

#### COOPERATION WITH LIMS SYSTEMS

Clarity Software

ENG

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To facilitate the orientation in the **Cooperation with LIMS systems** manual and **Clarity** chromatography station, different fonts are used throughout the manual. Meanings of these fonts are:

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

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

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

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

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

Note:Notifies the reader of relevant information.Caution:Warns the user of possibly dangerous or very important information.

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

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

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

## 1 Clarity cooperation with LIMS systems

**Clarity** can be connected to any **LIMS** using the **import/export** of **text files**. The results can be exported in various formats to the **LIMS** and the sample info can be imported from a text file to **Clarity** sequence to be processed.

Most LIMS systems will be able to handle the import/export of the text data directly.

The tasks usually comprise from import of sample data information generated by **LIMS** to **Clarity** sequence table and exporting the results from **Clarity** in a format suitable for import to the **LIMS**.

## 2 Import data to Sequence

Common approach is to copy the range of selected cells from a spreadsheet and paste it to the sequence table as you are used to do so in Excel, but we recommend to use the import functions provided in **Clarity** which can automate the data import from **LIMS** to **Clarity**.

To create a sequence table from a text file, the suggested procedure will be using the *File - Import...* command in the *Sequence* window  $\bigcirc$ .

65	Instrument 1 - Sec	uence Demo1													- 🗆	×
File	Edit Sequence	View Window	Help 🚺													
	New	Ctrl+N	6 🖬 🛛 🛛 🖂	<b>₹</b> ₹.))	► I► 101	0		1	E 🛛 🕄	-						
	Open	Ctrl+O	Cample ID	Comple	Sample	ISTD1	Sample	Inj.Vol.	File	Sample	1.4	Method	Report	0000	Open	Drint
E.	Save	Ctrl+S	Sample to	Sample	Amount	Amount	Dilut.	[µL]	Name	Type	LVI	Name	Style	open	Calib.	FILL
EZ.	Save As	Ctrl+Shift+S	Halocar	Std_1	0,400	2,000	1,000	5,000	%Q	Stan	1	Demo1	Calibration			
			Halocar	Std_2	1,000	2,000	1,000	5,000	%Q	Stan	2	Demo1	Calibration	- H-	H	
	Send Sequence by E	-Mail	Halocar	Std_3	5,000	2,000	1,000	5,000	%0	Stan	4	Demo1	Calibration	- H-		
	Import	1	Halocar	Sample	5,000	2,000	1,000	5,000	%Q Vial	Unkn		Demo1	Analysis			
	Export	-														
æ	Report Setup	Ctrl+Alt+P	1													
6	Print Preview	Crt1+Shift+P														
	Driet To DDE															
8	Pline to PDF															
<b>1</b>	Send Printed PDF by	/ E-Mail														
	Print	Ctrl+P														
	1 Demo1															
	Close Window															
_			-				Single	Analysis:	Disabled - No	configur	ed de	etector Vial: 1	/ Inj.: 1		File N	lame:

Fig. 1: Importing Sequence

In **Step 1** you can select the file to import (will be remembered). The default directory for browsing the files can be changed, see <u>the chapter "Setting of custom</u> export and import directories".

De	limiter				<table and="" borders="" second="" second<="" th="" the=""><th>~</th><th>Decimal Delimiter</th><th>, <comma></comma></th><th>~</th></table>	~	Decimal Delimiter	, <comma></comma>	~
Pre	view:						First Row Is Header		
1	Run	SV	EV	I/V	Sample ID	Sample	Sample Amount	ISTD1 Amount	Sample
_	1	1	1	1	Halocarbons	Std_1	0,400	2,000	
2			2	1	Halocarbons	Std_2	1,000	2,000	
2	1	2	-						
234	1	3	3	1	Halocarbons	Std_3	5,000	2,000	

Fig. 2: First step of importing Sequence

In the **Step 2** you can map the text file columns to the *Sequence* table columns – in case the same column headers will be used, it will be set automatically for most of them, the settings can be remembered (check box *Save Import Settings*). The imported file must contain at least the *File Name*, other fields will be replaced by

defaults values (new sequence) or from preceding line (append to existing sequence).

Sequence Column	Imported Column	Create New
SV	SV	Annual Science
EV	EV	Append to Existing
IN	I/V	
Sample ID	Sample ID	Save Sequence and Delete Import File
Sample	Sample	<u> </u>
Comments	Sample	
Sample Amount	Sample Amount	Save Import Settings
ISTD1 Amount	ISTD1 Amount	
ISTD2 Amount	Sample Dilut.	Show Sequence Ontions
ISTD3 Amount	File Name	
ISTD4 Amount	Sample Type	
ISTD5 Amount		
ISTD6 Amount		
ISTD7 Amount		

Fig. 3: Second step of importing sequence

If you check *Show Sequence Options*, the respective window will be shown. Here you can adjust sequence options as needed.

Sequence Options					×
Description:					
1					
Sequence mode					
O Passive					
<ul> <li>Active</li> </ul>					
Idle time:	0	[min]			
🗌 Idle time	e also before first inje	ection			
Run lines:					
1-5					
Counter (%n)			Solve conflict o	of filename	
Start at:	0		Automatical	lly	
	<b>O</b> 1		<ul> <li>Manually</li> </ul>		
Reset when:	Run sequence				
	Open instrume	nt			
	○ Never				
Current value:	1				
Calibration and sequ	ence usage				
Calibration used a Clone on first rec Standard addition Calibration brack	as specified by user alibration (safe calibr n measurement eting	ation usage)			
After sequence is fin	ished				
Send shutdown n	nethod:				
Run shutdov	in method				0
Sample typ	e: Bypa	iss 🗸	Vial no.:	1	
			Ini. vol. [µl.]:	0	
Perform shutdow	n		,		

Fig. 4: Sequence Options dialog

Note also the TEMPLATE.SEQ in the COMMON folder (located in C:\CLARITY by default) – this file is used to create a new sequence and can be amended to contain the desired sequence options and repeatedly used calibration standard and control samples lines – just to add the unknowns.

To automate the operation you can use the command line parameter:

seq\_import\_append

- This parameter imports specified file and adds it to the opened sequence using the current settings for manual sequence import; functional from **Clarity** version **2.8.3**).
- Supported file type is \*.TXT.
- Syntax: seq\_import\_append=c:\tmp\seq.txt
- Possible values: valid path.
- Implicit value: none.

When using the *Single Run* dialog in **Clarity**, it is possible to use command line parameter, which preset the *Sample* name in the *Single Run* dialog. Remember to add the %Q variable to the *Chromatogram File Name*, then the measured chromatogram will contain the *Sample* in their names. The syntax is:

#### set\_sample\_name

- Sets sample name parameter for the next single run. It is possible to set the Instrument by the i=(number of Instrument) parameter.
- Syntax: set\_sample\_name=text
- Possible values: Any non-empty text.
- Implicit value: None.

## **3 Export Results Data**

There may be two approaches to transfer the results to **LIMS** – either your method is robust enough, that you can do so automatically after the run is finished or (more commonly) you will want to export the results after reviewing and amending them in **Clarity**.

First you have to set the format of exported data. To do so navigate to *Setting - Export Data* in *Instrument* window.

🕂 Instrume	ent 1						— c	
Instrument Me	thod Analysis	Evaluation		Window	Help 📐			
			😏 Exp	ort Data				
-//		-	🖌 Use	r Options		1.1.1	1.11	-1
=			Тос	lbars	•	M		
Method Setup	Single Analysis	Sequence	Devi	ce Monitor	Data Acquisiti	Chromatogram	Calib	ration
C Durali								
🔮 кеаду								
Setting export dat	a parameters			•				

Fig. 5: Export Data menu in the Instrument window

Please check the **Reference Guide** or **Help** for a detailed description of the available options – some experimenting to obtain the exported data in a convenient format may be necessary. Note that the entire summary table can be exported for all the opened chromatograms. In the *File Name* field enter the export path without the file name. The file name will be generated from the chromatogram file name and the appropriate suffix will be added. If you leave the File Name field blank, data will be exported to the same directory where the original chromatogram is located or to directory which was set in the *User Options - Directories* tab (for more details see the chapter **Setting of custom export and import directories** on pg. **12**).

*Note:* Setting of *Export Data* dialog is saved into used desktop .DSK file. When multiple user accounts are meant to export in the same format they either must use shared desktop file, or the setting must be done for each of them separately.

Export Content Result Table In Fixed Format All Signals Results Table Special Results Summary Table Column Moments	Chromatogram Chromatogram Call Data Displayed Data Call X Axis Jime Step: 0 min	Text Format Field Separator Field Separator Dejmited by: , <comma> Decimal Separator . <dot></dot></comma>
Calculation Parameters Chromatogram Chromatogram Chromatogram NGA Amounts NGA Summary DHA Results DHA Group Results Table Ljeaders Full Format	Character Encoding: ANSI	Text Qualifier  * <double quotes="">  Export to  Clipbgard  Text Ejle  .txt Excel Excel 97-2003 Workbook (*.xlsx) Excel 97-2003 Workbook (*.xlsx)  Excel statut table only)</double>
ile Name: C:\ExportedData\(name b C:\ExportedData\	y chromatogram).csv	Append (Text and dBase Files only)

Fig. 6: Export Data dialog

The export of data can be performed in various ways:

• Automatically after each single run according to the settings in *Post Run Setting* tab in the *Single Analysis* dialog accessible from the *Instrument* window:

ingle Analysis						×
Open in Chromatogram Window     Print Results	Report Style					
Print Results To PDF	Analysis				Edit	
Export Data Open in Calibration Window						
Open Chromatogram with stored C Include Chromatogram in SST	alibration					
Export Chromatogram in AIA Form	at					
Export Chromatogram in TXT Form	at					
Export Chromatogram in EZChrom	Ascii Format					
🗹 Export Chromatogram in Multidete	ctor Format					
Parameters						•••
Analyzic Post Run Sattings Licer Varia	hlec					
Post Run Settings Osci Van	0103					
Control						
Send method	Run	Stop	Abort	101	Snapshot	
Chromatogram File Name (Data\Instru	ment 1 - 31.05.2023 1	3 36 18)				
%e - %R		/				
Enable File Overwrite		Counter	1	Data	Recovery	
OK Cancel						

Fig. 7: PostRun Setting dialog

• Separately for each line in sequence (the respective columns are hidden by default):

đ	Instru	ument	1 - 5	iequ	ence	Ethanol	in blood																	-	- 🗆 🗙
Eil	e <u>E</u> di	t <u>S</u> eo	quenc	e )	/iew	Window	v <u>H</u> elp		玐	Å.	/ /	0													
		ß	6	ē		ວ 🤉 🖌	🗈 🖻	οE	e i	Ξ.	•• 1	• iii O	- 6 8		۶ 🖻	8= -									
	Status	s Run	SV	EV	I/V	Sample ID	Sample	Samp le	ISTD 1	Samp le	Inj.V ol.	File Name	Sample Type	Lvl	Method Name	Report Style	Open	Open Calib.	Print	Print to PDF	Export Data	Export AIA	Export TXT	Export EZChrom	Export Multidetector
1			1	1	1	blank		0,00	0,20	1,00	2,00	%q_%R	Blan		Ethanol i	Analysis	$\checkmark$								
2			2	2	1	std1	0.4	0,00	0,20	1,00	2,00	%q_%R	Stan	1	Ethanol i	Analysis	$\checkmark$								
3			3	3	1	std2	0.8	0,00	0,20	1,00	2,00	%q_%R	Stan	2	Ethanol i	Analysis	$\checkmark$								
4			4	4	1	std3	1.4	0,00	0,20	1,00	2,00	%q_%R	Stan	3	Ethanol i	Analysis	$\checkmark$								
5			5	5	1	std4	1.9	0,00	0,20	1,00	2,00	%q_%R	Stan	- 4	Ethanol i	Analysis	$\checkmark$								
6			6	6	1	std5	2.4	0,00	0,20	1,00	2,00	%q_%R	Stan	5	Ethanol i	Analysis	$\checkmark$								
7		$\checkmark$	6	6	1	std5	2.6	0,00	0,20	1,00	2,00	%q_%R	Stan	6	Ethanol i	Analysis	$\checkmark$								
8			7	7	1	0442		0,00	0,20	1,00	2,00	%q_%R	Unkn		Ethanol i	Analysis	$\checkmark$		$\checkmark$	$\checkmark$	$\checkmark$				
9			8	8	1	0445		0,00	0,20	1,00	2,00	%q_%R	Unkn		Ethanol i	Analysis	$\checkmark$		$\checkmark$	$\checkmark$	$\checkmark$				
10																									
For	help p	ress F1											Sin	gle Ar	alysis: Ready -	Ready to start	run Vial:	1/Inj.: 1	1		File	Name:			Ac

Fig. 8: Export option in column of the Sequence table

• Or using the *Batch* on selected chromatograms or entire sequence after they have been reviewed:



Fig. 9: Batch menu in the Instrument window

Select *File Type* and files to be exported from the list on the left. Select what action to perform from *Post Run Options* and click Proceed.

Fig. 10: Batch dialog

The *Run Program* option can be used to start some application such as MS Excel macro or simple .bat file using the exported file name as parameter (variable %e). This could be used to automatically invoke the import of exported data to the **LIMS**.

## 4 Perform export in the Chromatogram window

In such case you need to export data from chromatogram you are just evaluating in the *Chromatogram* window, you can use the menu command *File* - *Perform Postrun...* 

• • • • • • •

*Note:* If this action is used on regular basis it is convenient to add it directly on one of the toolbars. To do so right-click one of them and use *Customize*. In *Commands* tab find the *Perform Postrun* command from *File* category and drag it to desired place.

PostRun Setting (From Chromatogram Window)	×
Open in Calibration Window	
Print Results	
Print Results To PDF	
Export Data	
Export Chromatogram in AIA Format	
Export Chromatogram in TXT Format	
Export Chromatogram in EZChrom Ascii Format	
Export Chromatogram in Multidetector Format	
Program to Run	
Parameters	
Sign	
Perform OK Cancel Help	

Fig. 11: Exporting data in the Chromatogram window

Please check the **Reference Guide** or **Help** for a detailed description of the available options. By clicking on the Perform button, the data will be exported according to the settings in the dialog.

#### **5** Review measured chromatograms

To review a series of chromatograms, the *File - Browse Through Chromatograms* can come in handy. By default it browses the folder of the opened chromatogram. To be used *Overlay* must be disabled.

Å	instrument 1 - Chromatogram "Data\PER		- #11; 21.04	4.2023 8:04					- 0	
File	Edit Display Chromatogram Method	Res	ults SST V	iew Windo	w Help		220	🗗 🎯		
<b>∕</b> ∿	Overlay Mode Off	e		. 🗨 🎜	<u>₩</u> + 2	** -				-
	Open Chromatogram Ctrl+O									
	Browse Through Chromatograms	M	First	Ctrl+F7				— Data\P	ERS01	7
	Open Chromatograms From Sequence	•	Previous	F7						
⊗	Close Ctrl+W		Next	F8						
	Close All Ctrl+Shift+W		Last	Ctrl+F8						
	Save Ctrl+S		5,3	1						
E7	Save As Ctrl+Shift+S			8						
	Send Chromatogram by E-Mail			2,86						
	Import Chromatogram									
	Export		4							
	Sign Verify		5.8	<u> </u>						
缹	Report Setup Ctrl+Alt+P	-		2		4		-	e	
ťQ.	Print Preview Ctrl+Shift+P	<b>1</b>		Time		-			ໍ້ເ	[min]
75	Print To PDF	le (IS	TD - Data\PERS	501)						
-	Send Printed PDF by E-Mail	unt	Amount%	Peak Type	Com	ound Name		Calibration	File (Peak Ta	able
	Print Ctrl+P	9]	[%]	Реак Туре	Comp	Journu Marrie		Ethanol		
¢	Perform Postrun	0,000 0,000	0,0					Open v	with stored ca	alibr
	1 Data\PERS01	D,648 D,000	16,2 0,0	Ordnr (by IST	ETHANOL			Bonort in f	t	
	Close Window	ISTD	Performanc	ISID1	I-BUTANO	L	Conditions	SST Re	sults	_
•*	For help press F1.		. c. of marie	e integra	aon m	icasai emerie	conditions		Over	rlay

Fig. 12: Open Chromatogram Sequentially menu in the Chromatogram window

Which chromatograms should be browsed can be selected in open file dialog. You can use the wildcards (\*, ?) to filter out the desired files and open first of them using *Browse Selected Chromatograms*.

	ram = C:\Clanty\Datariles\DElv	101\Data			×
Look In: 📒 Da	ata	v 🕇 🛃 🛤			
Name 🔺		Size	Туре	Created	Last Change
Kample_Vial_	6-1.prm	953 kB	PRM Chromatography	26.05.2023 22:13	26.05.2023 22:13
Kample_Vial_	6-2.prm	962 kB	PRM Chromatography	26.05.2023 22:13	26.05.2023 22:13
Sample_Vial_7-1.prm		962 kB	PRM Chromatography	26.05.2023 22:13	26.05.2023 22:13
A Sample_Vial_	.7-2.prm	964 kB	PRM Chromatography	26.05.2023 22:13	26.05.2023 22:13
A Sample_Vial_	8-1.prm	961 kB	PRM Chromatography	26.05.2023 22:13	
Sample_Vial_	.8-2.prm	963 kB	PRM Chromatography	26.05.2023 22:13	
Sample_Vial_	9-1.prm	963 kB	PRM Chromatography	26.05.2023 22:13	
A Sample_Vial_	.9-2.prm	961 kB	PRM Chromatography	26.05.2023 22:13	26.05.2023 22:13
File Name	Sample_Vial_6-1.prm; Sample_	Vial_6-2.prm; Sample_	_Vial_7-1.prm; S Signals:	als	Open in Overlay
File Name File Type	Sample_Vial_6-1.prm; Sample_ Chromatogram files (*.prm)	Vial_6-2.prm; Sample_	_Vial_7-1.prm; S Signals: All sign Signal : Signal :		Open in Overlay     Open in Overlay     Replace Opened Chromatogram(s
File Name File Type Version	Sample_Vial_6-1.prm; Sample_ Chromatogram files (*.prm) Recent	Vial_6-2.prm; Sample_	Vial_7-1.prm; S Vial_7-1.prm; S V All sign V Signal : V Signal : V Signal :	als L   2	Open in Overlay Open in Overlay Replace Opened Chromatogram(s Browse Selected Chromatograms
File Name File Type Version Details for:	Sample_Vial_6-1.prm; Sample_ Chromatogram files (*.prm) Recent	Vial_6-2.prm; Sample_	Vial_7-1.prm; § Vial_7-1.prm; § Vall sign Signal : Signal : Signal :	als L 2 3	Open in Overlay V Open in Overlay Replace Opened Chromatogram(s Browse Selected Chromatograms
File Name File Type Version Details for: Created By:	Sample_Vial_6-1.prm; Sample_ Chromatogram files (*,prm) Recent <varies></varies>	Vial_6-2.prm; Sample_	_Vial_7-1.prm; S Signals: Signal : Signal : Signal : Created:	aks	Open in Overlay V Open in Overlay Replace Opened Chromatogram(s Browse Selected Chromatograms 3.2007
File Name File Type Version Details for: Created By: Modified By:	Sample_Vial_6-1.prm; Sample_ Chromatogram files (*.prm) Recent <varies></varies>	Vial_6-2.prm; Sample_	Vial_7-1.prm; 5 Signals: Signal Signal Signal Signal Created: Modified:	als	Open in Overlay V Open in Overlay Replace Opened Chromatogram(s Browse Selected Chromatograms 3.2007 5.2023
File Name File Type Version Details for: Created By: Modified By: Sample ID:	Sample_Vial_6-1.prm; Sample_ Chromatogram files (*.prm) Recent <varies> <varies> <varies></varies></varies></varies>	Vial_6-2.prm; Sample_	Via_7-1.prm; £ Signals: Signal Signal Signal Signal Signal Signal Signal Signal	als	Open in Overlay
File Name File Type Version Details for: Created By: Modified By: Sample ID: Sample:	Sample_Vial_6-1.prm; Sample_ Chromatogram files (*.prm) Recent <varies> <varies> <varies> <varies></varies></varies></varies></varies>	Vial_6-2.prm; Sample_	Vial_7-1.prm; s Signals: Signal	From to 23.00 From to 24.00 From to 26.00 Varies>	Open in Overlay V Open in Overlay Replace Opened Chromatogram(s Browse Selected Chromatograms 3.2007 5.2023 to 11,80 min
File Name File Type Version Details for: Created By: Modified By: Sample ID: Sample: Signature:	Sample_Vial_6-1.prm; Sample_ Chromatogram files (*.prm) Recent <varies> <varies> <varies> <varies> <varies></varies></varies></varies></varies></varies>	Vial_6-2.prm; Sample_	Vial_7-1.pm; £ Signals: Signal Signal Signal Signal Signal Created: Modified: Description: Time: Has PDA Data:	Prom to 23.00 From to 23.00 From to 26.02 <varies> From 0,00 min No</varies>	Open in Overlay V Open in Overlay Replace Opened Chromatogram( Browse Selected Chromatograms 3.2007 5.2023 to 11,80 min
File Name File Type Version Details for: Created By: Modified By: Sample ID: Sample: Signature: GLP Mode:	Sample_Vial_6-1.prm; Sample_ Chromatogram files (*.prm) Recent <varies> <varies> <varies> <varies> <varies> <varies> off</varies></varies></varies></varies></varies></varies>	Vial_6-2.prm; Sample_	Vial_7-1.prm; { Signals: Signal Signal Signal Signal Signal Created: Modified: Description: Time: Has PDA Data: Has MS Data:	From to 23.00 From to 23.00 From to 26.02 <varies> From 0,00 min No</varies>	Open in Overlay V Open in Overlay Replace Opened Chromatogram( Browse Selected Chromatograms 3.2007 5.2023 to 11,80 min

Fig. 13: Open chromatogram with filter

For this reason, it is strongly recommended to use the *%variables* to create filenames automatically and to include all the info which could be used for searching/sorting the files.

During the reviewing chromatograms, you can export data from them using the *Perform Postrun* dialog as described in in the chapter **"Perform export in the Chromatogram window"** on pg. **9**.

# 6 Setting of custom export and import directories

By default data are exported to directories where the original chromatograms are located. Also when importing files to Clarity, default directory for browsing the files will be located in the current project. If you need to set a default directory for those actions, for example on a network drive, you can set it in the *User Options*. In the *Instrument* window, click the *Setting - User Options*... menu command and select the *Directories* tab.

#### Note:

Same as *Export Data* dialog this setting is saved into used desktop .DSK file. When multiple user accounts are meant to export in the same directories they either must use shared desktop file, or the setting must be done for each of them separately.

User Opt	tions (Ac	Iministrator - Clarit	y)					?	×
General	Graph	Axes Appearance	Signals & Curves	Gradient & Auxiliary	Signals	Directories			
Print to	PDF Dire	ctory:							
					Defa	ult			
Export	Directory								
U:\Ex	, portFrom	Clarity\			Defa	ult			
Import	Directory								
					Defa	ult			
Hint: Le	ave dire	ctories empty for exp	oorting files to the s	ame directories as chr	omatog	grams.			
				ОК		Cancel	Apply	He	aln al
Hint: Le	eave dire	ctories empty for ex	porting files to the s	ame directories as chr	omatog	grams. Cancel	Apply	He	elp

Fig. 14: Setting of the export and import directories

Once you set for example the *Export Directory* item, all the data export will be performed to the one selected.

### 7 Synchronization with other programs

Clarity allows a cooperation with other programs using the **DDE** (Dynamic Data Exchange). DDE is a technique the Windows system uses for transferring data between individual applications running under Windows.

For more details about this topic see the **D070-DDE-Synchronisation.pdf** datasheet which can be found on the web www.dataapex.com.