can be used for finding out who did what and when, including file operations, changes to settings, events that take place during data acquisition and system messages. Therefore this is an essential tool for troubleshooting and managing Clarity. To access the *Station Audit Trail*:

1. Select *Window - Station Audit Trail* from the *Instrument, Chromatogram, Calibration, Sequence or Data Acquisition windows.* 

🅂 Instrun	nent 1									-	×
Instrument N	lethod Analysis	Evaluation	Setting	Wir	ndow	Help					
E,	4	<i>.</i>	-(	Ľ ▲ Å		/ All	m	 М		/	
🕑 No me	ethod sent				Singl	e Analys	is		8	3	
Status:	Ready to ser	nd method or s	tart seque	63 68	Sequ	ence on Audit	Trail				
Sent method:	none			<u>.</u>		Acquisit					
								📑 WOR	K1	<u>●</u> Be	'n
Show Station Au	idit Trail Window										//

2. Click on the Session tab (a) if you would like to see the log from the time Clarity was started or on the Daily Audit Trial tab for the present day events.

File	Edit			Wind	_			A PA PA					
	ē (0		4	41	Y	© - 🖌	1						
	OK	Tim	ne 👌	<i>y</i>	Тур	Analyst	Instrument	Area	Description			Info	
	ok	07.08.2018	10:4	2:07	Z	Abraham	Instrument	Acquisitio	Acquisition was stopped by detection of stop of all	Clarity 8.0.0.	125 FULL,	SN: 088-000888	
	ok	07.08.2018	10:4	2:07	<u>.</u>	Abraham	Instrument	Acquisitio	Running - Acquisition running: Instrument was abo	Clarity 8.0.0.	125 FULL,	SN: 088-000888	
	ok	07.08.2018	10:4	2:07	i		System	Message	Do you want to abort running analysis? YES	Clarity 8.0.0.	125 FULL,	SN: 088-000888	
	ok	07.08.2018	10:4	1:18	2	Abraham	Instrument	Acquisitio	Ready - Ready to start run: Acquisition was starte	Clarity 8.0.0.	125 FULL,	SN: 088-000888	
	ok	07.08.2018	10:4	1:18	-5		Instrument	Files	Open File D: \Clarity \DataFiles \DEMO1 \Calib \Exam	Clarity 8.0.0.	125 FULL,	SN: 088-000888	
	ok	07.08.2018	10:4	1:17	i	Abraham	Instrument	Detector	VD: Method sent to sub-device.	Clarity 8.0.0.	125 FULL,	SN: 088-000888	
	ok	07.08.2018	10:4	1:17	i	Abraham	Instrument	Acquisitio	Method 'D: \Clarity \DataFiles \DEMO1 \Demo1.met (	Clarity 8.0.0.	125 FULL,	SN: 088-000888	
	ok	07.08.2018	10:4	1:17	4	Abraham	Instrument	Files	Open File D: \Clarity \DataFiles \DEMO 1 \Calib \Exam	Clarity 8.0.0.	125 FULL	SN: 088-000888	
	ok	07.08.2018	10:3	8:34	5	Abraham	Instrument	Files 🞱	Open File D:\Clarity\DataFiles\Common\Chromato	Clarity 8.0.0.	125 FULL	SN: 088-000888	
ו	ok	07.08.2018	10:3	8:32	4	Abraham	Instrument	Files	Open File D: \Clarity \DataFiles \DEMO1 \Demo1.met	Clarity 8.0.0.	125 FULL,	SN: 088-000888	
1	ok	07.08.2018	10:3	8:32	4	Abraham	Instrument	Files	Open File D: \Clarity \DataFiles \Projects \DEMO1.prj	Clarity 8.0.0.	125 FULL	SN: 088-000888	
2	ok	07.08.2018	10:3	8:32	1	Abraham	Instrument	Instrume	Open Instrument	Clarity 8.0.0.	125 FULL	SN: 088-000888	
3	ok	07.08.2018	10:3	8:32	ä,	Abraham	Instrument	Files	Open File D:\darity\Cfg\Clarity.dsk	Clarity 8.0.0.	125 FULL	SN: 088-000888	
4	ok	07.08.2018	10:3	8:29	4		System	System	Command line parameter(s): DataApex.ini parame	Clarity 8.0.0.	125 FULL	SN: 088-000888	
5	ok	07.08.2018	10:3	8:29	ő.		System	System	Start System, Version: 8.0.0.125	Clarity 8.0.0.	125 FULL	SN: 088-000888	
6		07.08.2018	10:3		<b>6</b>		System	System	End System	Clarity 8.0.0.	125 FULL	SN: 088-000888	
7		07.08.2018			<b>1</b>	Abraham	Instrument	Instrume	Close Instrument			SN: 088-000888	
3	ok	07.08.2018	10:3	8:24	Ö.	Abraham	Instrument	Files	Save File D: \Clarity\DataFiles\Projects\DEMO1.pri	Clarity 8.0.0.	125 FULL	SN: 088-000888	
9		07.08.2018			T				No method sent - Ready to send method or start s	Clarity 8.0.0.	125 FULL	SN: 088-000888	
5		07.08.2018			ġ.		Instrument		Open File D: \Clarity\DataFiles\Common\Calibration				
1		07.08.2018	10:3	7:04	4	Abraham	Instrument	Files	Open File D:\darity\DataFiles\COMMON\Template.	Clarity 8.0.0.	125 FULL	SN: 088-000888	
2		07.08.2018			a,		Instrument		Open File D: \Clarity DataFiles \Common \Chromato				
3		07.08.2018			a s		Instrument		Open File D: \Clarity\DataFiles\DEMO1\Demo1.met				
4		07.08.2018			4		Instrument		Open File D: \Clarity \DataFiles \Projects \DEMO1.prj				
5		07.08.2018			<b>H</b>	Abraham	Instrument	Instrume	Open Instrument			SN: 088-000888	
6		07.08.2018			4		Instrument		Open File D:\darity\Cfg\Clarity.dsk			SN: 088-000888	
7		07.08.2018			a.				Close Instrument			SN: 088-000888	
B		07.08.2018			ď.		Instrument		Save File D: \Clarity\DataFiles\Projects\DEMO1.prj				
č	JK		2010		-	, an an ann			instanting and and and a solution for the start				
	ession	Daily A			010	00.07	Global						

#### More Info:

The *Daily Station Audit Trail* is stored in one separate file every day the station is running. These files can be opened by using the command File - Open Audit Trail (Append).

3. Click on the *Instruments* or *System* icons (b) if you want to filter out events or operations.

4. Click on the *Properties* icon <sup>(C)</sup> if you want to set up which events and operations should be recorded on the *Session* or *Daily Audit Trail* on each one of the tabs.

Audit Trail S	Settings						×
Messages	Chromatogram	Calibration	GPC Calibration	Sequence	Method	Other	
			Session	Daily Au	dit Trail		
Export Me	ssages (Batch)		$\checkmark$	$\checkmark$	]		
Detector B	Error Messages		$\checkmark$	$\sim$	1		
LC Error M	lessages		$\checkmark$	$\checkmark$	]		
GC Error N	lessages		$\checkmark$	$\sim$	]		
AS Error N	lessages		$\checkmark$	$\checkmark$	]		
CE Error N	lessages		$\checkmark$	$\checkmark$	]		
Other Mes	sages		$\checkmark$	$\sim$	1		
			[	ОК	C	ancel	Help

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

More Info:

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

To access the *Local Audit Trail* (Chromatogram, Calibration, Sequence and Method):

1. Select Window - Chromatogram, Calibration or Sequence Audit Trail from the corresponding window or Click on the Audit Trail button on the Method Setup window for the Method Audit Trail.

More Info:

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

### 15.5 Controlling Clarity from an external application

It is possible to send commands to Clarity using Windows command line parameters and also to read its status through Windows Dynamic Data Exchange (DDE).

- For more information on the commands go to our <u>List of commands</u> in the **Clarity Reference Guide**.
- You can also find the list of variables which will give you information on Clarity status on our DDE datasheet.

# **16 Clarity in Network**

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

### 16.1 Clarity in network overview

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

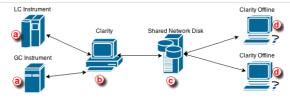
### What does the solution Clarity in network offer?

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

### What does the solution Clarity in network not offer?

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

# **16.2 Multiple Clarity stations in a network**



More Info:

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

Clarity in network is a solution that consists of at least one Clarity, at least one Clarity Offline and a reliable computer network as the most basic setup.

Simplified scheme of the possible configuration is displayed in the diagram above. LC and GC instrument (a) is controlled via Clarity (b). Chromatograms, calibrations and methods are all saved (using directory configuration) on a shared network disk (c). Clarity Offline (d) could then be used for evaluation of acquired chromatograms and preparation of methods which are saved (using directory configuration) on the shared network disk. Clarity (b) is able to send those pre-prepared methods to corresponding instruments.

Note that this shared network disk is then accessible to all computers within this computer network therefore a much wider configuration can be implemented than the one described above.

Following step-by-step guide will help you configure the Clarity in network solution.

# <u>Procedure A</u> - Firstly we will configure Clarity **b** which will acquire data and save them to the shared network disk.

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

Instrument Direct	cories for Projects X
Instrument 1	U:\Shared
Instrument 2	C:\Clarity\DataFiles
Instrument 3	C:\Clarity\DataFiles
Instrument 4	C:\Clarity\DataFiles
E	All As Instrument 1
Existing projects (e you copy/move the	.g. DEMO projects) will not be visible from changed location unless m manually
Audit Trail	C:\Clarity\Cfg\Audit_Trails\
0	K Cancel Default Help

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

Clarity -	Directories $ imes$
<u> </u>	The directory U:\Shared does not have the proper structure. Do you want to create necessary subdirectories and copy Common files?
	<u>Y</u> es <u>N</u> o

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

📐 Cla	arity $ \times$	
System	Login Dialog X	
	Enter User Name:	
ø	Administrator	
<b>a</b>	Select Project:	
	<new project=""></new>	
2	All Possible Instruments	
6	OK Cancel Help	
-	Help, press F1	

9. Fill project name and click OK.

Create Project or S	ave as	×
Laboratory LC		
	OK Cancel	Help

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

# <u>Procedure B</u> - Secondly we will configure Clarity Offline **(d)** which will be used for data evaluation from shared network disk.

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

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

📐 Cla	rity — ×
System	Login Dialog X
• ©	Enter User Name: Administrator
è	Select Project:
	All Possible Instruments
6	OK Cancel Help
For	Help, press F1

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

### 16.2.1 Migrating Clarity Project into a Network

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

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

### We will migrate our Clarity project into shared network disk.

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

#### More Info:

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

Backup (	WORK1)					-		×
Create A	Archive Restore	Archive						
File List	t:			Sele	cted Size:		147,	73 kB
	File Name	Date	Size Anal	yst Descr	iption			
1 DE	EMO1	29.08.2006	1,41 kB Administrator	Demo project with	n GC examples			
2 DE	EMO2	29.08.2006	1,42 kB Administrator	Demo project with	n HPLC examples			
3 DE	EMO3	29.08.2006	1,10 kB Administrator	Demo project				
4 DE	EMO4	29.08.2006	1,09 kB Administrator	Demo project				
5 DE	EMO_DHA	04.10.2011	1,63 kB Administrator	Detailed Hydrocar				
6 DE	EMO_EA	23.12.2004	1,25 kB Administrator	Elemental Analysis	s DEMO data			
7 DE	EMO_GPC	03.05.2004	1,28 kB dataapex	DEMO data GPC n	nodule			
8 DE	EMO_MS	11.11.2012	1,82 kB Administrator	MS Extension DEM	10 Data			
9 DE	EMO_NGA	11.06.2009	1,86 kB Administrator	Natural Gas Analy	sis DEMO data			
10 DE	EMO_PDA	04.05.2004	1,22 kB kauf	DEMO data for PD	A			
11 W	ORK1	25.10.1994	1,85 kB DataApex Ltd.	Default project fo	r Instrument 1			
12 W	ORK2	25.10.1994	1,64 kB DataApex Ltd.	Default project fo	r Instrument 2			
13 W	/ORK3	25.10.1994	1,38 kB DataApex Ltd.	Default project fo	r Instrument 3			
14 W	ORK4	25.10.1994	1,13 kB DataApex Ltd.	Default project fo	r Instrument 4			
			b	Select All Files	Delete	Selected Fi	les	
	File Type: Pro	jects		alibration Standards	Without Con	noressina		
			(d)	rom Common	Move to Arc	hino 🍙		
Ta	arget U:\Shared	1			Move to Arc	iive 🕑		
				cluding Common				
				ОК	Cancel Arc	() hive	Help	

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

📐 Cla	arity		
System	Login Dialog >		
	Enter User Name:		
٥	Administrator	]	
	Select Project:		
	WORK1 V		
L1	<new project=""></new>	1	
	WORK1		
6	OK Cancel Help		
0	L		
For	Help, press F1		

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

### 16.3 Remote control of Clarity over a network



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

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

#### **Requirements:**

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

### .....

### More Info:

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

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

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

### More Info:

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

omputer Name	Hardware	Advanced	System Protect	ion Remote
Remote Assist	tance			
Allow Rem	ote Assistan	ce connectio	ns to this comput	er
What happen	s when I ena	able Remote	Assistance?	
				Ad <u>v</u> anced
Remote Deskt	top			
Choose an op	tion, and the	n specify wh	o can connect.	
O Don't allow	v remote cor	nections to t	his computer	
Allow remo	te connectio	ons to this co	mputer	
			puters running Ri hentication (reco	
Help me choo	se			<u>S</u> elect Users

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

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

#### More Info:

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

You will to provide this information in step 5.

#### More Info:

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

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

#### More Info:

- Click Start and select Control Panel.
- Double-click User Accounts.
- Select Change your Windows Password under User Accounts.
- Click Create a password for your account and follow the instructions on the screen.
- 5. To start Remote Desktop from the computer you want to work from (a).

### More Info:

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

퉣 Remote	Desktop Connection	-		×
	Remote Desktop Connection			
	MAREKE DATAAPEX\MarekP sked for credentials when you cons	v	]	
Show Q	ptions	Connect	H	elp

#### More Info:

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

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

#### This solution then enables you to:

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

# Possible situations that may arise using the Remote Desktop Connection:

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

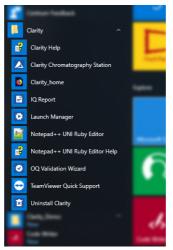
- However, if you try to connect to a PC when there is logged in someone else, e.g. another analyst, he will be asked if he allows the remote connection to put through. If he declines the remote connection you will not be able to connect.
- PC that you are connecting to must be turned on, it is not possible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

# **17 Utilities**

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

# 17.1 Checking that the software has been installed correctly (Installation Qualification - IQ)

The **Installation Qualification** (IQ) is a procedure confirming that the software has been installed successfully and that the files are in the correct version.



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

E IQ				- 1		×
ile Help						
Acquisition and hardware de	evices Maratnon <unknown> UNI Pump Control <unknov DEMO 7890 DemoSN</unknov </unknown>	vn>				
Installation Q	ualification Te	st: Passe	d			
		st: Passe	d	File date	Status	1
Files			Size	File date 30.06.2018, 20:01	-	1
Files	Path c:\clarity_demo\bin\utils		Size 38225		1 Passec	1
Files File advantecchf122scfc.rb	Path c:\clarity_demo\bin\utils \uni_drivers\advantec	Version	Size 38225 385536	30.06.2018, 20:01	1 Passec	1

#### More Info:

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

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

### 17.2 Editing Clarity user profiles using the Launch Manager

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

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

Select Cla	rity Profile		-		×
Select a Clarity	y profile, and double-click	on it, or click Laun	ch to run Clar	ity.	
The profile ma	y modify your current Cla	arity configuration.			
Name Default		Description Default setting			
Barbara		Barbara's confi			
☑ Close this v	vindow after launching Cl	arity			
Laund	h Edit Profiles	s Clo	ise	Help	
					~
dit Profiles - Barba	ra				×
Profiles					
Name		pened: 03.08.201	8, Last Edited	: 03.08.20	18 <b>b</b>
Default Barbara	Descri	ption: ara's configuration			
DdrDdrd			D		
			Duplicate	Crea	
		Rename	Delete	Short	cut
	General				
	Configuration:	<last used=""></last>			× *
۲	Instrument 1	Instrument 2 👩	Instrument	3 🚯 In	strument 4
	Open Instrument				
	Login User Name:	Barbara			
	Desktop:	Barbara.dsk			× »
	Project:	DEMO_DHA.prj			~
	Frojecti	preside Terrational			
	Method:	<from project=""></from>			×
					×

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

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

### More Info:

The list of configuration files is retrieved from the installation directory (configuration files are located in C:\CLARITY\CFG by default). If you click on >, a menu will pop up with operations on the configuration files.

Notice that Clarity always controls the Instrument type when loading the configuration file. If \*.cfg file is damaged or created in later version of Clarity, one of following error messages would appear and Clarity would be closed.

Clarity - Configuration X		
<u> </u>	Configuration file D:\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.	
	OK	
Clarity - Configuration		
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.		

- If you select the <Last Used> option, Clarity will start with the last configuration it was opened with or if Clarity is running, the present configuration will be preserved.
- 7. Select the Desktop, Project, Method and Sequence files that will be loaded when opening each of the instruments (d). Check *Open Instrument* to open given instrument at start.
- 8. Click on the *Refresh Files* button (e) to reload all the files displayed in the Edit Profiles dialog.
- 9. Once the profile is configured, *Close* the Edit Profiles dialog and *Launch* the profile either by double clicking on the profile or by selecting a profile and clicking on the *Launch*.

# 17.3 Creating a duplicate configuration using the Launch Manager

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

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

## pg **22**.

More Info:

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

Setup Con	trol Modules		Number of Instruments: 4				
ne	Used		🔇 Instrument 1	😚 Instrument 2	🚱 Instrument 3	😚 Instrument	t 4
AS			Name				
			Instrument 1			34.27	a.
🖻 💼 Agilent 1100			instanci i				
M FLD : Detector 1	Instrument 1		Instrument Type	e			-
M FLD : Detector 2	Instrument 1		LC				
A FLD : Detector 3	Instrument 1					~	
A FLD : Detector 4	Instrument 1				-		
FLD : Spectral Det A DAD : Detector 1	Instrument 1		Name		From		
A DAD : Detector 1	Instrument 1 Instrument 1			t. Pump : HP1100LC			-
M DAD : Detector 2	Instrument 1			t. Pump: HP1100LC			
M DAD : Detector 3	Instrument 1			t. Pump: HP1100LC			
A DAD : Detector 4	Instrument I			t. Pump : HP1100LC	4 Agilent 1100		
Ouart, Pump : HP1	Instrument 1	>	🖻 🚔 Detecto				
Ouart. Pump : HP1	Instrument 1			Detector 1	Agilent 1100		
Quart, Pump : HP1	Instrument 1	<		Detector 2	Agilent 1100		
Quart. Pump : HP1	Instrument 1	<		Detector 3	Agilent 1100		
AS : Sampler 1	Instrument 1			Detector 4	Agilent 1100		
GC	instanticite i	<<<		: Detector 1	Agilent 1100		
Detector				: Detector 2 : Detector 3	Agilent 1100		
Balance				: Detector 3 : Detector 4	Agilent 1100 Agilent 1100		
Thermostat					Aglient 1100		~
Valve			Data Inputs & O				
Fraction Collector					Device		Number
Capillary Electrophoresis			Ext. Start Dig. In	out:		$\sim$	$\sim$
Auxiliary			Ready Dig. Outp				
			Miscellaneous Se	ttings			
			Units	Setup	M	ethod Options	

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

Default FLD +DAD		New Duplicate C	reate ortcut
	General Configuration:	fid+dad.cfg	© »
	Open Instrument		Instantent
L	Desktop: Project:	<from .psw="" clarity.dsk="" or=""> <from desktop=""></from></from>	<ul><li>✓</li><li>✓</li></ul>

More Info:

- This step will create a duplicate configuration (.cfg file) based on the current Clarity setup (as described in step 2.). It prevents Clarity from overwriting a default configuration.
- Create a new profile (FLD) with a different configuration (fld.cfg), proceed with steps 4.-5. Once done, your profile should look similar to the image below.

Name Default FLD +DAD FLD	Descri	pened: Never, Last Edited: 03.08.2 ption: New Duplicate Rename Delete	Create Shortcut
ŀ	General Configuration:	fid.cfg Instrument 2 🔇 Instrument 3	> >>
	Login User Name: Desktop:	<from .psw="" clarity.dsk="" or=""> <from desktop=""></from></from>	~ <b>»</b>
	Project: Method: Sequence:	<from project=""> <from project=""></from></from>	×

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

Select Clarity Pr	ofile		-		×
Select a Clarity profile	, and double-click on	it, or click Launch to	o run Cla	rity.	
The profile may modif	y your current Clarity	configuration.			
Name	Des	cription			
Default		ault settings			
FLD +DAD		_			_
FLD 🕘					
Close this window	after launching Clarit	,			
Launch	Edit Profiles	Close		Help	

- Clarity has launched with the selected profile, open System Configuration. Since the configuration has been duplicated from the initial configuration, both detectors are present. Click on the Setup... button to invoke Agilent 1100 Setup dialog.
- 10. On the *Agilent 1100 Setup* dialog **click** on the *Common* tab (8) and then click the *Remove* button (b).

Agilent 1100 Setup	p ×	:
Communication protocol	GPIB O TCP     Auto Detect	
GPIB Board: Address:	gpb0 1 ~	
IP Address: Port:	192 . 168 . 254 . 11 9100	
	Add Remove (b)	
(g) Common FLD	DAD Quart. Pump AS	
,	OK Cancel Help	

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

Remove module	×
Module	(j)
	$\sim$
G1321 Aglent 1100 FLD, SN : 1	
G1315 Agilent 1100 DAD, SN : 2	
G1311 Agilent 1100 Quart. Pump, SN : 3	
G1313 Agilent 1100 AS, SN : 4	

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

# **18 Extensions**

Chapters describing topics related to specific Extensions.

# 18.1 GPC operations

Following chapters describe specific procedures concerning GPC.

## 18.1.1 Creating a GPC calibration

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

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

Calibration Type				
Narrow Calibration		~	Number of Signal	1
Calibration Descriptio	n:	Ť	Number of Signal	-
Use Flow Rate Cor	rrection		NormHt based or	Normal MW Distribution
🗹 Use Universal Calil	bration		Integral Percentages	Decreasing with M
Use Simplified Com	nputations of M Averages			
Signal	Flow Marker RT [min]	Curve Fit Type		
Signal 1	0,000	Linear		
Daariikaa Kaa Gaarii W	inden C		- Far1 - K F# (+=10.0	FT 14.1
Recalibration Search W			] [%] K [dL/g*10/	-
Recalibration Search Wi Peak Height	indow 5		[%] K [dL/g*10/ [%] Alpha	-5] [14,1 [0,7

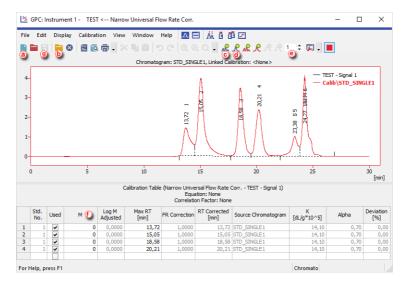
*Caution:* Once selected, the Calibration Type can't be changed later. More on GPC Calibration Options can be found in the *GPC Extension* manual, accessible on www.dataapex.com.

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

- 5. **Open integrated chromatogram of a standard:** select *File Open Standard...* or click on **b** in the *Calibration* window.
- Add peaks in the chromatogram of the calibration standard to the calibration file: select *Calibration Add All* or click on *R* ⓒ (if you have multiple peaks in your chromatogram) or select *Calibration Add Narrow Peak* or click on *R* ⓓ to add desired peak from your standard.
  - *Note:* If you have multiple chromatograms of standards, you can repeat these steps to add the desired peaks: open the standard and click *Add Narrow Peak*, then open another standard and click Add Narrow Peak, repeat for all standards. The number in field (e) is connected to the used standard and is not connected to the concentration level. Setting a peak on already used number will overwrite the values with a newly added one.

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

7. **Fill in the appropriate molecular weight** values for the respected peaks into the *M* column (f).

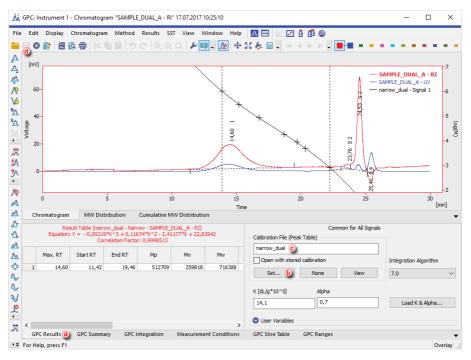


8. Save the calibration file from *File - Save* or click on  $\mathbf{F}(\mathbf{g})$ .

# 18.1.2 Applying a GPC calibration to a chromatogram

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

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



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

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

5. Save the chromatogram: select *File - Save* or click on  $\mathbf{F}$  **(**.)

## 18.1.3 Setting a GPC calibration in the template method

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

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

2. Open the template method by selecting the Open... icon (a).

Method Setup Universal	-		×
New Oper Save Save as Report setup Audit trail Send method by Help			
Common for all detectors			
Calibration File Universal View			
Set (b) New (c) Clone None			
Integration Algorithm 7.0 V			
Author dataapex			
Description Universal calibration with flow rate correction			
Created Modified			
03.05.2004 16:51:43 26.03.2018 1:11:42			
Event Table Measurement Integration Calculation Advanced GPC Integration GPC Calculation GPC Ranges			
		Send Me	thod

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

# **18.2 PDA Operation**

Pick the desired topic in the following chapters.

## 18.2.1 How to set Clarity instrument to display PDA data

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

Instrument Type Setting	:	×
Туре	Options	
⊖cc	MS	
●LC	ToF	
() CE		
⊖ GPC	DHA	
OEA	NGA	
⊖ cc-cc	✓ PDA	
		1
	OK Cancel Help	

# 18.2.2 How to open PDA chromatogram

- 1. In the Chromatogram window, click the Open Chromatogram icon 🧮
- Choose a chromatogram that has PDA data.
   More Info: Notice that chromatogram containing PDA data has the flag in the *Detail Info* section, just below the list of chromatograms.
- 3. After choosing chromatogram(s) click OK.
- 4. Next suggested topic is: "How to work with PDA chromatogram" on the next page.

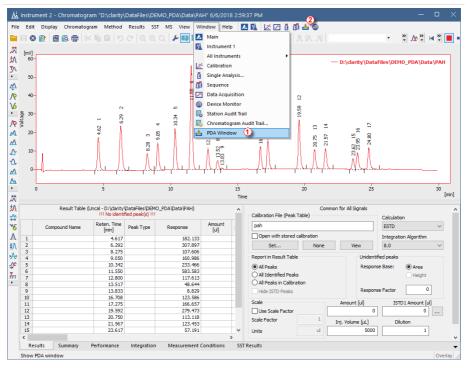
Open Chromatogram - D:\clarity\DataFiles\DEMO_PDA\Data X							×	
Look In:	Data		~	ተ 🛃 👩	문 🖩 V St	₩ C		
Name 🔻		Size	Туре		Created	Last Chan	ge	
Taxanes.pr		839 kB		Chromatog	6/30/2018 10:4		8 10:41 PM	
Quinones.p	rm	529 kB		Chromatog	6/30/2018 10:4		8 10:41 PM	
PAH.prm				Chromatog			8 10:41 PM	
Ai aromates.p	rm	902 kB	PRM	Chromatog	6/30/2018 10:4	6/30/2018	3 10:41 PM	
File Name	Taxanes.prm			Sig	gnals:		OK	
File Type	Chromatogram files (	(*.prm)		~	Signal 1 200-300		Cancel	
Method	6/6/2018 3:00:10 PM	1, IA: 8.0 Re	v.0	~			Overlay Mo	de
Analyst:	Administrator			Version:	Clarity			
SampleID:	Taxanes mixture			Range/Ra	te: <varies></varies>			
Sample:	Taxanes mixture			Time:	60,00 min			
Signature:	Not signed				ata: Yes			
GLP Mode	Off			GCxGC:	No			
			يى ا	h	Mh	h	\	ſ

## 18.2.3 How to work with PDA chromatogram

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

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

#### 18 Extensions

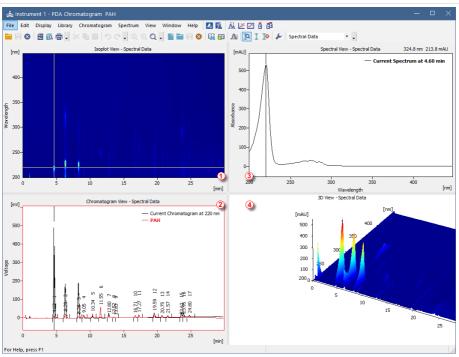


• After invoking, it will open *PDA Chromatogram* window which is covered below.

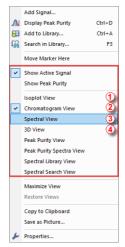
## How to display PDA data

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





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

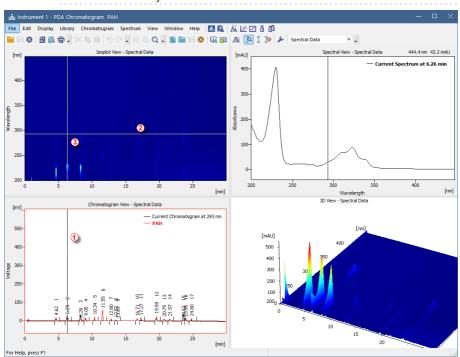


#### How to use markers in PDA Chromatogram

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

More Info:

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



- To change wavelength: drag the horizontal marker (2) to desired position.

Notice that the cross cursor changes to  $\frac{1}{2}$  once the move is possible.

• To change both, wavelength and time, move to the junction where the two

markers meet ③. Once the cross symbol changes to 👯, left mouse click + hold + drag to your desired position.

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

## 18.2.4 How to set PDA method

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

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

Method Setup Test_PDA	-		I	×
New Open Save Save as Report setup Audit trail Send method by Help				
Common for all detectors				
PDA Spectrum: FLD: PDA				
Peak Purity Options 3 Restrict Wavelength Range From: 190 To: 900 nm				
Absorbance Threshold: 5 %				
All O Five Use Background Correction				
Library Search Options 6				
Match Criteria: Correlation V				
Match Factor Threshold: 900 (0 1000) Max. Number of	Hits:		3	
Restrict Wavelength Range From: 190 To: 900 nm Use Background Co	rrectio	on		
Restrict Retention Time Relative: 1 %	aks	0		
Event Table Measurement Acquisition PDA Integration PDA Method Calculation Advanced			×	
R OK Cancel	:	S <u>e</u> nd	i Meth	bd

## 18.2.5 How to display peak purity

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

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

More Info:

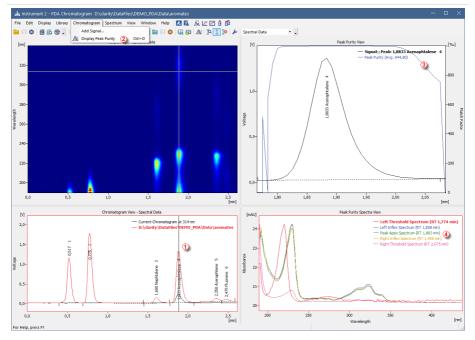
See "How to work with PDA chromatogram" on page 220

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

More Info:

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

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



## 18.2.6 How to work with PDA library

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

#### More Info:

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

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



#### Manage libraries:

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

#### Add compounds:

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

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

- 3. **Save library**: to keep any changes made in the library, click the *Save Library* ricon.
- 4. **Close library**: click the *Close Library* <sup>(2)</sup> icon. If you have unsaved changes you will be prompted to either save the changes or discard them.

#### View library:

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

More Info:

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

## 18.2.7 How to search in PDA library

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

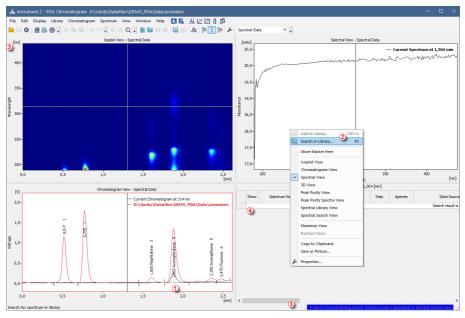
#### Most common ways to search in library:

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

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

#### Problems arising while using Search in Library

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



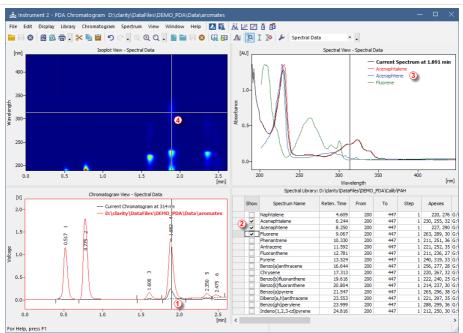
- After you **Search in Library** (2) for corresponding spectrum, you may notice that the blue ribbon (3) at the bottom of the window informs you that *O spectra found during the search*.
- Library Search View is also empty (4).
- Possible reason for such behavior can be that the *Library Search Options*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

Spectral Library Search	Options					×
Match Criteria	Least Square	~		Copy From	Current M	ethod
Match Factor	800	<b>(</b> 0 1000]				
Max Hits	3	]				
Restrict Wavelength R	lange	From:	200	To:	360	nm
Restrict Retention Tim	e (5)	Relative:	20 9	%		
Libraries:						<u>6</u>
Пран						
L	ОК	Cance	el 🛛		[	Help

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

## 18.2.8 How to view specific spectra in overlay

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



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

#### More Info:

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

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

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

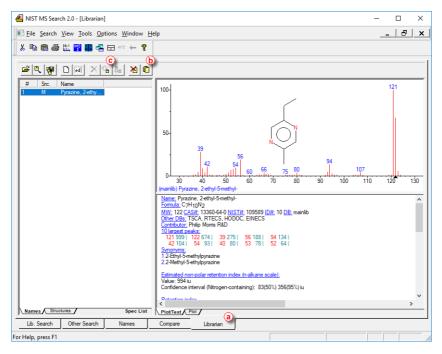
## **18.3 MS Operation**

Pick the desired topic in the following chapters.

## 18.3.1 Creating and filling your own MS library

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

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



To be able to add selected compounds (or spectra) to own library, such compounds must be selected in the Librarian tab. To do so, you can either

perform the Single Compound Search or use Add Spectrum to Library

#### Add Spectrum to Library

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

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

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

#### Single Compound Search

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

button add the spectrum into the library.

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

## 18.4 SST operations

Following chapters describe specific procedures concerning SST.

## **18.4.1 Using SST for quality control**

The optional SST Extension allows to set up limits for selected parameter. It compares measured values against those preset limits and perform actions based on the result. The SST works with calibrated chromatograms and the evaluation is based on the compound name in Chromatogram.

Here we provide an example on how to create SST method which can be used to check if the control samples are within expected limits and how to set up sequence to be checked by different SST methods.

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

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

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

More Info:

- When the SST Result is based on *Each Individual Value* than it compares each evaluated value with the Upper Limit or Lower Limit.
- When the SST Result is based on *Mean of All Values* than it compares average value of all opened chromatograms with linked calibration with the Limits. So pay attention to all opened chromatograms.
- You may hide the inactive rows and columns by using the SST Show All Columns and SST Show All Rows items in the menu
- The result of the check is displayed by the green tick mark or red cross. You can validate several different parameters at the same time this way.

• You will see similar result now:

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

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

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

More Info:

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

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

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

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