DataApex
Clarity™
CHROMATOGRAPHY SOFTWARE

COOPERATION WITH LIMS

Clarity Software ENG

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Contents

To facilitate the orientation in the **Cooperation with LIMS** 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.

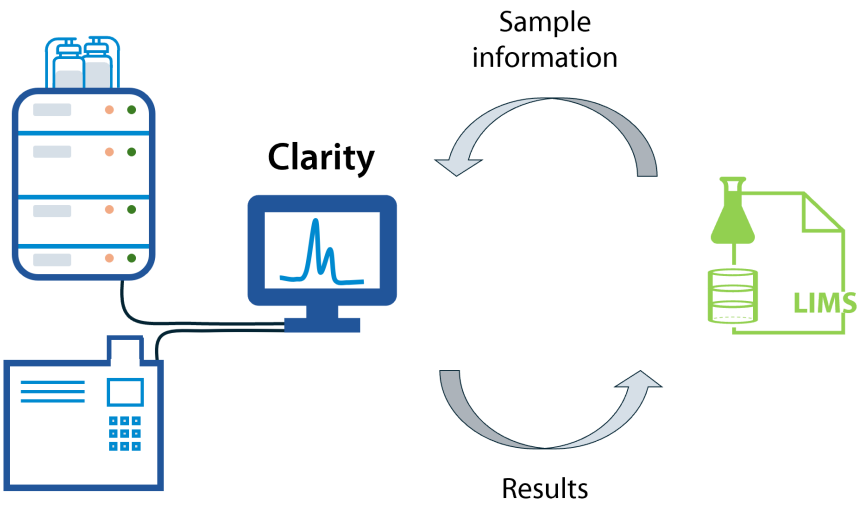
1 What is LIMS?

A Laboratory Information Management System (**LIMS**) is a software platform used for organizing, tracking, and storing laboratory data, including sample information, analytical results, and documentation. Clarity can cooperate with any **LIMS** by exchanging data through simple import and export functions. This allows laboratories to integrate chromatographic analysis into their broader data-management workflow without requiring any special connectors or extensions.

1.1 Cooperation between Clarity and LIMS

Clarity and **LIMS** exchange data in both directions:

- **From LIMS to Clarity**: The **LIMS** generates a text file containing sample information, such as *Sample Name* or *ID*. This file is imported into Clarity and the information is used for measurements.
- **From Clarity to LIMS**: After the analysis is completed and the results are reviewed, Clarity generates a file (most commonly .TXT) with the measured and calculated results. This file is exported from Clarity and then imported into the **LIMS** for further storage or processing.



2 Workflows in Clarity supporting cooperation with LIMS

Clarity provides several standard workflows that facilitate smooth data exchange with a **LIMS**. These workflows cover all steps from importing sample information, through reviewing measured data, to exporting results back to the **LIMS**. They can be combined or automated depending on the needs of the laboratory.

2.1 Setting up custom export and import directories

By default, Clarity exports data to the folder where the original chromatograms are stored, and imported files are browsed within the current project directory. If you routinely use specific locations, such as shared folders on a network drive, you can define custom default directories in *Settings - User Options…*, under the *Directories* tab accessible from the *Instrument* window.

Once a custom *Export Directory* is set, all exported files will be saved to that location, regardless of where the chromatograms are stored. Similarly, setting a custom *Import Directory* ensures that the import dialog opens in the predefined location.

Note: These settings are saved in the desktop file (.DSK). If multiple users need to work with the same directories, they must either share the same desktop file or configure their settings individually.

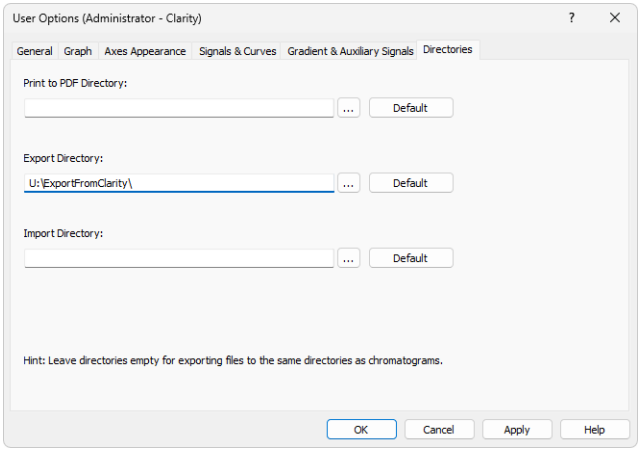


Fig. 1: Setting of the export and import directories

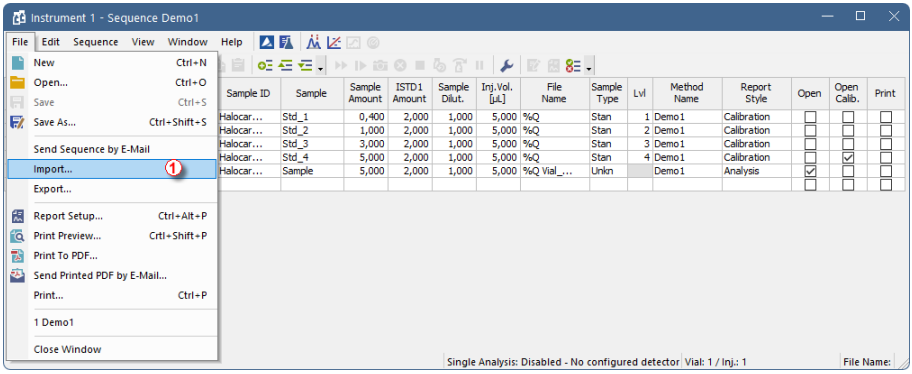
2.2 Import sample information to sequence

The recommended way to transfer sample information from a **LIMS** into Clarity is by importing a text-based file.

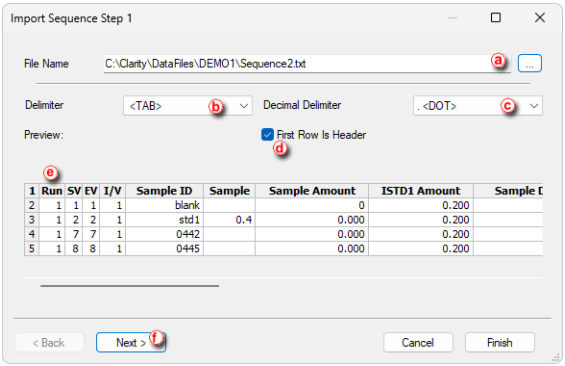
Clarity supports several file formats for this purpose, including *.txt, *.csv and *.prn. Values have to be in delimited format and separated by an arbitrary delimiter.

To create a sequence table from an imported file follow the steps below:

1. Open the *Sequence window* and select *File - Import…* ① . This opens the *Import Sequence Step 1* dialog, which opens in the directory defined in chapter "Setting up custom export and import directories".



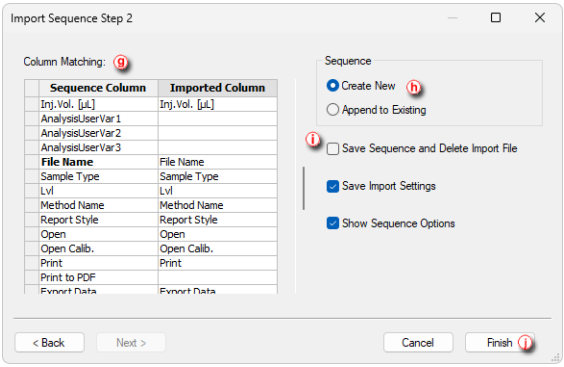
2. Select the file to be imported ⓐ .
3. Select the character used as delimiter ⓑ (possible options are *<TAB>*, *<SPACE>*, *<COMMA>* or *<SEMICOLON>*) and decimal delimiter ⓒ (possible options are *<Windows Locale>*, *<COMMA>*, *<DOT>* or *<SEMICOLON>*).
4. If the text file to be imported contains column headers in the first row, use *First Row Is Header* ⓓ checkbox. This row is used for matching in the *Import Sequence Step 2* dialog.
5. Preview of the first five rows of the imported sequence table is displayed in the bottom part of the dialog ⓔ .
6. Click *Next* to continue ⓕ .



7. Set the *Column Matching* ⓖ to match the imported columns with the ones present in Clarity *Sequence table*. *Start vial number* and *File Name* are required columns and are therefore shown in bold.

If the imported file contains column headers (the *First Row is Header* option was selected in Step 1), Clarity will try to match the columns automatically based on their names. Any manual changes will overwrite this automatic matching. Clarity will remember the final matching for future imports.

8. Select whether you want to save imported sequence as a new file or just append it to currently opened one ⓗ .
9. You can also use three additional checkboxes ⓘ to adjust the import behaviour:
   - *Save Sequence and Delete Import File* - invokes *Save as* dialog to save the imported sequence and deletes the imported file.
   - *Save Import Settings* - stores current settings so they will be used automatically for future imports.
   - *Show Sequence Options* – opens the Sequence Options dialog immediately after the import finishes, allowing you to adjust additional parameters before the sequence is created.
10. Press the *Finish* button to complete the import and close the dialog ⓙ .



Clarity also provides command-line parameters that can be used to automate the import process (full list of all available command-line parameters together with their detailed description can be found in ***Reference Guide***):

seq_import

Imports the specified *.TXT file as a sequence and replaces the currently opened sequence. The command is ignored when a sequence is already running. The imported sequence is loaded under the default name *Noname*, therefore the *seq_save_as* command must be used to save it before starting a run.

- Example: Clarity.exe i=1 seq_import="C:\CLARITY\DataFiles\<PROJECT>\seq.txt"

seq_save_as

Saves the active sequence under the specified name. The command is ignored when the sequence is running.

- Example: Clarity.exe i=1 seq_save_ as="C:\CLARITY\DataFiles\<PROJECT>\results.seq"

seq_import_append

Imports the specified file and appends its content to the currently open sequence. It uses the same settings as when the import is performed manually.

- Example: Clarity.exe i=1 seq_import_ append="C:\CLARITY\DataFiles\<PROJECT>\seq.txt"

2.2.1 Editing the template for new sequences

Clarity allows you to customize the template from which all new sequences are created. By modifying this template, every newly created sequence will automatically contain predefined parameters, calibration standards, control samples, or any other recurring lines needed for your workflow.

How to edit sequence template:

1. Select *File - Open…*from the *Sequence window* to display the *Open Sequence* dialog.
2. Navigate to the COMMON directory (located in C:\CLARITY\DATAFILES by default) and open the file TEMPLATE.SEQ. (Special templates are available for EA and GPC Extensions)
3. Edit the sequence as needed – including *Sequence Options*, default parameters, calibration standards, control samples, or other recurring rows.
4. Save the template.

Any new sequence created using *File - New* will now use the updated template and automatically include all predefined settings and lines.

The TEMPLATE.SEQ file in the COMMON directory is shared by the entire Clarity station, so any changes apply to all instruments using this directory. It is however possible to set custom locations of the Project directories for each *Instrument* with it own COMMON directory and therefore separate sequence template files. For more information, please refer to User Guide, chapter Setting up project directories.

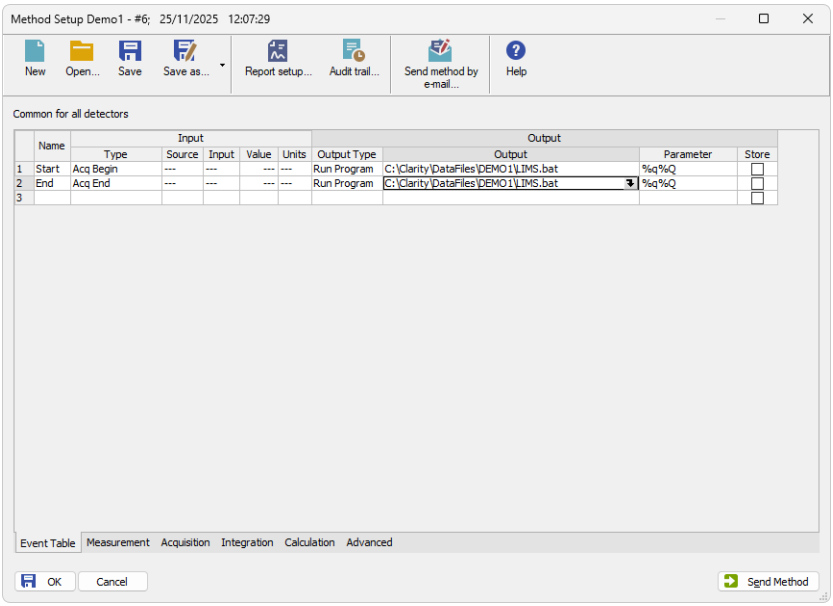
Caution: When importing a sequence file, the TEMPLATE.SEQ settings are ignored. The sequence is created strictly according to the import settings, regardless of any template configuration.

2.3 Communication with LIMS during measurement

During measurement, Clarity can also pass real-time information to a **LIMS**. These notifications allow the **LIMS** to track the progress of individual samples by receiving a message when a measurement starts or when it finishes. There are multiple ways to obtain such notifications.

Exporting through Event Table

The *Event Table* allows Clarity to trigger actions automatically at specific points during acquisition. The *Event Table* can set in *Method Setup* dialog with the following events:



- *Acq Begin*: triggered at the start of acquisition. Suitable for sending a message such as “Sample XYZ has started measuring.”
- *Acq End*: triggered at the end of acquisition .Suitable for sending a message such as “Sample XYZ has finished measuring.”

Both events use *Run Program* as the *Output Type*, because the notification is implemented by calling an external script. The *Output* field contains the path to the external script, and the *Parameter* field defines which Clarity variables (e.g., %Q for *Sample Name*) are passed to the script.

Export in Sequence table

In addition to the *Event Table*, Clarity can also send parameters to the **LIMS** using special columns available in the *Sequence Table*. This method links the notification directly to a specific sequence line and does not rely on acquisition events and effectively mirrors an *Acq End Event Table* action.

To enable this, three special columns must be displayed in the *Sequence Table* by using left-click *Setup Columns...*.

- *Run Program* - a checkbox that determines whether the action should be executed for this sequence line after the run finishes.
- *Program To Run* - defines the external program or script to execute.
- *Parameters* - contains the parameters passed to the program.

2.4 Reviewing measured chromatograms

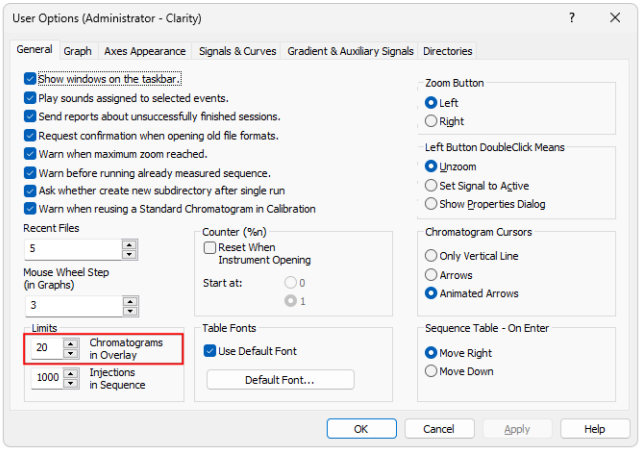
Clarity provides two complementary ways to compare results from several chromatograms:

- *Overlay mode*, which displays multiple chromatograms simultaneously in a single graph.
- *Browse Through Chromatograms*, which allows reviewing them one by one in sequence.

Both approaches can be used to evaluate differences between chromatograms, verify results, and prepare data for reporting or further processing.

2.4.1 Comparing chromatograms using Overlay mode

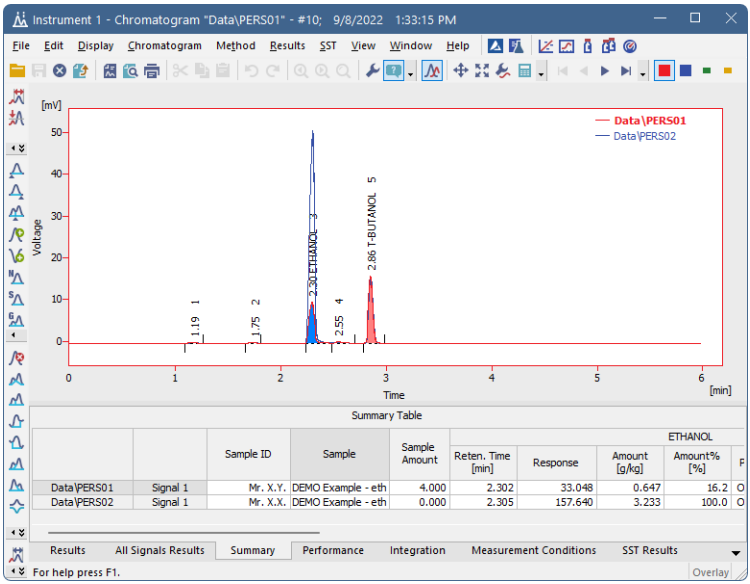
The default maximum number of chromatograms that can be open in Overlay mode is 20. If your workflow requires comparing a larger number of chromatograms (for example, when producing a summary report), this limit can be changed in the *User Options* dialog, accessible from the *Instrument* window by using *Setting - User Options...*.



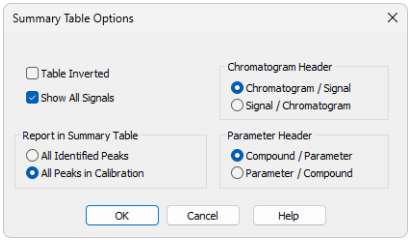
To view chromatograms in *Overlay mode*, follow these steps:

1. Open the chromatograms using *File - Open Chromatogram...*.
2. In *Open Chromatogram* dialog select desired chromatograms and click *Open in Overlay*.
3. 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.

Caution: *Summary Table* is based on calibration, meaning only calibrated peaks will be present in it.



4. Right click on the *Summary Table*to access options for adjusting its layout or content, including the *Inverted* view, which switches the table from a horizontal format to a vertical one for easier inspection of individual results.
5. To see all signals, select 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*.



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

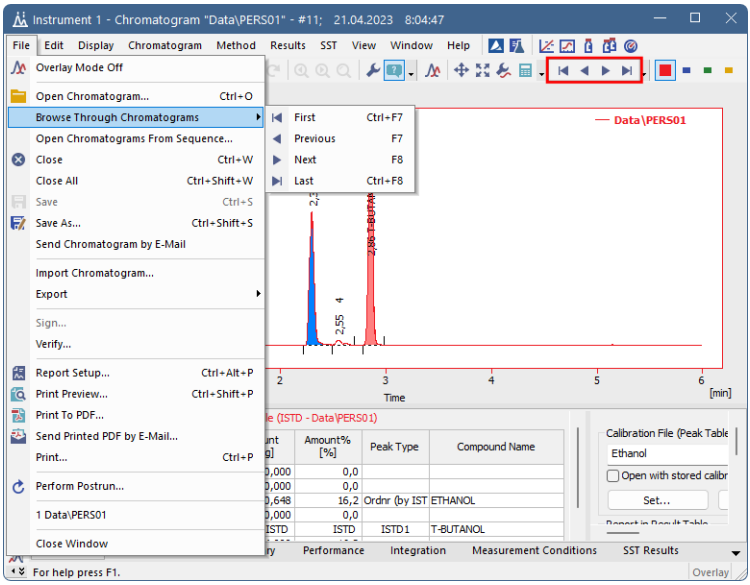
2.4.2 Comparing chromatograms by browsing them sequentially

In addition to *Overlay mode*, Clarity also allows reviewing multiple chromatograms one after another using the *Browse Through Chromatograms* function. This method is useful when you want to visually inspect each chromatogram individually, especially when working with large batches.

To use this feature, the *Overlay mode* must be disabled.

To browse chromatograms, follow these steps:

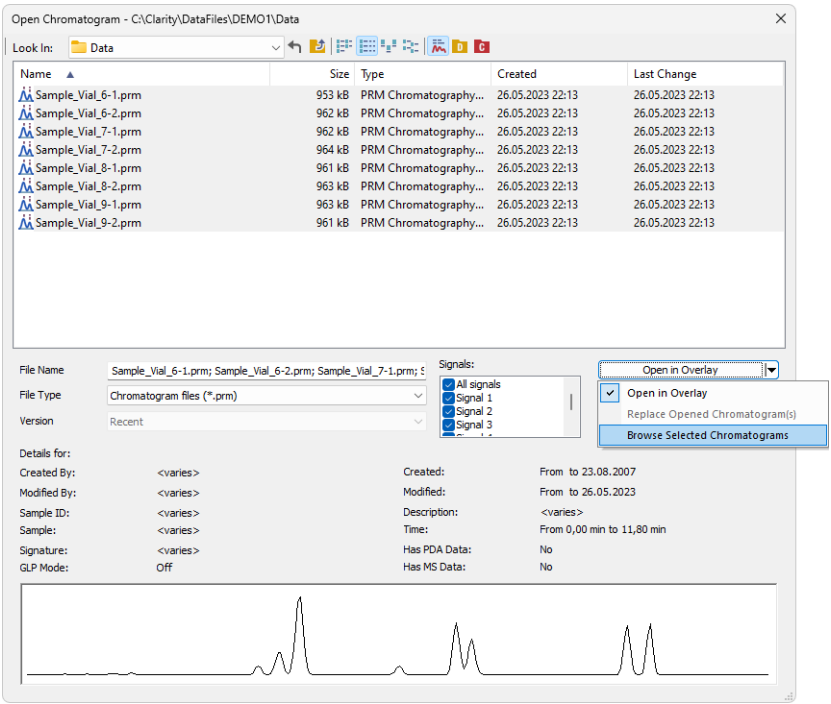
1. You can browse the chromatogram by using *File - Browse Through Chromatograms* or by using the navigation controls in the toolbar. By default, Clarity browses the folder of the currently open chromatogram.



2. In the *Open Chromatogram* dialog, select the chromatograms you want to review. You can also filter the list by typing simple wildcard patterns (*, ?).

   Caution: Using *%variables* when creating chromatogram file names is strongly recommended, as it ensures that useful information, such as sample name, injection number, or date, is included automatically. This makes it much easier to search, sort, or filter chromatograms when browsing through them.

3. When you have the desired files selected, you can open them by using *Browse Selected Chromatograms*.



When reviewing chromatograms—either one by one or in Overlay—you can export the currently displayed chromatograms using the *Perform Post-run Actions...* command, as described in Export of Results chapter.

2.5 Batch processing

Reprocessing whole sequence allows recalculation of results for all chromatograms in a sequence after changes to integration, calibration, or calculation parameters. This ensures that all results are consistent and reflect the current evaluation settings before further processing, reporting, or export to external systems such as **LIMS**.

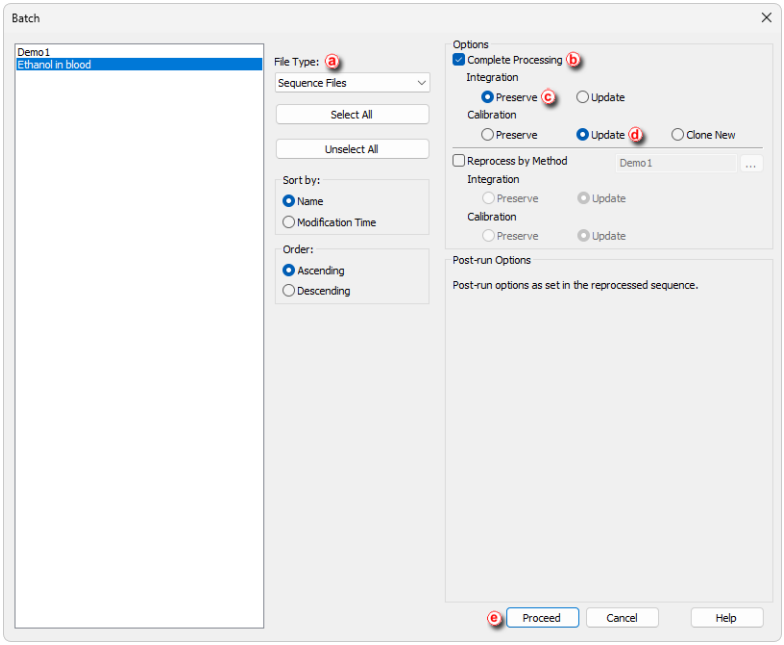
Reprocessing does not modify raw chromatographic data. Only calculated results and derived outputs are updated.

The steps below describe a process, where *Integration* is reviewed and if necessary, updated manually in each chromatogram, or sequence is already measured using a method with optimized integration parameters.

1. Open the *Batch* dialog by using *Analysis - Batch* in the *Instrument* window.
2. Set *File Type* to *Sequence Files* ⓐ .
3. Select the Sequence you want to reprocess.
4. Check the *Complete Processing* ⓑ checkbox.

5. Under *Complete Processing*, adjust the processing behavior as required:
   - Select *Preserve* ⓒ in the *Integration* to keep manually adjusted integration.
   - Select *Update* ⓓ in the *Calibration* to perform recalibration using updated integration.
6. Click *Proceed* ⓔ to start with the batch processing.

The sequence is processed row by row. All selected recalculations and post-run actions defined in the sequence are performed.



Caution: The operations during *Batch* reprocessing are done row after row, injection after injection. In some situations it is necessary to perform the *Complete Processing* in two steps - first just the recalibrations, second the post-run actions (either using the *Complete Processing* again with the *Integration* a *Calibration* settings set to *Preserve*, or through running the post-process on selected chromatograms only through procedure described in Performing Post-run Options from Batch section). For example, if the sequence is using calibration bracketing the unknowns are measured before second standards set and if the unknowns were reported during the recalibration step, the responses from the second standard set would be missing in the report.

2.6 Export of results

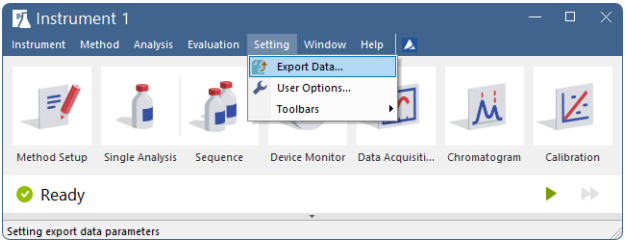
Before exporting data to a **LIMS**, it is recommended to review the chromatograms in Clarity to ensure that all results and calculated values are correct (see chapter

Reviewing measured chromatograms).
Once the results have been verified, Clarity offers several ways to perform the export, depending on the workflow and user preference.

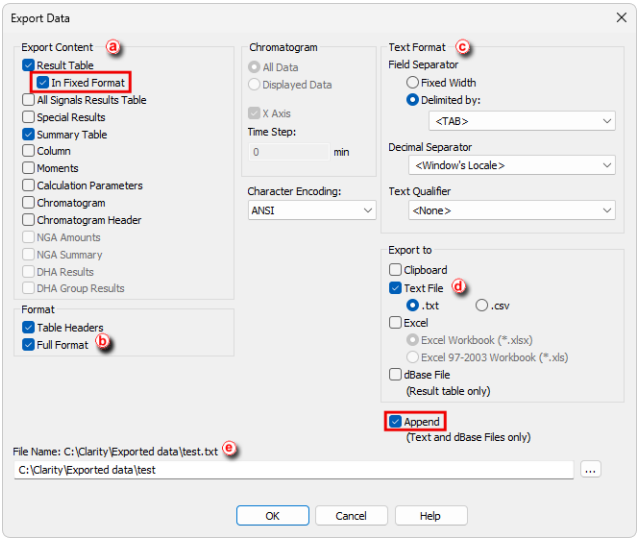
2.6.1 Setting up the Export Format

First, it is necessary to set the format of exported data. To do that, follow these steps:

1. Open *Export Data* dialog by using *Settings - Export Data* from the *Instrument* window.



2. In the *Export Content* section ⓐ , select which data you want to include in the exported files. It is recommended to export the *Result Table* with *In Fixed Format*. This will ensure that the data will be exported always in the same format regardless of the setting on the screen. However, *Fixed Format* can only be used if the predefined set of exported columns meets your needs—if you require custom or user-defined columns, leave this option unchecked.



3. Select *Full Format* ⓑ option. This will add the file name, date and time before each *Result Table* row to allow for easy sorting, which is particularly useful when

using the *Append* option.

4. Select the desired file formatting in *Text Format* ⓒ section.
5. Select *Export to - Text File* ⓓ and choose preferred suffix. In the *File Name* ⓔ field, specify the directory where the export files should be created. If the field is left empty, Clarity automatically uses the chromatogram name as the file name and saves the exported file either to the chromatogram directory or to the directory defined in the *User Options – Directories* tab (for more details, see chapter "Setting up custom export and import directories").
6. Check *Append* to export all results to a single file.

Note: The settings defined in the *Export Data* dialog are stored in the active desktop file (.DSK). If multiple users need to export data in the same format, they must either share the same desktop file or configure their settings individually..

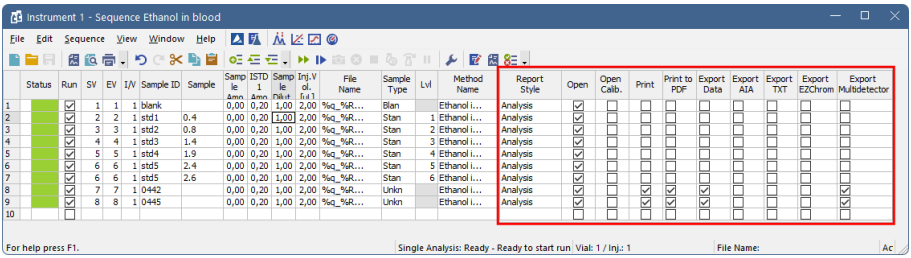
2.6.2 Ways to Export Results

Depending on the workflow and user preference, Clarity provides several ways to execute the export:

Export for individual lines in a sequence

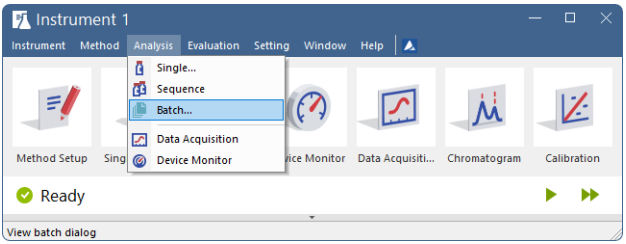
In the *Sequence* window, select checkbox in the *Export Data* column for row(s) to be exported. Note that the export is performed immediately after the run is finished, without any possibility of manual review of the results.

Columns defining export in the *Sequence table* are hidden by default; you can display them using the *Setup Columns...* command and use them to define the export format for each sequence line.

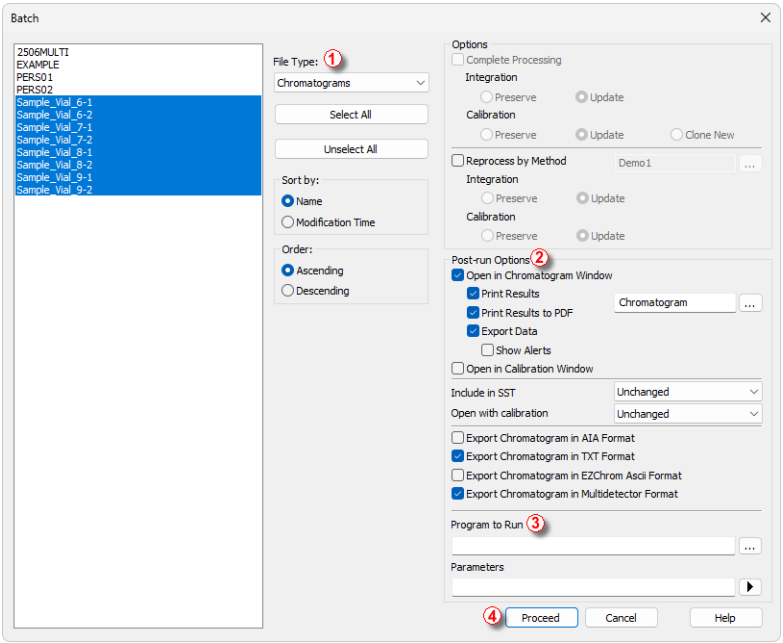


Export on demand for selected chromatograms

This can be done using the *Analysis - Batch* after the results have been reviewed.



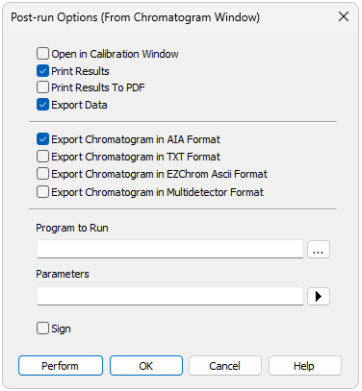
1. Select *File Type* ① and files to be exported from the list on the left.
2. Select what action to perform from *Post Run Options* ② .



3. The *Program to Run* ③ option can start an external application and pass the exported file name to it, allowing the **LIMS** to import the data automatically.
4. Click *Proceed* ④ .

Export directly from the Chromatogram window

This option lets you export data from the chromatogram you are currently reviewing by selecting *File - Perform Post-run Actions...*, which opens the *Post-run Options (From Chromatogram Window)* dialog and performs the export according to the defined settings.



If this action is used on a regular basis, it is convenient to add the command directly to the toolbar. A toolbar button executes the action immediately using the configured settings, without opening the dialog. If you need to modify these settings, you must access the command through the menu (*File - Perform Post-run Actions…*).

To add the command to a toolbar, right-click any toolbar and select *Customize...*. In the *Commands* tab, find the *Perform Post-run Actions...* command in the *File* category and drag it to the desired position.

The toolbar configuration is stored in the active .DSK file.

2.7 Synchronization with other programs

Clarity allows communication 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.

More details can be found in the D070 datasheet available on our website.