DataApex
Clarity™
CHROMATOGRAPHY SOFTWARE

COOPERATION WITH LIMS SYSTEMS

Clarity Software ENG

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Contents

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 ① .

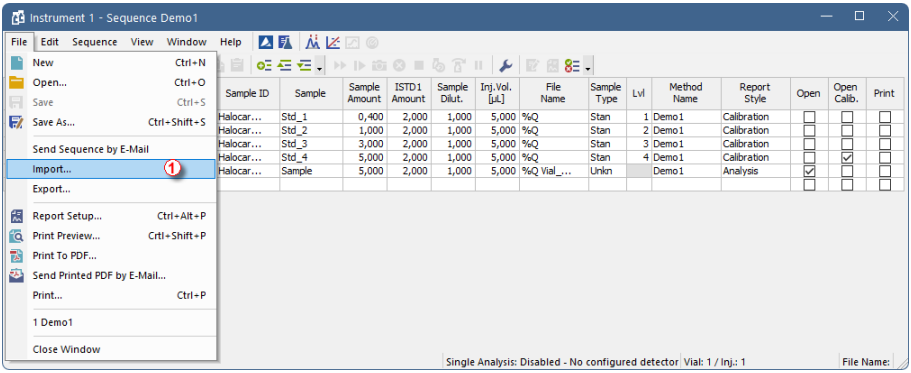

Fig. 1: Importing Sequence

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

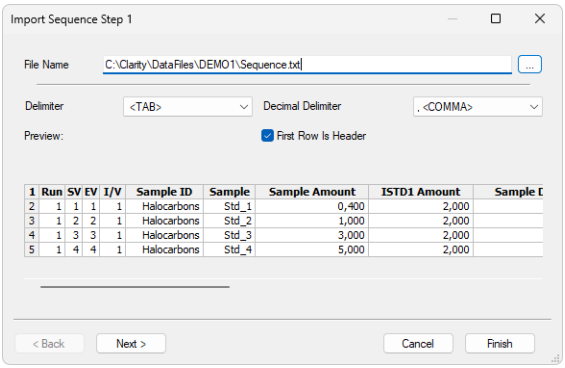

Fig. 2: First step of importing Sequence

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).

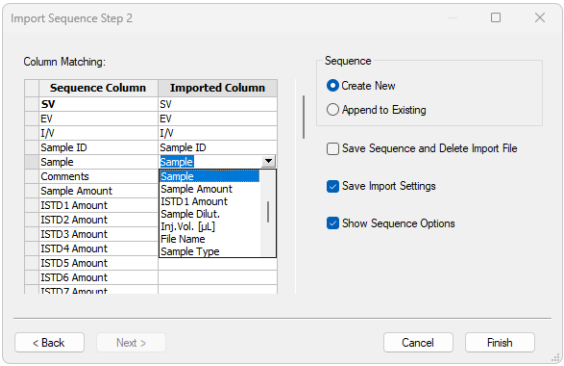

Fig. 3: Second step of importing sequence

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

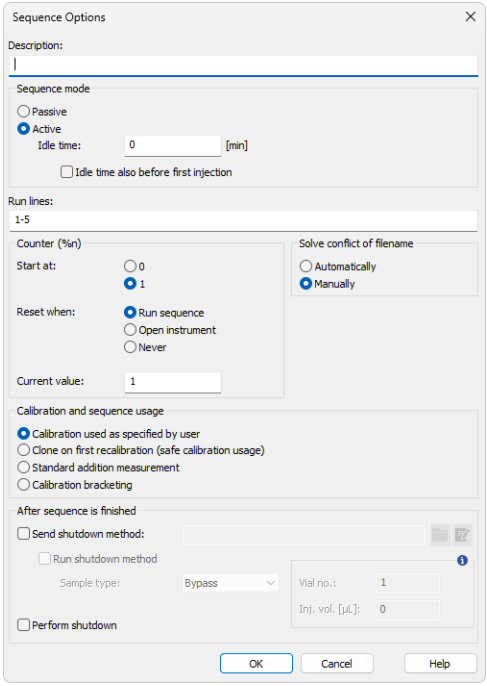

Fig. 4: Sequence Options dialog

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.

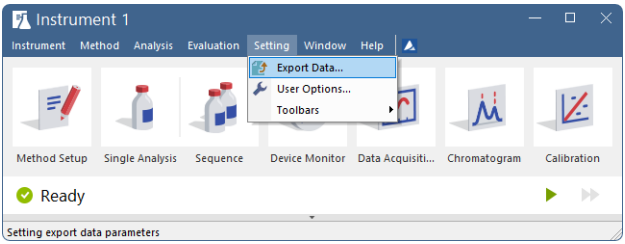

Fig. 5: Export Data menu in the Instrument window

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.

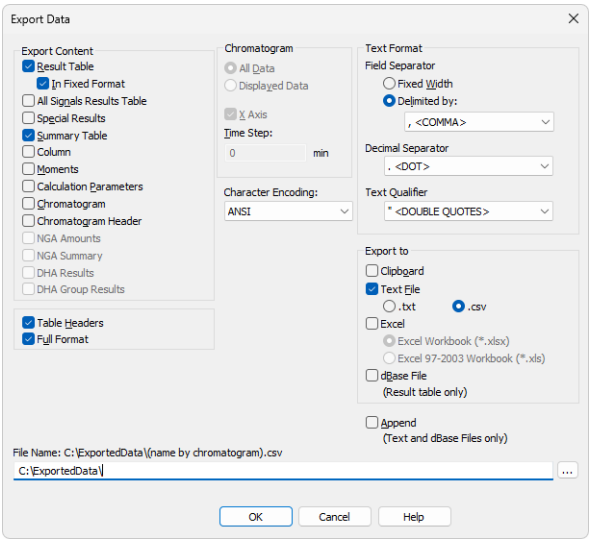

Fig. 6: Export Data dialog

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:

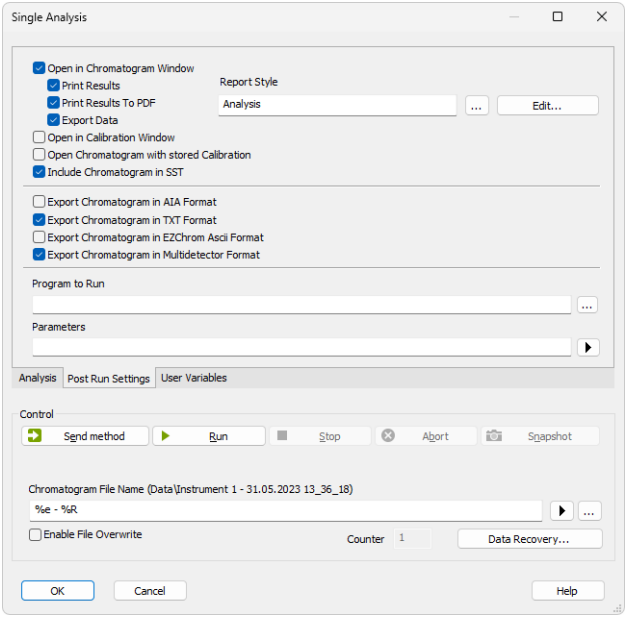

Fig. 7: PostRun Setting dialog

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

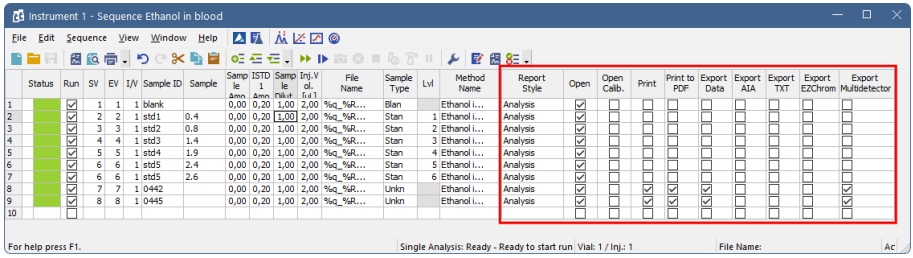

Fig. 8: Export option in column of the Sequence table

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

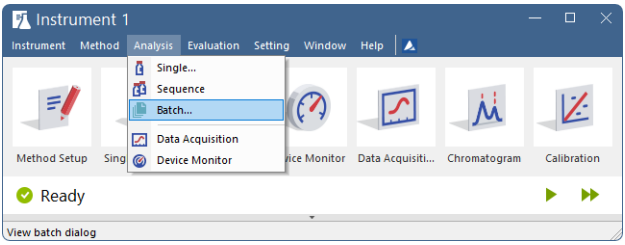

Fig. 9: Batch menu in the Instrument window

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.

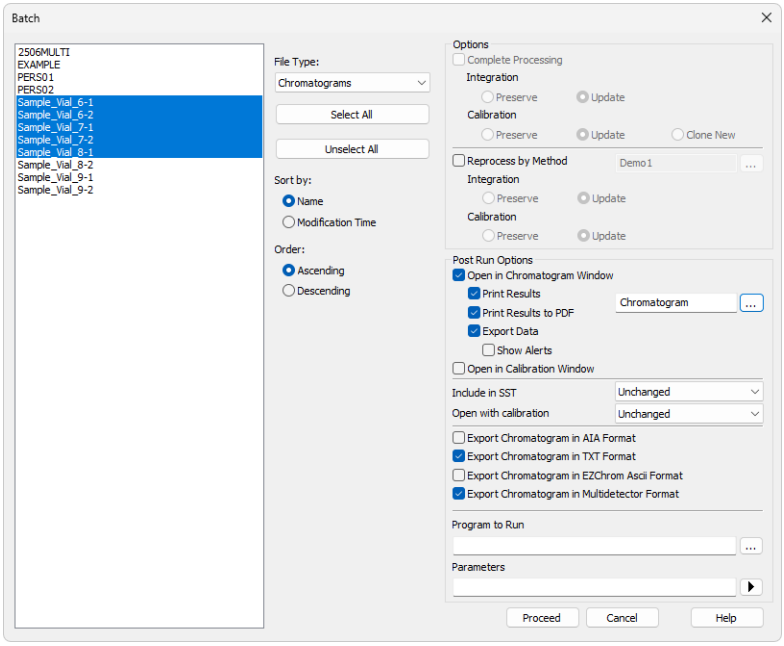

Fig. 10: Batch dialog

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.

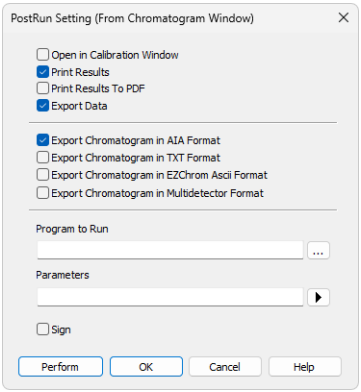

Fig. 11: Exporting data in the Chromatogram window

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.

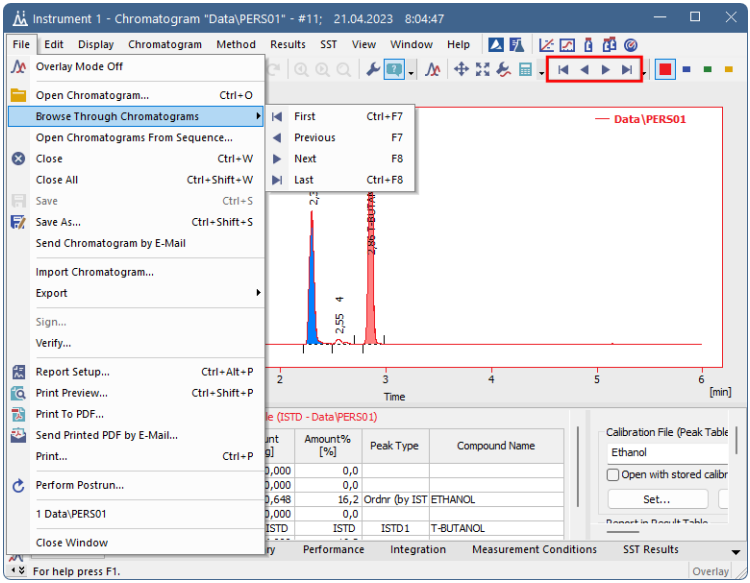

Fig. 12: Open Chromatogram Sequentially menu in the Chromatogram window

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*.

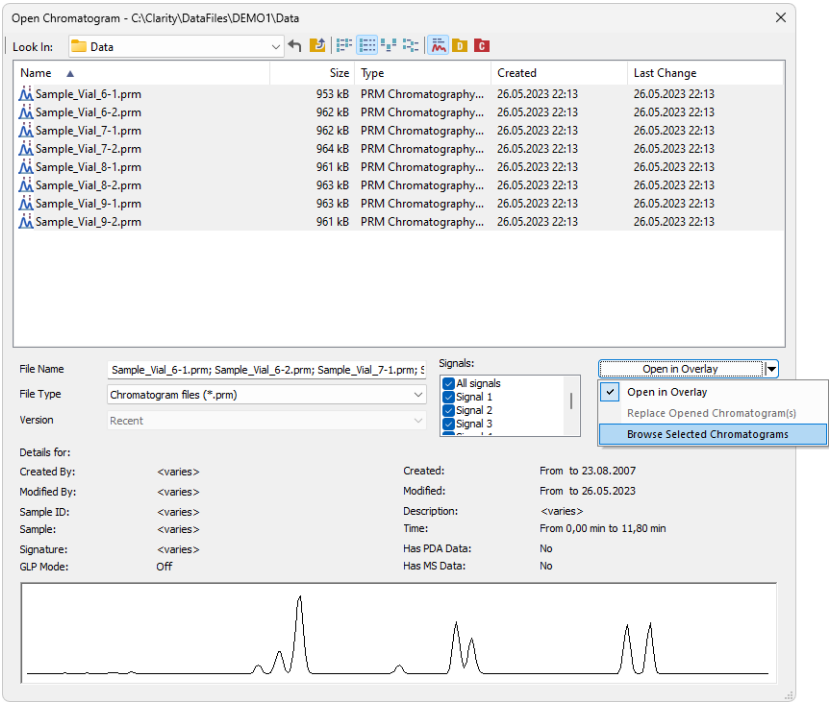

Fig. 13: Open chromatogram with filter

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.

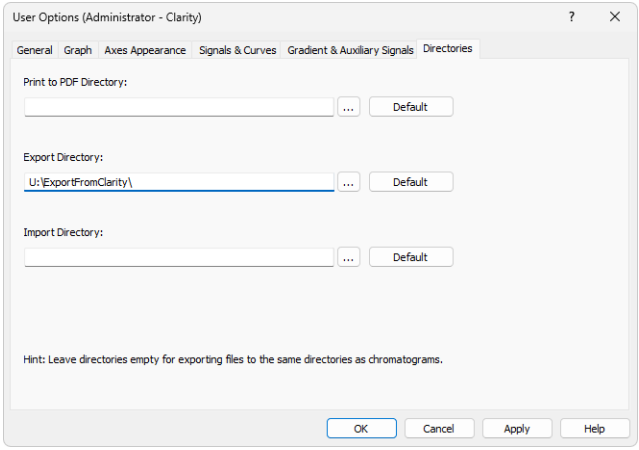

Fig. 14: Setting of the export and import directories

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.