



OpenLab ChemStation

## Concepts and Workflows



# Notices

## Document Information

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Agilent Technologies  
Hewlett-Packard-Strasse 8  
76337 Waldbronn, Germany

## Software Revision

This guide is valid for revision LTS 01.11 Update 07 or higher of Agilent OpenLab ChemStation.

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## In This Guide...

Agilent OpenLab ChemStation provides great flexibility for research and method development laboratories by supporting advanced features and workflows of Agilent GC, LC and CE instruments with add-on software and advanced method development. This guide describes all the concepts of OpenLab ChemStation in detail.

This manual also explains the efficient use of the data acquisition, analysis, and reporting functions in ChemStation to boost your lab's productivity.

**Table 1** Terms and abbreviations used in this document

Term	Description
AIC	Agilent's Analytical Instrument Controller
ChemStation	OpenLab ChemStation
Control Panel	OpenLab Control Panel
Microsoft Control Panel	Part of the Microsoft Windows operating system
LTS	Long-term Support
Single Run	Individual analysis of a single sample that is triggered by running a method or queueing a method. Single runs may also be submitted as a series of method runs defined in the sequence table.

### 1 Basic Concepts of ChemStation

This chapter explains the principles of working with ChemStation, including remote control, the graphical interface and the ChemStation views.

### 2 Working with Methods

Methods are a vital part of how OpenLab ChemStation works. OpenLab ChemStation is a chromatography data system with great flexibility for method development. This chapter explains the concepts of methods in detail.

### **3 Data Acquisition**

OpenLab ChemStation offers seamless instrument control of Agilent LC, GC, CE, CE/MS, and LC/MS systems. It supports advanced features and workflows of Agilent GC and LC instruments with add-on software and provides flexibility for research and method development laboratories. This chapter contains an introduction to the process of acquiring analytical data.

### **4 Automation/Sequences**

This chapter describes the concepts of automation. It explains how to work with sequences in ChemStation, what happens when a sequence is run and how to customize sequences.

### **5 Run Control**

This chapter explains the concepts of Run Queue and Queue Planner. It explains how to add single samples, sequences, pauses, or commands to the Run Queue. It also describes the Command Scheduler in which you can schedule events to make your everyday lab work easier.

### **6 Data Analysis and Review Concepts**

You can analyze and review your data with ChemStation. This chapter outlines the ChemStation data analysis and data review options.

### **7 Calibration**

This chapter explains the concepts of calibration.

### **8 Reporting**

This chapter describes the concepts of Intelligent Reporting and Classic Reporting.

### **9 CE specific Concepts and Functions**

This chapter is relevant only if you use ChemStation to control CE instruments.

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This chapter explains the principles of working with ChemStation, including remote control, the graphical interface and the ChemStation views.



## Introduction

ChemStation provides full instrument control of Agilent's LC, GC, CE, CE-MS and LC-MS instrumentation. It offers tools for data acquisition, analysis and interpretation using a multi-technique, multi-vendor instrument control. Start the chromatography software from the OpenLab Control Panel, where you access all functions provided by OpenLab Shared Services.

## About the ChemStation Software

### Data Integrity

ChemStation files such as data, methods, or sequences are stored in various local folders. To ensure data integrity, ChemStation offers the *Secure File I/O* function. If you enable this function, all folders will be protected against modifications from outside ChemStation or in **Open** or **Save As** dialogs.

For more information, refer to the *Folder Protection with Secure File I/O* chapter in the *OpenLab ChemStation Configuration Guide* (CDS\_CS\_configure.pdf).

### Central Data Storage

A central data storage system can hold all kinds of electronic data independent of any proprietary data formats. ChemStation raw data (and other human-readable documents, such as workbooks) are stored together with *metadata*; this allows the data to be searched very easily. ChemStation methods, sequence templates, report templates, and data files (sequences and single runs) can be uploaded to the central repository, and later downloaded back into the ChemStation if required.

Agilent provides two systems for central data storage:

- *OpenLab Server* is available as a single-server solution providing centralized data management for small to medium laboratories with up to 30 instruments. It provides the necessary security in support of regulatory compliance. Please see OpenLab Server documentation for further information.
- *OpenLab ECM* is available as a single-server solution or a multi-server, distributed solution for comprehensive data management needs for laboratories with a few instruments to 100s of instruments. It also provides the necessary security in support of regulatory compliance. Please see OpenLab ECM documentation for further information.

For more information on the concepts of ChemStation with central data storage, refer to the *OpenLab ChemStation with Content Management Systems - Administrator's Guide*.

## Methods and Sequences

The analytical method fully describes how a particular separation is performed. It contains all parameters for instrument control, data acquisition and evaluation, including integration, quantification and reporting. The system may be set up to acquire data from a number of samples by different methods. The control file for this sort of operation is called a sequence. It holds the individual sample information, references to the appropriate methods, automatic recalibration specifications, and reporting instructions for a summary report across all runs in the sequence. For further information on methods and sequences, see [“Automation/Sequences”](#) on page 78 and the online help system.

## System Configuration

The configuration of the instrument system is done through the OpenLab Control Panel which starts the configuration editor program. It allows you to define your instruments, their LAN addresses, the directories for your data, sequences and methods and the initial screen size of the ChemStation software. In addition, you can activate or deactivate Intelligent Reporting and 3D Spectral Evaluation, and you can define the method download options.

## Acquisition Method Viewer

With the Acquisition Method Viewer, you can check the acquisition parameters stored in a method, independently of the current instrument configuration. You can choose to either apply this method in its original version to the instrument, or to resolve this method against the current instrument configuration.

## Method Download Options

The method download options define the behavior of ChemStation, if the last selected method from the previous instrument session differs from the current instrument settings. You can choose among the following options:

- **Download method to instrument**

The last selected method is downloaded to instrument. The instrument settings will be overwritten. This behavior corresponds to ChemStation revisions C.01.03 or lower.

- **Upload method from instrument**

The instrument settings are uploaded into the last selected method. The method will be marked as modified.

- **New method from instrument**

The instrument settings are uploaded into a newly created ChemStation method.

- **Always ask user to choose an option**

At ChemStation startup, a dialog is shown where you can choose on of the options described above. In this dialog, you can also compare the instrument settings for each module with the settings in the last selected method.

When comparing the differences, you can either display the entire list of settings, or display only the differences.

## Data Model

The ChemStation software is designed around a data model based on a memory structure called a register. Registers are multipurpose structures that can hold analytical data and information for both two-dimensional information (for example, time/intensity) and three-dimensional information (for example, time/intensity/wavelength).

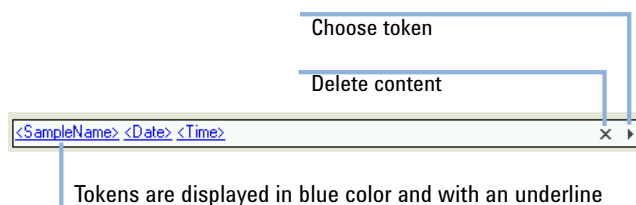
ChemStation provides commands and functions to construct, expand, extract and, where it does not alter primary data, edit registers. For further information, see the online reference in ChemStation under **Help >Commands**.

## File Naming Conventions

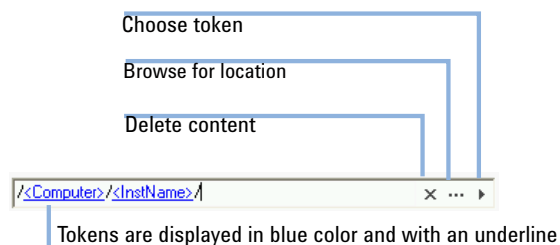
### File Names and Tokens

In most of the ChemStation dialogs where you enter a path name or file name, you can use tokens to dynamically generate suitable names. Depending on the file or path name that is set in a given dialog, different tokens are available. In the following screens, several tokens are used as examples.

The control for file names has the following appearance:



The control for path names has the following appearance:



In each corresponding dialog, the resulting file name or path name is displayed additionally.

You have the following options to work with this type of fields:

- Add static text.
- Click the Arrow button ( ► ) to choose a token from the list.  
Press the **Arrow Down** key to choose a token from the list.
- Right-click one of the tokens already used to replace it by another token from the list.
- Click the X button to delete the current content of the field.
- Click the button with the three dots ( ... ) to browse for the required path.

## Naming Conventions

Make sure you only use the following characters for ChemStation items such as file or directory names, names of sequence templates, or names of ChemStation methods:

---

A-Z, a-z, 0-9, \_ (underscore), - (hyphen)

---

Check your names for leading or trailing blanks. They are not allowed, but are easily overlooked.

### NOTE

If you use tokens, file names or directory names are automatically created based on information such as instrument names, operator names, or sample names. Make sure that these names follow the same naming convention.

### NOTE

Automatically created file names may include specific characters for Front and Back injector location. These characters may be localized. They are valid even if they are not part of the characters listed above.

The following reserved device names cannot be used as the name of a file. Also avoid these names followed by an extension (e.g. Nul.txt):

- CON, PRN, AUX, NUL
- COMx (where x is a number from 1 to 9)
- LPT1x (where x is a number from 1 to 9)

### NOTE

English, Japanese, and Chinese operating systems are used to test naming conventions. Agilent cannot give a support statement for non-English operating systems and their special characters.

## Maximum Length of ChemStation file names and subdirectories

The Agilent ChemStation specifications for file names and subdirectories are listed below:

**Table 2 Maximum length of ChemStation file names and subdirectories**

DataFile/Subdirectory/Path	Max. Input Length	Auto append	Example
Data file name of single sample	60	.D	Demodad.d
Data file name in a sequence, using prefix/counter	60	.D	longname000001.d
Data file name in a sequence, using a name pattern	60	.D	05-1-sampleA.d
Method	60	. M	def_lc.m
Sequence		. S	def_lc.s
Libraries		. UVL	demodad.uvl
Customized Report Templates		. FRP	areapct.frp
Data file subdirectory	40		demo (in sample information)
Data sequence subdirectory	40		demo (in sequence parameters)
Data Path	149		C:\Users\Public\Documents\ChemStation\1\data
Method Path			C:\Users\Public\Documents\ChemStation\1\methods
Sequence Path			C:\Users\Public\Documents\ChemStation\1\sequence
Libraries Path			C:\Users\Public\Documents\ChemStation\speclib
Customized Report Template Path			C:\Users\Public\Documents\ChemStation\repstyle

All ChemStation logbooks report system messages in an extended format and information strings are printed over multiple lines. Certain reports, e.g. Sequence report, may truncate filenames to fit all information onto the report template.

All paths are limited to 260 characters by the Windows operating system. Some of the characters are invisibly used by the operating system. Therefore you may need to use shorter names even all specifications listed above are met.

## Data Files

A data file comprises a group of files, by default stored in the DATA directory or in a subdirectory of this folder as a subdirectory with a data file name and a .D extension. A data file name can be defined manually using up to 42 characters (including the extension). Each file in the directory follows a naming convention (see “[File Naming Conventions](#)” on page 13). Additional data directories can be added using the **Preferences** settings.

**Table 3** Data files

Name	Description
*.CH	Chromatographic/electropherographic signal data files. The file name comprises the module or detector type, module number and signal or channel identification. For example, ADC1A.CH, where ADC is the module type, 1 is the module number and A is the signal identifier and .CH is the chromatographic extension.
*.UV	UV spectral data files. The file name comprises the detector type and device number (only with diode array and fluorescence detector).
*.ms	LCMS spectral data files
REPORT.TXT, REPORT.PDF	Report data files for the equivalent signal data files. Note: the PDF filename can be different if you use Unique PDF file naming.
Acq.MACAML	The file contains information on the method used during data acquisition. The information is stored in the ACAML format. ACAML files are used by Intelligent Reporting.
Sequence.ACAM_	The file contains the single injection results. The information is stored in the ACAML format. ACAML files are used by Intelligent Reporting.
SAMPLE.MAC or SAMPLE.XML	This file is used to store the sample values
SAMPLE.MAC.BAK or SAMPLE.XML.BAK	Backup of the original sample.mac. The .bac file is created during reprocessing, when the sample parameters (like multipliers) are updated the first time. It stores the original sample values used during acquisition.
RUN.LOG	Logbook entries which have been generated during a run. The logbook keeps a record of the analysis. All error messages and important status changes of ChemStation are entered in the logbook.
LCDIAG.REG	For LC only. Contains instrument curves (gradients, temperature, pressures, etc.), injection volume and the solvent descriptions.
ACQRES.REG	Contains column information. For GC it also contains the injection volume.



**Table 3      Data files**

Name	Description
GLPSAVE.REG	Part of the data file when Save GLP Data is specified.
M_INTEV.REG	Contains manual integration events.

## Software User Interface

The ChemStation user interface is designed into views that group software functionality according to typical analytical tasks. The following standard views are present in all software configurations:

- the Method and Run Control view for controlling and acquiring data from the instrument
- the Data Analysis view for reevaluating data that has been acquired
- the Review view for reviewing the data using specific report templates
- the Report Layout view for designing specific report layouts

Additional views are present if additional data evaluation modules have been ordered or for certain instrument configurations that support instrument diagnostics and verification procedures.

The Navigation Pane contains the Navigation Buttons, to allow rapid switching between the ChemStation views, and the tree-based ChemStation Explorer. The contents of the ChemStation Explorer are view-dependent, giving access to different ChemStation elements.

Each view consists of a set of standard user elements including menus and toolbars. The standard toolbar provides rapid access to the common system specification information such as methods and sequences. The **Method and Run Control** view additionally incorporates a system status bar, a sample information area, which may be configured for single runs or automated runs, and a schematic instrument interface diagram for GC, CE and LC configurations. The schematic instrument interface diagram uses hot spots to allow rapid access to instrument parameters and an animated graphical overview of the status of each analysis as it proceeds. The schematic instrument diagram may be turned off if it is not required, to save memory and other Windows resources. The **Run Queue** tab also integrated in this view displays all sequences, samples and commands that are scheduled for the instrument and also allows you to organize and process this workload (see [“Using the Run Queue”](#) on page 145).

The **Data Analysis** view extends the standard toolbar to specific data analysis modes including recalculation, reprocessing, integration, calibration, reporting, annotation, signal comparison and additional specialized modes if the modules are installed. Each of these separate data analysis modes are supported with a mode-specific toolset.

The **Review** view is available if Intelligent Reporting is selected for the instrument. This view allows you to review the data in a very flexible way. You can select any combination of data files as a basis for the review, and apply any existing report template to the selected data. The selected report template defines the way in which the data is shown and which type of information is included in the generated report. The toolbar provides functions for printing and exporting the generated reports.

The **Report Layout** view allows you to define the layout of a specific report template or report style. It also uses a set of toolbars specific to this task. The type of Report Template editor shown in this view depends on the type of reporting that is configured for the instrument. You can either use Classic Reporting or Intelligent Reporting (see ["Reporting"](#) on page 189).

## Navigation Pane

A Navigation Pane, available on the left side of all ChemStation views, is designed to speed access to many key ChemStation elements, as well as enabling quick switching between views. The Navigation Pane contains the tree-based ChemStation Explorer and a configurable button area. It also includes an autohide feature so that the ChemStation workspace is not compromised, and offers standard features such as resizing, and re-arranging of the navigation button area.

## Navigation Buttons

The Navigation Buttons allow the ChemStation view to be switched by clicking on the specific Navigation Button. The Navigation Button section can be minimized, expanded and re-arranged.

## ChemStation Explorer

The contents of the Navigation Pane are view-dependent. For Method and Run Control, Data Analysis, Review, and Report Layout, the ChemStation Explorer allows you to navigate to the different ChemStation elements. By default, these elements for data, methods and sequences are based on the configuration editor settings. New nodes for methods, sequences, data location can be specified using the "Preferences" option in the view menu.

**Table 4**      **Navigation Pane items**

Navigation Buttons	ChemStation Explorer Elements
Method and Run Control	Sequence templates / Master methods, Result Set methods
Data Analysis	Data / Master methods, Result Set methods
Review	Data / Report templates
Report Layout	Classic Reporting: Master methods Intelligent Reporting: Report Templates
Verification (LC and LC/MS)	Verification view-specific shortcuts
Diagnosis (LC/MS)	Diagnosis view-specific shortcuts
Tune (LC/MS)	Tune view-specific shortcuts

## Data Acquisition

The status of the instrument is continually monitored and updated on the display, along with the elapsed run time of the analysis both when the software is a visible window and when it is iconized. The transactions that occur during the analysis, including any errors and the instrument conditions at the start and the end of the analysis, are recorded in the system's logbook, an extract of which is stored with every data file.

The instrument conditions, such as flow, temperature, pressure and solvent composition for liquid chromatographs may be recorded and stored with each data file. These instrument parameters can be displayed and plotted to testify to the quality of each analysis. The exact nature of the parameters recorded depends both on the technique and the capabilities of the configured instrument.

All regular data acquisitions - single samples as well as sequence runs - are first added to the Run Queue and then started from there. For more information, see ["About the Run Queue"](#) on page 143.

One or more display windows may be used to monitor the data being acquired by the instrument in real time. The data are displayed in real measurement units such as mAU, Volts, degrees or bar. The windows may each show multiple overlaid chromatographic/electropherographic signals or instrument parameters, such as pressure. The display default settings may be adjusted and are remembered by the system so users can set their own preferred settings as the instrument default. The window has zoom capability and the cursor may be used to display a specific signal's response at any point in time.

During an analysis, the complete functionality of ChemStation can be used through the offline copy. While acquisition is running, the Data Analysis part of the online session of an instrument is not accessible, and data review has to be performed in the offline copy.

A snapshot function is available for users who wish to start processing data before the analysis is completed. The snapshot has to be taken in the offline copy of the instrument sessions and is immediately present for review.

The layout of the signal and status information windows, including the components of the schematic instrument interface diagram is saved automatically.

For further information on Data Acquisition, see [“Data Acquisition”](#) on page 69 and the online help system.

## Retention Time Locking

A retention time is the fundamental qualitative measurement of chromatography. Most peak identification is performed by comparing the retention time of the unknown peak to that of a standard. It is much easier to identify peaks and validate methods if there is no variation in the retention time of each analyte. However, shifts in retention time occur frequently. Routine maintenance procedures such as column trimming alter retention times. In a multi-instrument laboratory running duplicate methods, the retention times for each instrument can differ from each other, even when run under nominally identical conditions. These differences in retention times will require at a minimum a recalibration with update of the retention time and may mean that each instrument session must have a separate calibration and integration event table, making it time-consuming to transfer methods from one system to another. Differences in retention time can require additional work when comparing data between instruments over time.

Retention time locking (RTL) allows a close match of retention times on one GC system to another system with the same nominal column type (same stationary phase, column diameter, length, and phase ratio (film thickness)). Using the retention time/pressure calibration from the initial Retention Time Locking setup, RTL determines the new inlet pressure needed to update (relock) the GC's method inlet pressure when an analyte peak has shifted. This *locked* method can now be loaded on another GC to update the inlet pressure to match retention times.

## Data Analysis

### Data Analysis — Options

"Classic" Data Analysis is a feature in ChemStation. An overview is provided on the next pages. For more details, see ["Data Analysis"](#) on page 153.

### Data Analysis — Display

The ChemStation Data Analysis view extends the standard tool bar with task-grouped data analysis functions including recalculation, reprocessing, integration, calibration, reporting, annotation, and signal comparison toolsets. The following key graphical operations are possible:

- single or multisignal displays selectable when loading the chromatogram/electropherogram,
- overlays of chromatogram/electropherogram from different samples,
- subtraction of one chromatogram/electropherogram from another,
- graphical vertical and horizontal alignment of signals to help visual comparison,
- signal inversion or mirroring to help visual comparison,
- displays of extended peak performance characteristics for specific integrated peaks,
- graphical zoom and scrolling functions,
- adjustment of display attributes including selection of tick marks, baselines, axes, retention/migration times and compound names (you can also select the font for the retention time (RT) and compound labels, adjust the size and orientation of the display, select the display as overlaid or separated and select scaling factors),
- the chromatogram/electropherogram display may include graphical overlays of instrument parameters depending on the capability of the configured instrument,
- user-defined annotations may be interactively added to the display, with the selection of font, size, text rotation and color (once defined, the annotations may be graphically moved, edited or deleted),
- copy the display to the Windows clipboard in both metafile and bitmap format,

- a *pick mode* function to display the values of individual data points in detector units, and
- export of time/intensity digitized points to the Microsoft Windows clipboard.

### **Data Analysis – Integration**

The ChemStation integrator algorithm is the second revision of a new generation aimed at improved ruggedness, reliability and ease-of-use.

### **Data Analysis – Quantification**

The ChemStation's calibration mode of the data analysis view allows simultaneous display of:

- the signal or signals being calibrated with an indication of the current compound's retention/migration time window,
- the calibration table whose display may be configured from a comprehensive selection of calibration parameters, and
- the calibration curve for the compound being calibrated.

All the calibration mode windows are linked so that changes in one are automatically reflected in all the others. This mode allows graphical selection and modifications of the calibration data.

Quantification is based on %, Normalized %, External standard, External standard %, Internal standard and Internal standard % calculations calculated on either peak area or height. Calibrations may be multilevel and include multiple internal standard definitions. Calibration histories are automatically saved and can be used to weight the recalibration calculations.

For information on calibration and quantitation, see "[Calibration](#)" on page 174.

### **Data Analysis – Batch Review**

The Batch Review report can be used to review results for each compound for each sample. It offers the following key graphical operations:

- define automatic or manual review and reprocess of (calibrated) data files
- recalibration of calibration table
- review compound tables of calibrated methods
- create specific batch reports

The Navigation Table offers several key graphical operations:

- standard table configuration features, such as sorting, drag-and-drop options, column selection, item grouping to specify a preferred navigation table configuration
- right mouse click functions to load a signal, overlay a signal, export data, print reports
- review signal details by expanding a line in the navigation table
- review signals and create ChemStation reports using a specific method

Batch Review allows saving manual integration events per run. It is possible to save manual events with the data file outside of Batch Review. To avoid conflicts with two sets of manual integrations, any manual events that have been stored with the data file will not be applied in Batch Review.

There are a few points to watch out for:

- The recalibration methodology in Batch Review differs from the recalibration in the original sequence. Pressing the update calibration button on the batch review toolbar causes the system to recalibrate with all calibration runs in the batch, creating a recalibrated calibration table. Pressing the Start button on the Batch Review toolbar will then recalculate amounts for each calibrated compound. The amounts for all samples will be calculated from the recalibrated calibration table.
- Clicking a line on the Batch Review sample table causes the associated data file to be loaded. Some large data files may take a significant amount of time to load. This is no different than using Load Signals to load the same data file.
- The Batch Review report gives results for each compound for each sample. Because some calibration tables have large numbers of compounds this may lead to quite large Batch Review reports.
- Batch Review allows saving manual integration events per run. It is also possible to save manual events with the data file outside of Batch Review. To avoid conflicts with two sets of manual integrations, any manual events that have been stored with the data file will not be applied in Batch Review.

If you use ChemStation with central data storage, the Batch view is by default disabled. It can be enabled by an entry in the [PCS] section of the ChemStation.ini file: [PCS] \_BatchReview=1. The ChemStation.ini file is located in the C:\ProgramData\Agilent Technologies\ChemStation directory.

## Data Analysis – Recalculation

The functions in the recalculation mode allow you to quickly generate results or reports for any subset of data shown in the Navigation Table. You can easily generate results for self-assembled data sets, independent of the sequences the samples were originally acquired in. You can use any method for recalculation. The method used will be copied to the single data files (DA.M). No calibration is done during recalculation.

## Data Analysis – Reprocessing

The functions in the reprocessing mode allow you to reprocess one entire sequence, using the methods defined in the sequence table and using the results of the calibration samples to calculate the sample results.

## Data Analysis – Last Results

In this mode, the data file method (DA.M) for each run is loaded. DA.M is an exact copy of the method which was used for the last data analysis (during acquisition, reprocessing, or recalculation). The Last Result mode allows you to reproduce the results of the last data analysis, even if the sequence method has been changed in the interim.

## Reporting

With ChemStation, you can choose for each instrument the type of reporting you want to use:

- *Classic ChemStation Reporting* that is unchanged compared to ChemStation B reporting. For details, see [“Classic Reporting”](#) on page 203.
- *Intelligent Reporting*: With Intelligent Reporting, you can ...
  - create report templates with drag and drop (“What you see is what you get” model)
  - generate reports in the new **Review** view by just choosing the data and the report template
  - use interactive reports for data review: define the search criteria to select the information that is relevant for you
  - generate cross sequence reports

For more details, see [“Intelligent Reporting”](#) on page 196.



## Data Export and Import

### ANDI

ChemStation can import and export data files in the andi (Analytical Data Interchange) chromatography format of the Analytical Instrument Association (AIA), revision 1.0, copyright 1992. Data import is supported at compliance level one (sample information and signal data) and data export at compliance level two (sample information, signal data and integration results).

### DDE

ChemStation includes commands and functions to support the dynamic data exchange (DDE) standard of the Microsoft Windows platform as both a DDE client and a DDE server. The command set includes commands to establish and terminate connections, transfer information in both directions and execute remote functions.

### ADF

The **ADFExport for OpenLab** tool allows you to export ChemStation data into the Allotrope Data Format (ADF). The tool is only available if the corresponding Add-on is installed.

A detailed description of the **ADFExport for OpenLab** tool is available in the *ChemStation ADF Export* online help.

## Customization

ChemStation can be customized using a powerful command set. These commands may be grouped to execute automatically a specific function; such a group is called a macro.

Users writing macros may define their own variables, build in conditional or looping constructs, perform physical I/O including file handling and user interaction, nest their macros and schedule and exchange data with other Microsoft Windows applications.

## Using Custom Commands or Macros in ChemStation

In ChemStation, custom commands can be used at the following locations:

- Run Queue  
see ["Using the Run Queue"](#) on page 145
- Queue Planner  
see ["Using the Queue Planner"](#) on page 149
- Run Time Checklist  
see ["Run Time Checklist"](#) on page 49
- Sequence Parameters  
see ["Sequence Parameters"](#) on page 82
- Command Scheduler  
see ["Schedule Commands"](#) on page 150

From each location you can also access the dialog to create or change commands and macros.

### Create Custom Commands

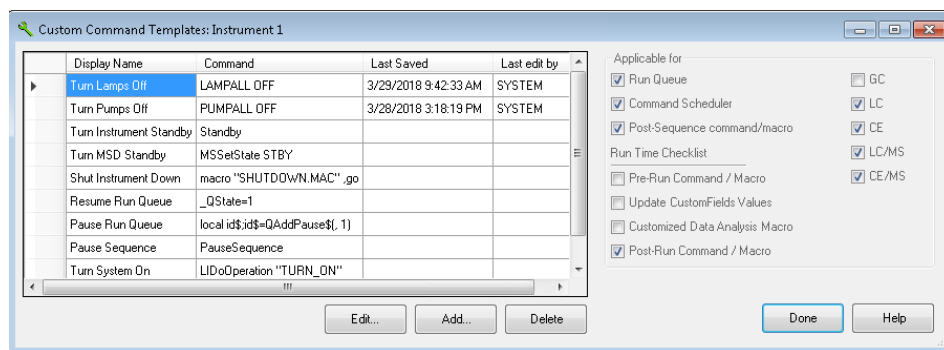
ChemStation offers several built-in commands that can be used by any user. If you have the required privilege, you can create your own custom commands and macros.

#### Prerequisites

You need the privilege **ChemStation:Security >Command Line**. Privileges are configured in the Control Panel.

- 1 From any location where commands can be used, select **Set up Custom Command Template ...**

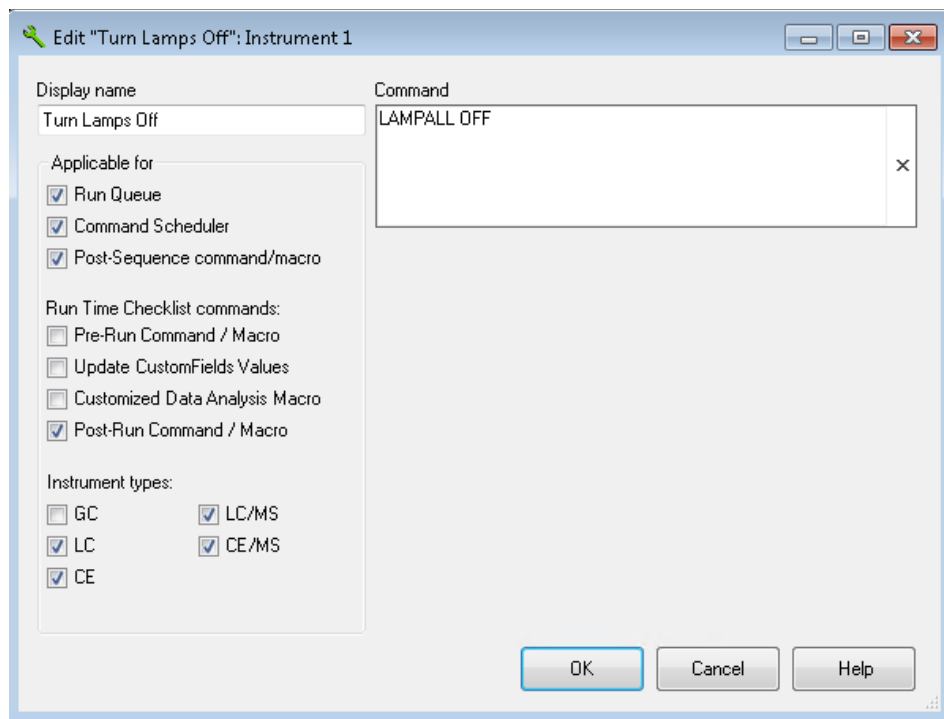
The **Custom Command Templates** dialog lists all built-in commands and custom commands that are available for the current instrument type.



- 2 Select the required command, then click **Edit....**

A dialog opens that allows you to set up the command properties.

- Display name that is shown in ChemStation to all users.
- Location where the command will be available (**Run Queue, Command Scheduler, Post-Sequence command/macro, Run Time Checklist** of the method).
- **Instrument types** for which the command applies.



3 Confirm your changes.

NOTE

Command definitions are saved separately with a method's run-time checklist, sequence template or a queue plan. That means, if you change or delete a definition, this is effective only within the scope of where you called the **Custom Command Templates** dialog. To apply the change to the dialog in another scope, you must explicitly update the relevant method checklist, sequence template or a queue plan.

For more information on customization, see the ChemStation online help on *commands* or *macros*.

## Automation

ChemStation can plan and execute both single samples and multi-method sequences.

The sequence parameter set may be defined to use automatically generated files or sequentially numbered files with a user-defined prefix of up to fifteen characters. The user may select to run full analyses or data reprocessing only sequences and can also select one of a series of technique specific shutdown commands (for examples about built-in commands, see [“Postsequence Operation”](#) on page 122) or a user-defined shutdown macro that runs when the sequence terminates either by error or after all the analyses are completed.

The sequence table, or list of analyses to run, is built in a spreadsheet-like user interface that allows users to specify vial numbers and sample names, sample types, analysis methods, sample quantification parameters including sample amount, a multiplier and dilution factor, calibration specification, data exchange parameter LIMSID and the number of repeat injections. Depending on the configured instruments and modules, more fields will be accessible, for example, if an Agilent 1100/1200 LC system includes a fraction collector, the **Fract. Start** column will appear in the sequence table. The appearance of the sequence table can be configured by the user. The user can jump between individual cells in the table and copy, cut or paste individual cells or entire rows or series of rows in order to build sequences efficiently and quickly.

Samples may be identified in the sequence table as unknown, calibration, blank, or control sample types. The sample type determines any special data evaluation treatment of the sample:

- Unknown samples are evaluated and reported according to the method specification.
- Calibration samples are used to recalibrate the quantification component of the method as described below.
- Blank samples are used to evaluate the reference signal for specific peaks, as defined by European Pharmacopeia. You can print the signal-to-noise ratio in customized reports. Please refer to the Reference Guide for details on the calculation and the required data fields.
- Control samples are evaluated against the limits for each component defined in the method. If the results lie outside any specified parameter range the execution of the sequence will be halted.

Calibration samples may be defined as simple, cyclic or bracketed. Simple recalibrations mean a recalibration occurs each time a calibration sample is defined in the sequence. Cyclic recalibrations occur at defined intervals during

analysis of a series of unknowns. In bracketing a series of unknown samples, two calibration sets are analyzed. The quantitative reports for the unknown samples are then calculated using a calibration table averaged between the two calibration sets.

The Sequence Preview functionality allows users to see the order of execution of the sequence. As soon as the sequence is queued, the sequence table also shows all samples run by run. The user can select individual sample entries to rerun or re-evaluate. When re-evaluating data that was already acquired, users can specify whether reprocessing uses the original sample quantification data or new data entered in the sequence's sample table.

Sequences may be paused to run single injection priority samples by another method, then restarted without disrupting the automation. Samples can be added to the sequence table while the sequence is executing.

Both the sequence and partial sequence tables may be printed.

For more information on sequences, see [“Automation/Sequences”](#) on page 78, and the online help system.

## Run Queue and Queue Planner

The Run Queue allows you to automatically run several single samples or sequences one after another. The first item added to the queue starts when the data system is ready, unless paused from the queue. You can add single samples, sequences based on Easy Sequence templates, classic ChemStation sequences, or pauses to the queue. Also each **Run Method** or **Run Sequence** command automatically adds an item to the Run Queue, and automatically starts this item in the queue.

Using the Queue Planner, you can prepare a series of single samples or sequences and save the plan to the file system. To start these planned samples and sequences, you simply open the plan and add it to the Run Queue. This function allows you to start lengthy tasks such as overnight or weekend jobs.

For more information, see [“About the Run Queue”](#) on page 143.

## Sample Locations

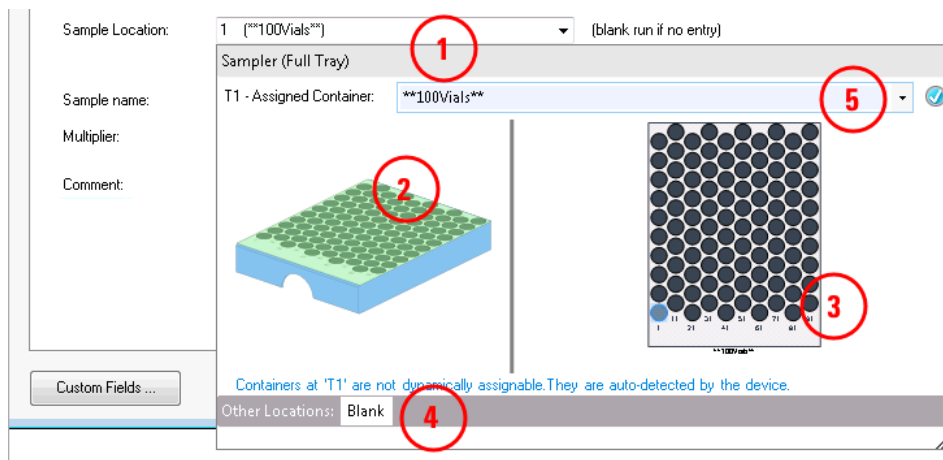
A graphical control allows you to pick the vial locations for your injections and for fraction collection.

Instead of typing the sample location manually, which requires a deep knowledge of the correct addressing format, you simply choose the drawer location, tray type, and vial location with a mouse click.

The graphical control to select sample locations is integrated in the following dialogs and toolbars:

- **Sample Info**
- **Sequence Table**
- **Filldown Options**
- **Fraction Collector (Start Position)**
- **Purify** taskbar in the **Data Analysis** view

The control contains the following elements:



**Figure 1** Sample location picker in the Sample Info dialog

- |   |  |
|---|--|
| 1 | Initial input field for the sample location. Click the arrow or press <b>F4</b> to open the graphical control, or enter the location string manually.                  |
| 2 | Graphic that visualizes the layout of the sample container device (injector or fraction collector). If several container locations are available, click to select one. |
| 3 | Visualization of the selected sample container. Click a sample location to select it and close the graphical control.  |

- 
- |   |   |
|---|---|
| 4 | Additional locations, as defined by the driver. For example, <b>Blank</b> for samplers, or <b>Next Location</b> , <b>Next Plate</b> , <b>Pooling</b> for fraction collectors. Click to select the location and close the graphical control. |
|---|---|
- 
- |   |   |
|---|---|
| 5 | <p>List of containers that are compatible to the selected device location.</p> <p><b>Use Current Configuration</b> selects the container as determined by the device/driver configuration at the time of injection.</p> <p>Use <b>&lt;empty&gt;</b>, for example, for fraction collector layouts to ensure that a container is not considered in the collection order during execution.</p> |
|---|---|
- 

There are primarily the following workflows:

- Use current configuration  
This is the default approach. When the sample or sequence is executed, the system automatically detects the device.
- Assign container to be applied on acquisition  
This workflow is for definable containers that cannot be detected by the system, for example, plates. You specify which container has to be used when the sequence or sample is executed.
- Assign container to be validated  
This workflow is for non-definable containers that are automatically detected by the device, for example, trays. When the sequence or sample is executed, the system validates the specified container. If the physical container does not match the specified one, the run will be aborted. This ensures that the correct container type is used.
- Prepare unassigned container  
This workflow is for containers that are filled in advance but are not yet inserted into the sampler. They are assigned to a drawer and position at a later point in time.

The graphical sample locations control is supported, for example, by the **Agilent LC RC.Net** drivers.



## Good Laboratory Practice

ChemStation is developed to internationally recognized design and development standards and has a number of features specifically to help users operating in a regulated environment. These features are in the area of complete method specification and verification that the methods are fit for their intended use, to check the operation of their system and ensure the traceability, originality and quality of the data.

### Development Process

The Certificate of Validation shipped with each software package documents the software development and testing steps executed as part of the development cycle. The development process is registered to the ISO 9001 quality standard.

### Method Specification and Use

- Global methods — the complete instrument and data analysis specification is stored in one place. Methods include individual compound range specifications to check that quantification results are not applied outside the calibrated range.
- The method change history log allows users of a validated method to automatically record how and when a method was changed. Users may optionally add a comment reason to the change history log. The change history log is automatically stored as part of the method in a binary format. To prevent unauthorized access to the records, it is protected by the user access scheme, described below. The change history log may be viewed and printed.
- Limits may be assigned on a compound-by-compound basis in each method for a number of chromatographic/electropherographic and system performance parameters, as described in the data analysis quantification section. Results exceeding these parameter ranges are used to control the execution of automated sequences as described in the automation section. They are indicated on the appropriate analysis report.
- System performance or suitability reports (see the Reporting section above) provide detailed analysis of the separation quality.

You can set up different roles and privileges in OpenLab Shared Services. The pre-configured roles **ChemStation Administrator**, **ChemStation Lab Manager**, **ChemStation Analyst**, and **ChemStation Operator** offer a basis for the roles in your environment.

## Method Robustness

Sequence summary reports (see “[Classic and Intelligent Reporting](#)” on page 195) provide a means to test methods for robustness. With classic reporting, the extended format reports for user selected criteria are reported as trend charts and may be used to determine the realistic operation limits. With intelligent reporting, you can create your own templates for sequence summary reports including trend charts with limit lines. These limits can then be incorporated in the method to ensure, through the analysis of control samples, that the method is operating within specifications.

## System Operation

The ChemStation verification kit, which is part of the standard software, automatically checks for the correct installation and operation of the data evaluation parts of the software by comparing results generated when the test is executed against prerecorded known values. The verification kit allows users to define their own data files and methods to be the basis of the test.

## Data Traceability, Originality and Quality

The run time logbook provides a transaction log of the complete system. It also records any unusual events (such as errors or parameter changes made during a run) as well as the instrument conditions before and after each analysis. A copy of the relevant logbook extract is saved with each data file.

The actual instrument conditions, such as pressure, flow, and temperature, that occurred during each analysis are also recorded if the configured instrument supports this capability. This data can be subsequently displayed graphically with the chromatogram/electropherogram to show the actual instrument conditions during that particular analysis, as well as being included on the report.

Methods saved with the data file record the actual method at the time of the analysis and allow the complete reconstruction of the reported data at a later date. The method is saved at the completion of all the analytical steps.

By default, all reports have time stamps and traceable page numbering (*page x of y* pagination style). The user may select the level of detail in each report ranging from simple summary reports to complete system details.

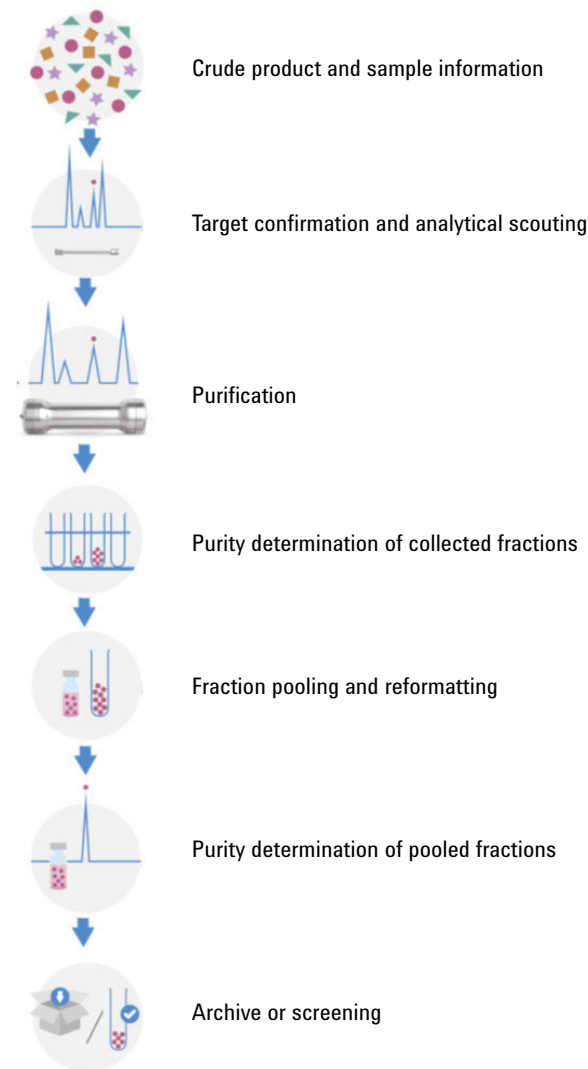
GLP Save register files, specified as part of the method configuration, save all the original data, including sample information, data analysis method, chromatographic/electropherographic signals, instrument conditions, integration and quantification results, report data and the run logbook in one checksum protected binary file. This is an uneditable binary format that ensures the

originality of the results. The file includes a revisioning scheme that indicates if data has been reprocessed.

Control sample types may be defined in the sequence table and used to automatically check the instrument performance against quality control sample results when the instrument is running unattended. Results that are outside the user-specified acceptable range will stop the automatic execution of the instrument.

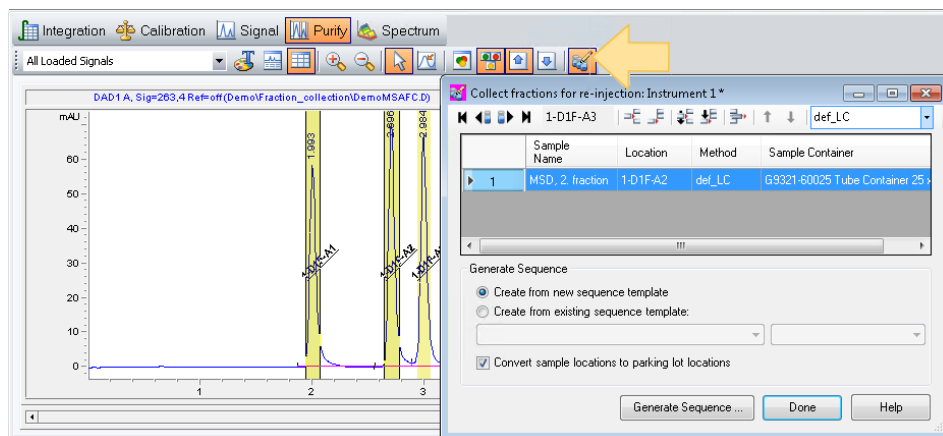
## Preparative Liquid Chromatography

ChemStation supports the automation of purification and preparation workflows. The typical workflow includes using a fraction collector with fraction pooling.



### Purity determination of collected fractions

In order to check the purity of your collected fractions, you can convert them into samples and add them to a sequence for re-injection. The list of fractions for the re-analysis is created in the **Collect fractions for re-injection** dialog accessible via the **Purify** toolbar in the Data Analysis.



In the dialog table, you set up the list of fractions for generating the sequence, and you can specify the method and the sample location.

Fraction list	Fractions can be added by selecting them from the chromatogram, the fractions table, or the sample container graphic.
Method	A drop-down list shows all methods stored on the computer. If your method is on another instrument that you will use for re-injection, you can type the method name in the field, or keep it blank for later.
Sequence	You can create a new sequence using the <b>Create from new sequence template</b> option. You can also append the fractions to an existing sequence using the <b>Create from existing sequence template</b> option.
Location	If you intend to transfer the sample container to a different instrument for re-injection of the fractions, select the <b>Convert sample locations to parking lot locations</b> check box. This converts the locations in the table to neutral parking lot locations that can be used on a different sampler.

Depending on the setup, the sequence can now be executed, or edited again in the **Sample List** of the **Sample Entry** tab. For more information, see [“Graphical Sample Entry”](#) on page 84.

## Fraction Pooling

Pooling is the collection of multiple fractions into the same collection vessel. ChemStation supports different pooling options:

- Inject several times from the same sample position, and collect into the same vessel(s)

In the **Sample Info** dialog, choose the required number of runs for the single sample, and select a fixed fraction start location for the first run.

- Inject from different sample positions, but collect into the same vessel(s)

To configure pooling, set the fraction collector start location for the first run and, if required, for the following runs.

## Fraction Collector Delay Calibration

The time a compound needs to travel between the point of detection in a detector and the point of collection in a fraction collector is called delay time. It can be determined by performing a delay time calibration.

The Delay Calibration Wizard guides you through this process of performing and evaluating a fraction collector delay calibration. The wizard is accessible in **Instrument** menu of the **Method and Run Control** view.

First, set up and run the delay calibration using **Perform Delay Calibration Run**. Then evaluate the results of the delay calibration using **Evaluate Delay Calibration Data**. The delay calibration is summarized in the **Delay Calibration Summary** report.

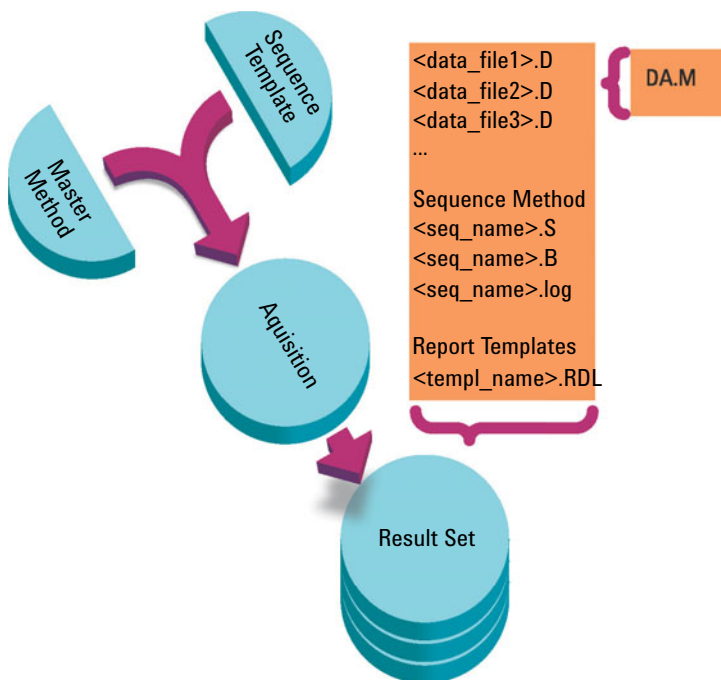
The data evaluation assists with working out the delay between the peak detector(s) and fraction collector module(s). Delay times are determined based on detector signals and the fraction collector's delay sensor signal of a calibration run data file. Delay volumes are calculated based on flow information.

For more information, refer to the ChemStation online help.

## ChemStation Data Structure

In order to strengthen the association between data files and methods, the usage of result sets has been introduced with ChemStation B.02.01 (result sets have been called sequence containers then):

- The data is stored with all necessary information needed for data analysis: copies of the sequence file, of all methods, and in case of Intelligent Reporting also of the report templates employed with the sequence. The sequence methods can be changed with sequence specific input and do not influence the original master method. The result set concept thus strengthens the meaning of a sequence as a set of data files and methods belonging together for result creation.
- Sequence data are not overwritten. Each sequence acquisition stores the resulting data files in its own result set with unique name.
- Data recalculation and reprocessing are both available in **Data Analysis** view via the Navigation Table.
- If you use a central data storage system (*OpenLab ECM 3.x*, *OpenLab ECM XT*, or *OpenLab Server*), the complete result set (sequence/methods/data files/report templates) is transferred to the central repository as one entity.



**Figure 2 Sequence Acquisition**

The methods in the folder ChemStation\x\methods<sup>1</sup> serve as master methods. They remain unchanged during acquisition and data analysis.

Similarly, the sequences in the public documents folder ChemStation\1\sequence serve as sequence templates that can be used to rerun (but not reprocess) a sequence several times.

Report Templates in the public documents folder ChemStation\REPSTYLE serve as a starting point for developing your own report templates.

<sup>1</sup> x is the instrument number. The folder is under public documents by default but can be configured during installation.



The data storage pattern varies depending on whether single run data or sequence data is acquired:

- 1 When a sequence is executed, a new folder is automatically created (**result set**) with a unique name in the specified subdirectory. When a single sample is run, the data file (\*.d) is written to the specified subdirectory.
- 2 For sequence data, the executed sequence template (\*.s) and all the methods (\*.m) involved are copied into the result set. The copies of the methods are called the **sequence methods** in order to distinguish them from the original master methods. If you use Intelligent Reporting, all involved report templates (\*.rdl) are copied into the result set as well.

All sequence-related tasks (for example, acquisition and data analysis) are performed on the copies of the sequence and the methods. Therefore, the sequence template and the master methods remain unchanged for future sequence execution.

Any changes performed on the sequence during sequence acquisition, for example, adding lines to the sequence table, are performed on the copy of the sequence file in the result set. The sequence template remains unchanged.

Similarly, any changes in the method, for example, updates in the calibration table in case of calibration runs, are reflected in the sequence methods, but not in the master methods.

While executing the sequence, all generated data files (\*.d) are stored in the sequence data folder, along with the corresponding batch file (\*.b) and sequence log file (\*.log).

- 3 Each data file contains a copy of the method used to create the run. The following method information is stored:
  - To view the original method parameters for each specific data file, right click the relevant line in the navigation table, then select **View ACQ Method**.
  - ChemStation offers to save a copy of the complete method (RUN.M) after each run (see [“Save Copy of Method with Data”](#) on page 68).
  - A copy of the data analysis parameters (DA.M) is always saved (see [“Save Copy of Method as DA.M with Data \(ChemStation Default\)”](#) on page 68).

## Remote Instrument Control

With a distributed system configuration, you can configure and launch your ChemStation instruments from any OpenLab Control Panel that is connected to the OpenLab Shared Services server.

### Launch Instruments

To configure or launch your instruments, you can use the *Configure Instrument*, *Launch online*, and *Launch offline* buttons in the OpenLab Control Panel. As in workstation or networked workstation configurations, the instrument configuration dialog runs on the local PC. However, with a distributed system configuration, the ChemStation application itself runs on an Analytical Instrument Controller (AIC) machine, and you access the application via a Remote Desktop connection to the AIC machine.

The remote ChemStation windows are shown independently of the OpenLab Control Panel; you can launch an instrument, close the Control Panel, and continue working with the instrument. Also you can run multiple instances of OpenLab Control Panel on the same client using different logon credentials. The different credentials will be propagated to the instruments you launch from the corresponding OpenLab Control Panel.

You can identify the instruments running on a remote AIC machine by the window title, which contains both the instrument name and the AIC name.

### Session Disconnect

Instruments running on an AIC are independent of the client from which you opened the Remote Desktop connection. If the client disconnects, for example, due to network failure, a sequence running on the instrument continues unaffected. To regain control over the instrument session once the network has recovered, simply click the *Launch online* or *Launch offline* button again.

To disconnect intentionally, click on the **Close** button or select **File >Exit**. The **Close** dialog offers an additional **Disconnect** button. By disconnecting, you cut off the Remote Desktop connection while leaving the instrument running.

#### NOTE

You can disconnect the Remote Desktop connection while a sequence is running.

To reconnect to this instrument session, simply click the *Launch online* or *Launch offline* button again in the OpenLab Control Panel. You can reconnect from any OpenLab Control Panel that is connected to the OpenLab Shared Services server.

If you click *Launch offline* to reconnect to an online instrument, or vice versa, you will get two instrument windows, one for the online instrument and one for the offline instrument.

### Session Takeover

You can take over an existing session by clicking the *Launch online* or *Launch offline* button in the **OpenLab Control Panel** on a different PC:

- If you launched an instrument from the OpenLab Control Panel on PC 1, then log on to an OpenLab Control Panel on PC 2 with the same user credentials and launch the same instrument there, you simply take over your existing session and continue on PC 2 with whatever you started on PC 1.

### NOTE

No warning is shown if the new user and former user have the same credentials.

- If another user has launched the instrument from the OpenLab Control Panel on a different PC, and you have the required privileges, you can also take over that session. You must have the **Take over ChemStation Remote Session** privilege, and if the other user has privately locked the ChemStation, you must also have the **Break Session Lock** privilege. For more information on user

management, privileges, or session lock configuration, refer to the *OpenLab ChemStation Configuration Guide* (CDS\_CS\_configure.pdf).

The current lock status of an instrument/session is shown by an icon to the left of the user name in the **used by** field of the **Instrument** panel and the **used by** column in the **Instruments** table:



The instrument/session is being used by another user; do not take it over.



The instrument/session is locked privately; do not take it over.



The instrument/session is either locked non-privately or is disconnected; it is available for another user to take over.

If you take over the session, the other user receives a message stating which user has taken over the session.

The report displays both the **Acquisition Operator** who is logged on as the current user and the **Sample Operator** who submitted the single sample or sequence to the Run Queue.

Online and offline instruments are included in the same session and are therefore always transferred together. If an online instrument and an offline instrument are already launched in a session, the takeover transfers control of both instruments, regardless of whether you clicked the *Launch online* or *Launch offline* button. If you click *Launch offline* and the session comprises only an online instrument, or vice versa, you will get two instrument windows, one for the online instrument and one for the offline instrument.

### Force Shutdown

To shut down non-responsive instruments that cannot be used anymore, you can right-click the instrument in the OpenLab Control Panel, and select **Force Shutdown** from the Control Panel on the ChemStation Client.

You must have the **Instrument Administration** privilege to use this function.

Forcing a shutdown will not immediately update the instrument status, leading to a temporary inconsistent status display until the status is automatically reset to "not started". It is recommended that you wait at least two minutes before launching a new ChemStation session.

## 2

# Working with Methods

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Methods are a vital part of how OpenLab ChemStation works. OpenLab ChemStation is a chromatography data system with great flexibility for method development. This chapter explains the concepts of methods in detail.

## What is a Method?

A method comprises all the parameters for acquisition and data analysis together with pre- and post-run tasks for a given sample, if they are needed.

The available methods (\*.m) files are visible in the ChemStation Explorer. For quick and easy navigation, you can add additional method locations to the ChemStation Explorer selection tree using the **Paths** tab of the **Preferences** dialog box.

There are different types of methods. Depending on the storage location, methods are either used as master methods, as a reference within the result set of a sequence, or as an actual record of the settings used during data acquisition.

## Master Methods

These are methods stored on the computer disk. Stored methods have a name with up to forty alphanumeric characters followed by the extension \*.M. The master method directories are configured in the Preferences (see "[Path Selection](#)" on page 70).

The Master Method is stored in a methods subdirectory, available in a Methods node of the ChemStation Explorer, and is not directly associated with any result set.

## Sequence Methods

When a sequence is run, copies of all the master methods used in the sequence are stored in the result set along with the sequence data files. These methods are directly linked to the sequence, and are also used when the sequence is reprocessed. Changes to these methods are by default not automatically propagated to the master methods. Changes take effect as soon as the sequence run starts or continues after a pause. Changes are also propagated to the data file methods (DA.M) when the sequence is reprocessed, and on any report generation.

## Data File Methods

A copy of the data analysis parameters is stored as the data file method DA.M with the data files. The data file method DA.M is automatically updated after each result generation (data acquisition, recalculation or report generation). It is also loaded by ChemStation when you recalculate results in the Last Result mode (see “[Last Result Mode](#)” on page 158).

If you use the **Save method with Data** option in the run time checklist, the method is stored additionally as run.m in the data file.

In the ChemStation Explorer, you can easily load either a master method or a sequence method by double-clicking on the method item.

## Parts of a Method

A method is identified by a name of up to forty alphanumeric characters. The file name always has the .M extension to identify it as a method. Methods are stored as directories that contain individual files relating to the components of the method.

Each method comprises four components:

- method information,
- instrument control,
- data analysis, and
- run time checklist.

### Method Information

This section is used to define descriptive information about the method.

### Instrument Control

Defines parameters that control the instrument or its components. With an LC instrument, parameters, such as mobile phase composition, flow rate, injection volume, detector wavelength, and so on, control the pump, the injector and the detector. With a GC instrument, parameters such as inlet temperature, inlet pressure, packed column flow setting, and so on control the instrument.

### Data Analysis

Defines parameters that control the data processing.

- *Signal Details*

Defines signals and their properties used for data evaluation.

- *Integration Events*

Defines timed events that will occur at specific retention/migration times on a chromatogram/electropherogram. These timed events can be used to change the way the signal is integrated.

- *Peak Identification*

Defines data processing parameters associated with the identification of peaks in the chromatogram/electropherogram.



- *Peak Quantification*  
Defines data processing parameters that affect the quantification calculations which determine the amount or concentration of sample component corresponding to each peak.
- *Calibration and Recalibration*  
Defines data processing parameters that affect the calibration and how often calibration is done.
- *Custom Fields*  
Defines the properties of sample or compound related custom fields that are available for the method. The custom fields allow you to add custom information to a sample or a compound in a sample.
- *Report*  
With Classic Reporting: defines the format of the report that is printed after a run.  
  
With Intelligent Reporting: specifies the report template used to generate the report after a run.

#### Run Time Checklist

Defines which parts of the method are executed when the method is run.

You can use the run time checklist to:

- acquire, store and process data to produce a report,
- execute only a portion of the method,
- acquire and store data without analyzing it,
- reanalyze existing data files,
- use your own commands for data analysis, pre- and post-run processing,
- save the analysis results in a register for GLP purposes, and
- save your method together with the data.

For more information about custom commands and how to set them up, see [“Using Custom Commands or Macros in ChemStation”](#) on page 26.

## Creating Methods

Creating a new method always means modifying a master method or sequence method and saving the modifications. You can either overwrite an existing method, or save a method as a new master method. Be aware that when you change a method, the disk version remains unchanged until you save your changes.

You have a choice of how to create a method. You can create a method to do either one or all parts of an analysis. For example, you can create a method to do only data acquisition. When you are ready to analyze the data and generate a report, you can then modify the method to do these data processing tasks.

### NOTE

Do not delete the default method (DEF\_LC.M, DEF\_CE.M or DEF\_GC.M). These method files are used as templates to create new methods.

## Editing Methods

You can edit an existing method using the Edit Entire Method item of the Method menu. You are guided through all the method dialog boxes and at the end you can save the method. This process is shown below:

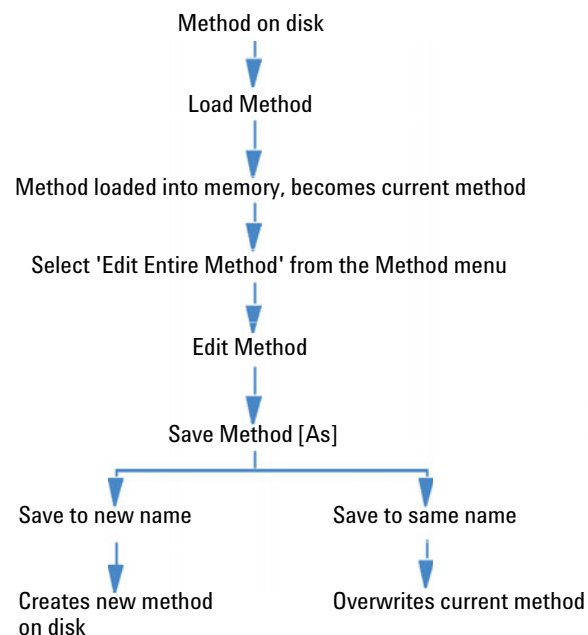


Figure 3 Editing Method

## Method Parts to Edit

Each method comprises four components that can be edited separately.

Some of the following subsections refer to specific dialog boxes, and some are generalized descriptions.

- *Method Information* comprises:
  - a text description about the method.
- *Instrument Control* depends on the configuration, and can comprise, for example:
  - oven parameters,
  - injector parameters, and
  - detector parameters.
- *Data Analysis* comprises:
  - signal details,
  - integration parameters,
  - quantification parameters,
  - calibration parameters,
  - custom field setup parameters, and
  - reporting parameters.
- *Run Time Checklist* comprises:
  - the parts of the method that will be executed.

## Method Directory Structure

### Folders

A method comprises a group of files stored in the method directory (\*.M). By default, master methods are stored in the instrument's method directory. This directory is, for example, in the public documents folder C:\Users\Public\Documents\ChemStation\x\METHODS, where x is the instrument number.

The path to the instrument can be defined during installation. Additional paths for master methods can be added using the preference settings.

Use ChemStation menu **File >Open Windows Explorer...** to open the instrument's data directory (for example, C:\Users\Public\Documents\ChemStation\1). Alternatively, use the shortcut to **Instrument Data** in the Start menu.

Sequence methods are stored in the result set, and data file methods are stored as DA.M in the data file subdirectory.

## Files

Method files with the .MTH extension contain parameter sets and are in UNICODE format. The file INFO.MTH comprises the method control parameters.

Method files containing the instrument parameters have the name of the related analytical module. For example:

**Table 5 Method file examples**

HPCE1.MTH	Comprises the acquisition method for the Capillary Electrophoresis.
ADC1.MTH	Comprises the Agilent 35900 acquisition method. If two identical instruments are configured, the method files are called ADC1.MTH, ADC2.MTH.
DAMETHOD.REG	For data evaluation.
LALS1.REG	Comprises parameters for the Agilent 1100/1200 Series autosampler when a classic modular LC system is configured. The method files for the other Agilent 1100/1200 Series modules follow the same convention Lxxx1.reg where xxx is the module acronym.
AgilentSamplerDriver1.RapidControl.xxx.xml	Comprises parameters for the Agilent 1100/1200 Series autosampler when a modular LC system is configured. Several .xml files are present for the various parts of the parameters (indicated by the xxx part of the file name). Similar .xml files are available for the other modules.

## Editing Methods in Online Mode

When an online ChemStation is idle, you can edit all parts of a sequence method. When a sequence is currently running, you can edit all acquisition parameters and some of the Data Analysis parameters, such as the settings under Specify Report.

The changes are saved and immediately set into effect for the current run and all following sequence lines that include the same method. This means that you can also change the method during a sequence pause or a partial sequence.

## Editing Methods in Offline Mode

You can edit a sequence method in an offline ChemStation, while the same method is used for a run in an online ChemStation. In this scenario, you can edit the Data Analysis part in the offline session. Once you save the changes in the offline session, the changed DA settings will be used for the next Data Analysis of the current sequence run within the online session.

Method updates concerning calibration are not taken into account. Also history entries are not merged, that is, if a method is running in an online session, and you change it in both online and offline session, the audit trail of the method will only contain the changes made in the offline ChemStation.

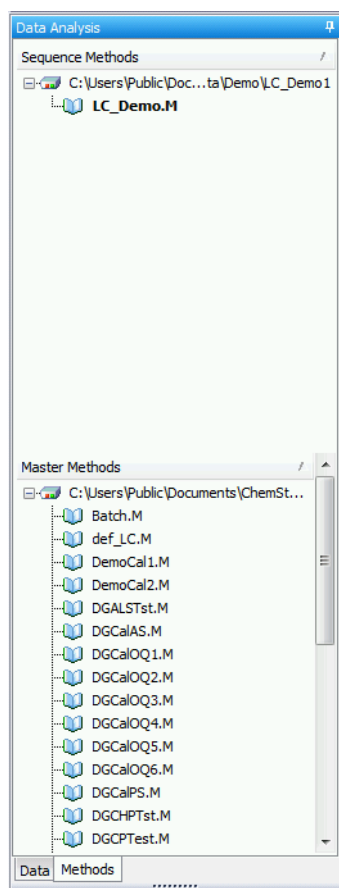
### NOTE

If the same master method is loaded in online and offline ChemStation of the same instrument, you can only edit the method in the online ChemStation.

## Administrrating Methods

### Methods Tree in ChemStation Explorer

The Methods Tree in the ChemStation Explorer is divided into two parts. The upper part shows the methods contained in the currently loaded result set. The lower part shows the methods in the master method directories, which you configure in the **Preferences** dialog.



The currently loaded method is always shown in bold.

By Drag & Drop you can easily copy master methods to sequence methods. The entire method (DA parameters and ACQ parameters) will be copied to the result set.

## Viewing the Acquisition Method

You can access the Acquisition Method Viewer via the menu **Instrument > Acquisition Method Viewer...** in the **Method and Run Control** view. The Acquisition Method Viewer is available for both Online and Offline ChemStation sessions.

With the Acquisition Method Viewer, you can check the acquisition parameters stored in a method, independently of the current instrument configuration. The dialog shows the instrument configuration at the time when the method has been saved in ChemStation. Data analysis parameters are not shown in this viewer. The Acquisition Method Viewer does not allow the user to make any changes to the loaded ChemStation method.

The Acquisition Method Viewer shows the method settings in read-only mode. It does not provide functionality to edit and save methods.

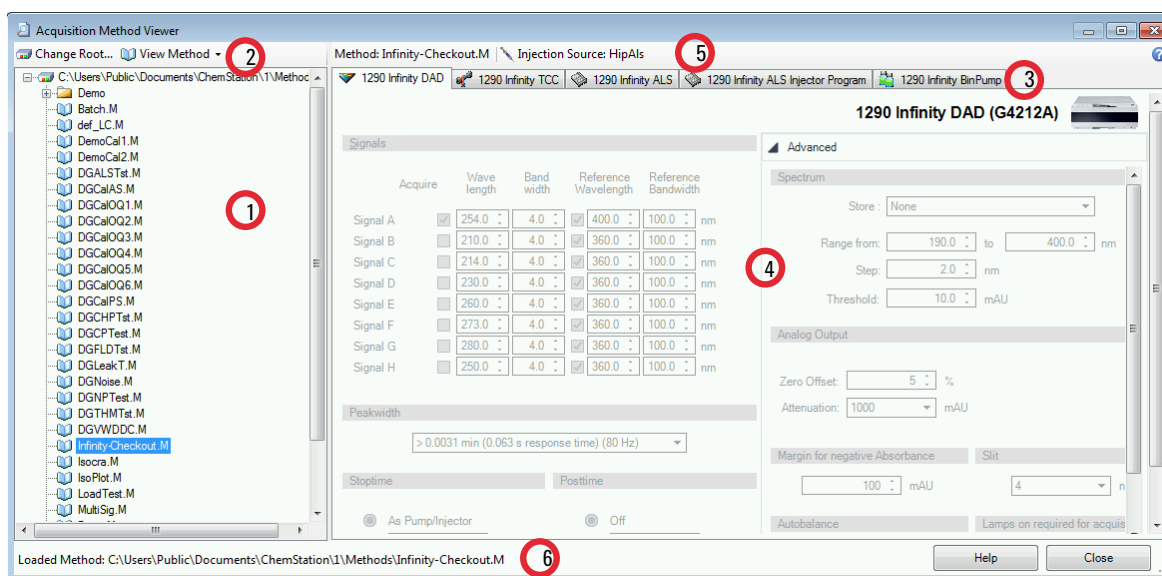


Figure 4 Acquisition Method Viewer dialog



1	Method browser
2	Toolbar
3	Module tabs (It shows method settings, pretreatment settings in a tab-control for all found modules in the used instrument configuration)
4	Method viewer area
5	Method Name, Injection Source Info
6	Status bar

In the method browser (1), the preferred method path is shown by default. Click **Change Root...** in the toolbar to select a different directory.

The toolbar (2) offers the following **View Method** options:

- **View with Original Configuration...:** Load the settings as stored in the method to the instrument.
- **View with Instrument Configuration...:** Apply the stored method to the current instrument configuration. This option is available for Online instruments only. The stored method might not be consistent with the current instrument settings; if possible, the settings are then automatically adapted, otherwise, you can check the details in the **Method Resolution Info** dialog. This dialog shows the list of inconsistencies and the differences between unresolved and resolved method.

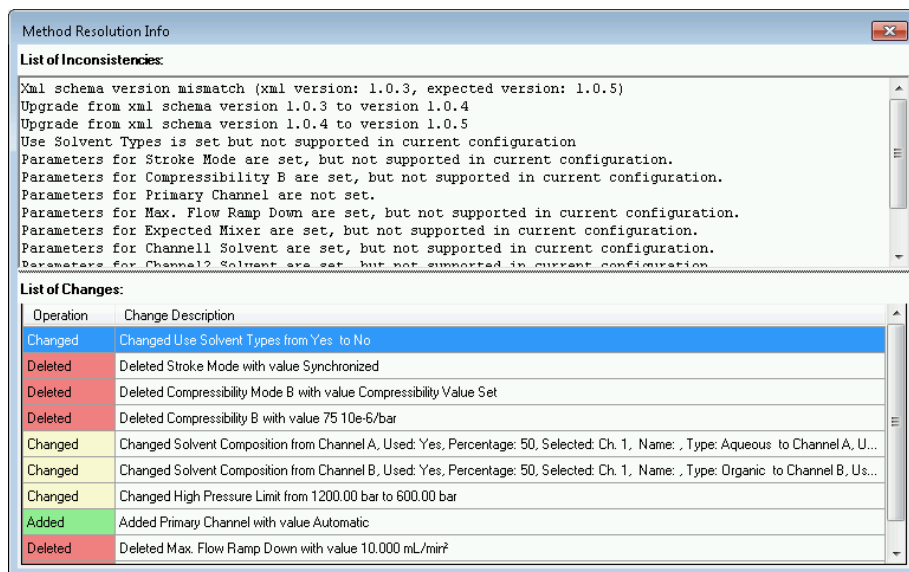


Figure 5 Method Resolution Info dialog

## Updating DA Parameters in the Master Method

The **Update Master Method** option is available from the **Method** menu and from the context menu of the sequence method in the ChemStation Explorer. The availability and exact behavior of this function depends on the current mode. In all cases, this function updates the data analysis parameters of the target method.

### NOTE

It is important to note that this feature updates the data analysis parameters *only* of the target method, and that it overwrites *all* data analysis parameters.

### Updating a Master Method in Reprocess or Recalculate Mode

In this mode, the **Update Master Method** command is only active for sequence methods of a result set. You can update the master method that you referred to when creating the sequence. The precondition is that the master method still exists in the master methods directory (the master method must have the same name as the sequence method).

You can also configure the sequence parameters to automatically execute this function during each sequence acquisition or reprocessing. For more information, refer to [“Administrating Methods”](#) on page 55.

### Updating a Master Method in Last Result Mode

In this mode, the **Update Master Method** command is active for both sequences and single samples. You can transfer the current data analysis parameters to the master method last used for data analysis. This method is shown in the **Analysis Method** column of the Navigation Table.

The command is available under the following conditions:

- The method file exists in the given location (that is, the name and the entire path must match).
- For sequences: The sequence run has been manually analyzed with a master method (not with the sequence method).

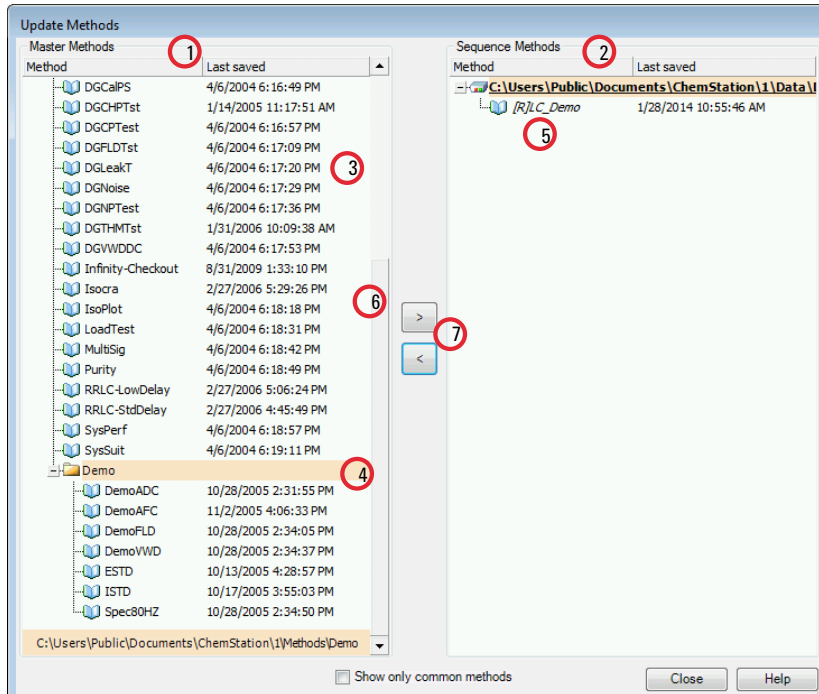
### Updating Any Master Method in Last Result Mode

In Last Result Mode, you can transfer the data analysis parameters to any master method, independently of the master method related to the current sequence or single run. To update any master method, select **Menu >Update any Master Method ...**, and select a method from the **Choose Master Method to update** dialog. The data analysis parameters will then be copied to the selected master method.

## Updating Methods

With the **Update Methods** dialog (see figure below), you can copy methods from the master method directory to the result set and vice versa. In both cases, the entire method is copied (DA parameters and ACQ parameters).

You can open the dialog from the **Method >Update Methods...** menu or from the context menu of the sequence method in the ChemStation Explorer. The function is available for result sets in Recalculate and Reprocess mode.



**Figure 6** Update Methods dialog

- 1 On the left side, you see the methods in all master method directories (as configured in the Preferences).
- 2 On the right side, you see the methods in the currently loaded result set.
- 3 For each method, you see the date when it was last saved. The tooltip of the date shows the method's last history entry.
- 4 Methods can also be stored in subfolders of the master method directory.
- 5 Read-only methods have an [R] prefix. The currently loaded sequence method is shown in italics.
- 6 Methods that are common for the sequence result set and the master method pool are shown in a bold font. The methods are matched only by name; if a method name exists in more than one pool each of the instances will be considered common.
- 7 You can copy methods between a master method pool and the sequence result set either by using Drag&Drop or by using the < and > buttons. You cannot overwrite methods that are marked as read-only.

## Saving a Method as New Master Method

You can save the data analysis parameters from DA.M as a new master method. However, the DA.M does not contain acquisition parameters. To provide a valid set of acquisition parameters for the new master method, you must therefore select another method as a template for the acquisition parameters (see figure below). The new master method will then contain your current data analysis parameters from the DA.M, and the acquisition parameters from the selected template method. The new method will be created in the folder where the acquisition template method is located.

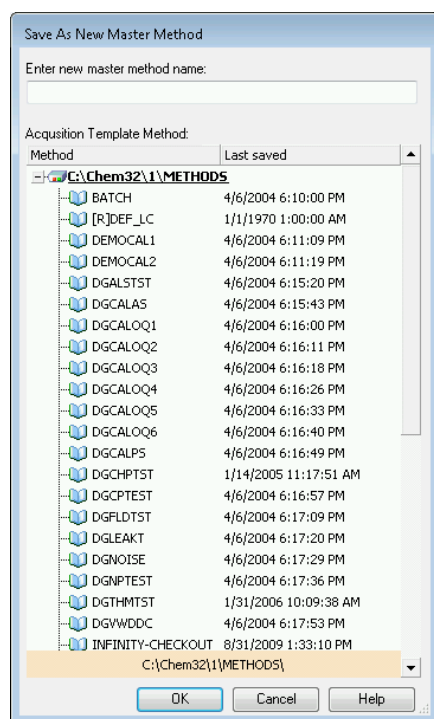


Figure 7 Save as New Master Method dialog

## What Happens When a Method is Run?

The **Run Time Checklist** dialog box specifies the parts of the method to execute when a run is started.

There are the following parts to the run time checklist:

- pre-run command or macro,
- data acquisition,
- standard data analysis,
- analysis method for second signal (GC only),
- update custom fields values,
- customized data analysis,
- save GLP data,
- post-run command or macro, and
- save copy of method with data (RUN.M).

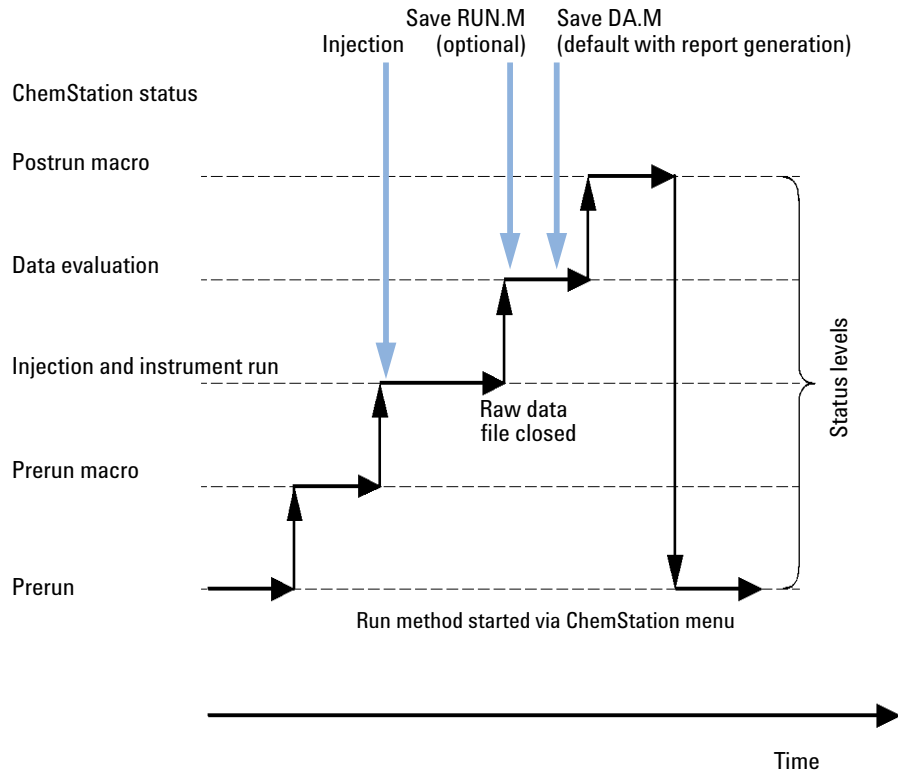
When running a method the specified parts of the method defined in the Run Time Checklist dialog box are executed. Use the menu **Method >Run Time Checklist...** to display or edit the specified parts of the Run Time Checklist.

For more information about commands and how to set them up, see [“Using Custom Commands or Macros in ChemStation”](#) on page 26.

## Method Operation Summary

The following list shows the flow of the method operation when all parts of the Run Time Checklist are selected.

- 1 *Prerun Command Macro*  
Does a task before the analysis is started.
- 2 *Data Acquisition*  
Does injector program.  
Injects sample.  
Acquires raw data.  
Stores data.  
Saves the acquisition parameters in the ACQ.TXT file.
- 3 Optional, as directed by the Run Time Checklist: *Save Copy of Method with Data* as RUN.M.
- 4 *Data Analysis (Process Data)*  
Loads data file.  
Integrates data file.  
Identifies and quantifies peak.  
Searches spectral library if available.  
Checks peak purity if available.  
Saves a copy of the method (DA.M).  
Prints reports (after updating custom fields values, if selected).
- 5 *Update Custom Fields Values*  
Executes your macros to update custom fields values before reports are printed.
- 6 *Customized Data Analysis*  
Executes your macros after reports have been printed.
- 7 *Save GLP Data*  
Saves binary register GLPSave.Reg
- 8 *Postrun Command Macro*  
Does a task after completion of the analysis, for example, generates a customized report.



**Figure 8 Method operation**

The figure below shows an overview of the ChemStation status during the method operation, where all parts of the Run Time Checklist are selected.

## Pre-run Command or Macro (Run Time Checklist)

If a pre-run command or macro is specified, it is executed before the analysis is started. This part is typically used for system customizing in conjunction with other software packages.



## Data Acquisition (Run Time Checklist)

- All parameters are set to the initial conditions specified in the current method.
- If specified the injection program is executed and an injection is made from the currently defined vial.
- The monitor display shows the progress of the analysis including chromatographic/electropherographic information, and spectral data if available.
- Data are acquired and stored in a data file.
- When the Data Acquisition is finished, the acquisition parameters of the currently executed method are stored as ACQ.txt for the data file by default.

## Data Analysis (Run Time Checklist)

When the stop-time has elapsed, the analysis is finished and all raw data is stored on the computer's hard disk. The data analysis part of the software starts when all the raw data is stored.

### Integration

- Chromatogram/electropherogram objects in the signal are integrated as specified in the Integration Events dialog box.
- The start of the peak, the peak apex, retention/migration time and the end of the peak are determined.
- Baselines are defined under each peak to determine final peak height and area.
- The integration results are created as an Integration Results list.

### Peak Identification and Quantification

- Using retention/migration times and optional peak qualifiers, the software identifies the peaks by cross-referencing them with known components defined in the calibration table.
- By using peak heights or peak areas the software calculates the amount of each detected component using the calibration parameters specified in the Calibration Table.

Spectra Library Search (for LC 3D, CE, CE/MS and LC/MS Systems Only, Available With Classic Reporting)

For all peaks that have UV-Visible spectra available, an automated search of a predefined spectral library may be done to identify the components in the sample based on the UV-Visible spectra. See *Understanding Your Spectral Module* for details.

Peak Purity Checking (for LC 3D, CE, CE/MS and LC/MS Systems Only)

For a peak with UV-Visible spectra, you can calculate a purity factor for that peak and store it in a register. Peak purity may be determined automatically at the end of each analysis as part of the method, if the Check Purity box is checked when specifying an automated library search or when selecting an appropriate report style. See *Understanding Your Spectral Module* for details.

Print Report

A report is generated with identities and amounts of components detected in the run.

#### NOTE

If you run an Update Custom Fields macro, reports will be generated *after* this macro has been executed.

## Update Custom Fields Values

ChemStation allows to define custom fields for a sample and for specific compounds. These custom field values can be included in your reports. By default, the values are static. **Update Custom Fields Value** enables you to modify the custom fields values before reports are generated. The updated fields are available in both Classic and Intelligent Reporting.

An example macro is available in the **Disk2 >UCL** folder.

Your Update Custom Fields macro will be executed as follows:

- 1 as a part of a Standard Data Analysis, shortly before reports are created
- 2 every time on creating a report/report preview in the **Data Analysis** view (even if Standard Data Analysis is not selected in the Run Time Checklist)

**NOTE**

During reprocessing, the custom fields values are always overwritten with the static values defined in the sequence/sample. The custom fields will be modified only shortly before reports are generated. Therefore, if you reprocess a sequence with a different method that does not contain the Update Custom Fields macro, the values will be reset to the defined static values.

## Customized Data Analysis

Enables you to run your own customized macros to evaluate your analytical data.

With Standard Data Analysis enabled, these macros run *after* reports have been generated. Results are therefore not available for reporting (neither Classic nor Intelligent Reporting). With Standard Data Analysis disabled, they run after data acquisition.

## Save GLP Data

Saves the binary register GLPSave.Reg together with the data analysis method in the data directory. This feature is designed to help prove the originality of the data and the quality of the individual analysis.

The GLPSave.Reg binary file contains the following information in a non-editable, checksum-protected, register file:

- key instrument set points (can be graphically reviewed),
- chromatographic or electropherographic signals,
- integration results,
- quantification results,
- data analysis method, and
- logbook.

These data are saved only if the Save GLP Data feature is activated by checking the check box in the runtime checklist. You can review, but not edit, GLP data in the data analysis menu of ChemStation.

## Postrun Command or Macro

If a postrun command or macro is specified it is executed after the data evaluation, for example, copying data to a disk for data backup.

## Save Copy of Method with Data

This is done after data acquisition, and only if **Save method with Data** is activated in the Run Time Checklist. It copies the method used for acquisition to the data directory, named as RUN.M. RUN.M contains DA and ACQ parameters. It is read-only and thus provides a means for you to reconstruct the analysis in the future even if the method changes in the meantime. You can see how changes in the method or in selected parameters have influenced your analysis, which can help you to optimize it.

## Save Copy of Method as DA.M with Data (ChemStation Default)

Independently of the marked items in the Run Time Checklist, a copy of the data analysis parameters of the executed method is saved as DA.M along with the report in the data file. This is done at the end of the *Standard Data Analysis* part, and also when you create a report in the Data Analysis view.

# 3

## Data Acquisition

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OpenLab ChemStation offers seamless instrument control of Agilent LC, GC, CE, CE/MS, and LC/MS systems. It supports advanced features and workflows of Agilent GC and LC instruments with add-on software and provides flexibility for research and method development laboratories. This chapter contains an introduction to the process of acquiring analytical data.

## What is Data Acquisition?

During data acquisition, all signals acquired by the analytical instrument are converted from analog signals to digital signals in the detector. The digital signal is transmitted to ChemStation electronically and stored in the signal data file.

## Path Selection

Flexible data storage for single runs and sequences allows you to specify various saving locations without reconfiguration. The **Paths** tab in the **Preferences** dialog box in the **View** menu gives you the opportunity to add multiple paths in addition to the default path<sup>1</sup> C:\Users\Public\Documents\ChemStation\x\DATA (where x is the instrument number). Using the **Add** and **Remove** buttons, existing paths can be deleted, or you can navigate to a selected location and add the path into the **Preferences**.

The default path cannot be removed from the list, but it can be changed in the **Configure Instrument** dialog from the Control Panel. For more information on changing the default paths, refer to the *OpenLab ChemStation Guide for Administrators*.

The ChemStation menu **File >Open Windows Explorer...** provides easy access to the actual instrument's data directory (for example, C:\Users\Public\Documents\ChemStation\1). Alternatively, use the shortcut to **Instrument Data** in the Start menu.

<sup>1</sup> Path can be defined during installation.

## Data Acquisition

### What is Data Acquisition?

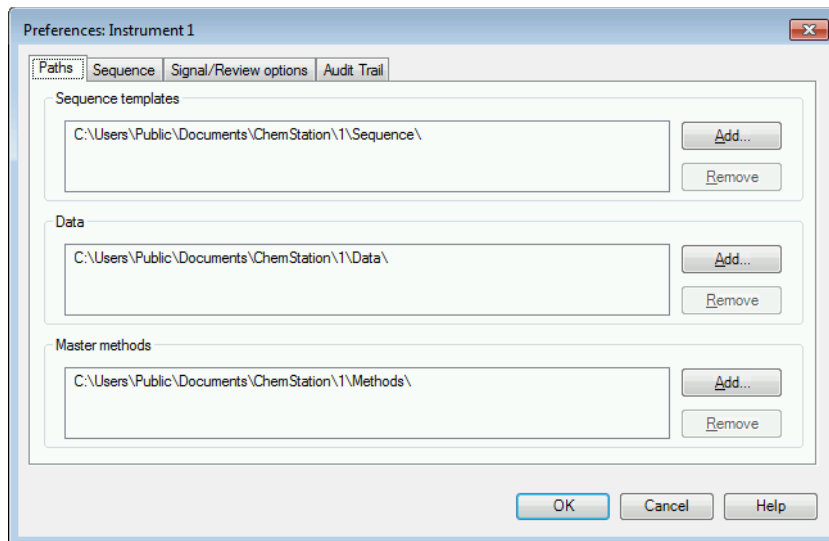


Figure 9 Paths tab in the Preferences dialog

All newly specified Data Paths are then available for selection in the **Sample Info** and **Sequence Parameters** dialog boxes when performing runs.

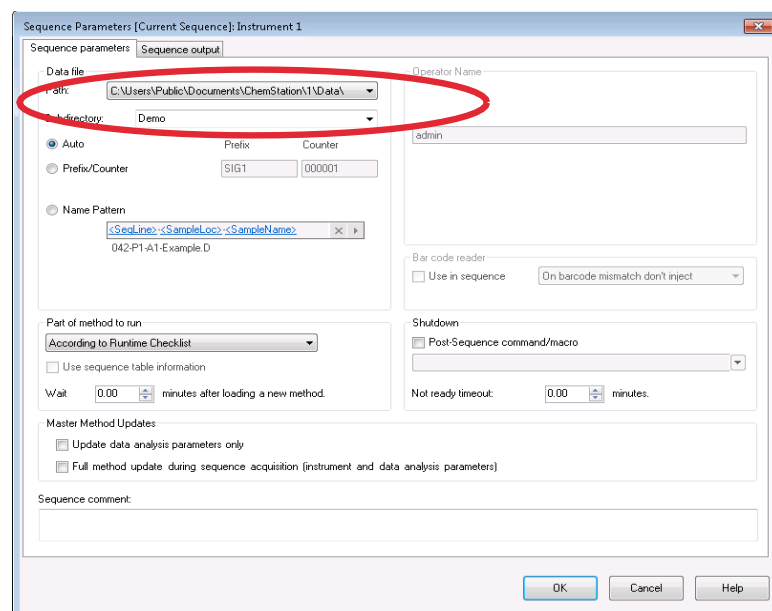


Figure 10 Data path selection in the Sequence Parameters dialog

## Online Monitors

### Online Signal Monitor

The online signal monitor allows you to monitor several signals and, if supported by the associated instrument, instrument performance plots in the same window. You can conveniently select the signals you want to view and adjust the time and response axes. For detectors that support this function a balance button is available.

You can display the absolute signal response in the message line by moving the cross hair cursor in the display.

### Online Spectra Monitor

The online spectra monitor shows absorbance as a function of the wavelength, or  $m/z$  for mass spectra. You can adjust both the displayed wavelength range and the absorbance scale.



## Logbook

The logbook displays messages that are generated by the analytical system. These messages can be error messages, system messages or event messages from a module. The logbook records these events irrespective of whether they are displayed or not.

## Status Information

### ChemStation Status

The ChemStation Status window shows a summary status of the ChemStation software.

When a single analysis is running:

- the first line of the ChemStation Status window displays run in progress,
- the second line in the status window displays the current method status, and
- the raw data file name is shown in the third line together with the actual run time in minutes (for a GC instrument, files for front and back injector are also displayed).

The Instrument Status windows provide status information about the instrument modules and detectors. They show the status of the individual components and the current conditions where appropriate, for example, pressure, gradient and flow data.

### Status Bar

The graphical user interface of the ChemStation system comprises toolbars and a status bar in the Method and Run Control View of ChemStation. The status bar comprises a system status field and information on the currently loaded method and sequence. If they were modified after loading they are marked with a yellow asterisk or cogwheel, depending on the instrument. A yellow EMF symbol points to usage limits that exceed the setpoints set for LC consumables (for example, the lamp). The status bar also shows the status of the Run Queue, which can be **Resumed**, **Paused**, or **Blocked**.

## System Diagram

If supported by the configured analytical instruments (for example, the Agilent 1200 Infinity LC Series modules, or the Intuvo 9000 GC system) you can display a graphical system diagram for your ChemStation system. This allows you to quickly check the system status at a glance. Select the **System Diagram** item from the **View** menu of the **Method and Run Control** View to activate the diagram. It is a graphical representation of your ChemStation system. Using the color coding described below the current status is displayed.

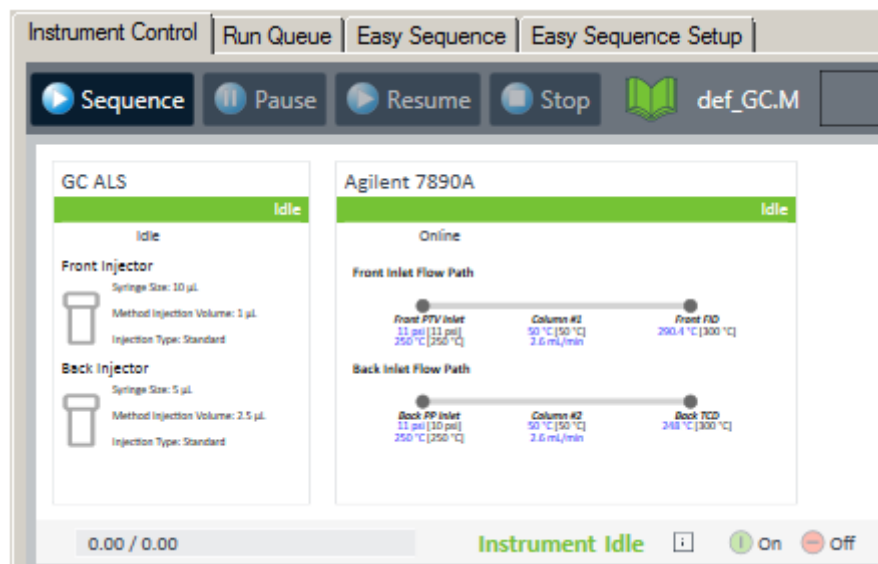


Figure 11 System diagram, for example for a GC

Table 6 Colors used to indicate the status of the module or instrument

Color	Status
gray	offline
green	idle
orange	not ready
red	error
cyan	standby (for example, lamps off)
purple	pre-run, post-run

**Table 6** Colors used to indicate the status of the module or instrument

Color	Status
magenta	injecting
blue	running or post-run

In addition, you can display listings of actual parameter settings. Apart from a status overview, the diagram allows quick access to dialog boxes for setting parameters for each system component.

See the instrument part of the online help system for more information on the system diagram.

## Rules and Alerts

For instrument drivers that support this feature (for example, 8890 GC), you can choose **Instrument >Manage Rules and Alerts...** to configure how the ChemStation will react to specific events during acquisition.

For example, a missing vial or vessel is a common error in chromatography. The ChemStation may, for example, continue, pause, stop, or abort a sequence.

### NOTE

The covered events and the possible behaviors depend on the instrument driver.

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This chapter describes the concepts of automation. It explains how to work with sequences in ChemStation, what happens when a sequence is run and how to customize sequences.

## What is Automation?

Automation is the unattended analysis of more than one injection.

The sequence part of the ChemStation software allows you to automate acquisition, data evaluation, and report generation.



## What Are Sequences and Sequence Templates?

A sequence is a series of instructions that automates the analysis of samples. It can be used to automatically inject each sample, and to acquire and analyze the data according to the method specified for that sample. Each sample vial in a sequence may be analyzed with a different analytical method and, thus, use different sets of chromatographic/electropherographic conditions and evaluation parameters.

Sequence files (\*.s) are “sequence templates” that can be used to run an acquisition multiple times; however, these templates are not used for reprocessing in **Data Analysis**. When the sequence template is run, a result set is created, containing all related files. If you reuse the sequence template, ChemStation creates a new result set for each reuse. For backward compatibility reasons, it is also possible to run sequences as a series of single runs. For details, see “[Sequence Execution Mode](#)” on page 115.

The available sequence templates are visible in the ChemStation Explorer. For quick and easy navigation, you can add additional sequence template locations to the ChemStation Explorer selection tree using the **Paths** tab of the **Preferences** dialog box.

It is possible to set up multiple sequences for an instrument and schedule them in an appropriate order. The **Run Queue** tab displays the total workload for the instrument (sequences as well as single samples, pauses, etc.). You can define the order of items to be processed directly in the Run Queue tab. For more information about the Run Queue, see “[About the Run Queue](#)” on page 143.

## Sequence Parameters

The **Sequence Parameters** dialog box contains information common to all sample vials in a sequence. To open it, select the **Sequence** menu in the **Method and Run Control** view.

The screenshot shows the 'Sequence Parameters' dialog box for the current sequence 'LC Zen Liquid'. The dialog has two tabs: 'Sequence parameters' (selected) and 'Sequence output'. The 'Sequence parameters' tab contains several sections:

- Data file:** Includes a 'Path' dropdown set to 'C:\Users\Public\Documents\ChemStation\1\Data\' and a 'Subdirectory' dropdown. Below these are radio buttons for 'Auto', 'Prefix/Counter', and 'Name Pattern'. The 'Prefix' field is 'SIG1' and the 'Counter' field is '0000001'. The 'Name Pattern' section shows a pattern '<SeqLine>-<SampleLoc>-<SampleName>' with an example '042-P1-A1-Example.D' below it.
- Operator Name:** A text field containing 'SYSTEM'.
- Bar code reader:** Includes a checkbox 'Use in sequence' (unchecked), a dropdown 'On barcode mismatch don't inject' (set to 'On barcode mismatch don't inject'), and a 'Reference field' dropdown set to 'Sample name'.
- Shutdown:** Includes a checkbox 'Post-Sequence command/macro' (unchecked) and a dropdown menu. Below this is a 'Not ready timeout' field set to '0.00' minutes and a checkbox 'Error Method' (unchecked) with a 'Browse...' button.
- Part of method to run:** A dropdown set to 'According to Runtime Checklist'. Below it is a checkbox 'Use sequence table information' (unchecked) and a 'Wait' field set to '0.00' minutes after loading a new method.
- Master Method Updates:** Includes two checkboxes: 'Update data analysis parameters only' (unchecked) and 'Full method update during sequence acquisition (instrument and data analysis parameters)' (unchecked).
- Sequence comment:** A large text area for entering comments.

At the bottom right of the dialog are three buttons: 'OK', 'Cancel', and 'Help'.

Figure 12 Sequence Parameters dialog

Use this dialog box to:

- select the data directory using the **Path** combo box,
- specify how the sequence processing should be done by choosing particular part of Methods and Run parameters, and
- specify what happens when the sequence is finished, for example, by using a **Shutdown** command macro. For more information about custom commands and how to set them up, see [“Using Custom Commands or Macros in ChemStation”](#) on page 26.

For example, you can choose to either:

- execute the run time checklist,
- do acquisition only, or
- do reprocessing only (for data acquired till ChemStation Rev. B.01.03. or for data acquired with the legacy option **Unique Folder Creation OFF**).

**NOTE**

Sequence data acquired with ChemStation revisions up to B.01.03 or acquired using the legacy option **Unique Folder Creation OFF** needs to be reprocessed using the **reprocess** option in the **Method and Run Control** view.

Sequence data acquired with ChemStation revisions B.02.01 and higher need to be reprocessed using the **reprocess** option in the **Data Analysis Navigation table**.

If the **reprocess** option is selected, you have the choice to use the sample data defined when the sample was originally analyzed, or by activating the **Use Sequence Table information** check box, you can use updated sample data by entering new data in the sequence table:

- specify if the barcodes should be used in the sequence and how to handle a barcode mismatch, assuming that a barcode reader is installed on the system.

## Graphical Sample Entry

The graphical sample entry offers an intuitive visual display of the Sample Container and the loaded samples. You can either manually create new samples, or load existing sequences for which you want to assign parameters that do not yet exist, such as a method or a container location (for example, for re-injection sequences generated from collected fractions).

*Sample Containers* refer to instrument trays or plates that hold samples/vials. Sample containers have different dimensions and different vial capacity depending on the instrument. Sample Container types describe the physical properties of a specific tray or plate in an XML format. Custom Sample Container types can be centrally stored and made available across the lab by importing an XML file containing the sample container type definition. The **Import Sample Container Type** button in the OpenLab Control Panel is used to import the custom Sample Container types.


You can choose a sample container in the **Sample Entry** tab. You can easily create new sample entries in the graphical user interface, simply by clicking in the container visualization. The sample locations will be color coded corresponding to the sample type.

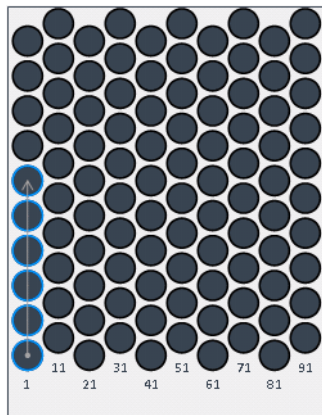
The screenshot displays the 'Sample Entry' tab in the OpenLab software. It features three main components: a 3D visualization of a sample tray, a 2D grid of sample locations, and a 'Sample List - New' table.

**Sample List - New Table:**

#	Sample Location	Sample Name	Method Name	Inj Volume	Sample Type	Cal Level	Update RF	Update RT	Sample Amount	Multiplier
1	Blank 1	def_LC			Blank		No Update	No Update	0	
2	Control 1	def_LC			Control Sample		No Update	No Update	0	
3	Calib 1	def_LC			Calibration	1	Average	Average	0	
4	Calib 2	def_LC			Calibration	2	Average	Average	0	
5	Sample 1	def_LC			Sample		No Update	No Update	0	
6	Blank 2	def_LC			Blank		No Update	No Update	0	

Figure 13 Sample entry tab

The **Selection Properties**  allow you to define the pattern for multiple samples. Using these options, you can display the ordering arrow. Simply drag the mouse over several locations.



**Figure 14** Ordering arrow

For all autosamplers that physically allow rearranging of plates, you can even drag entire plates to other positions or drawers. The vial locations are automatically adjusted in the sample list. The container configuration can be saved with the sequence template, or exported to PDF.

You can also prepare plates that are not associated with any specific position or drawer. These *parking lots* correspond to the plates you prepare on your bench. They are saved together with the other settings in the sequence template. You can load this sequence template at a later point in time for the relevant instrument, and then assign the prepared plates to the correct position and drawer.

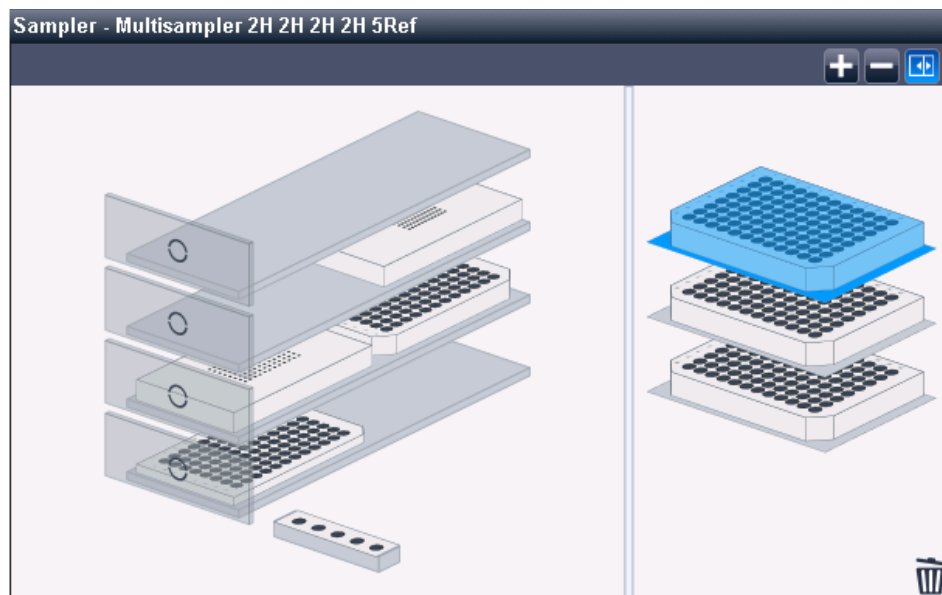


Figure 15 Multisampler in the Sample entry tab

The **Sample List** table offers many functions that help you editing the table, such as:

- Copy cell ranges
- Append copied cells or lines
- Group samples by specific information
- Filldown with intelligent auto-increment
- Re-order single or multiple selected rows
- Copy individual cell content or selected table regions to the clipboard

In the sample list, you prepare the same information as in the Sequence Table (see “[Sequence Table](#)” on page 88). When finished, submit the sample list as a sequence to the Run Queue.

**NOTE**

Once the sequence runs, you cannot edit the sample list anymore. Online editing is only possible in the Sequence table.

**NOTE**

To continue editing this sequence template in ChemStation, first save it using the **Save** button in the **Sample Entry** tab. Then load the sequence template again using the **File** or **Sequence** menu.

**NOTE**

The container configuration is not updated in the graphical hotel presentation in the instrument dashboard.

## Sequence Table

The sequence table determines which methods are used to process the sample vials and the order in which the data for the vials is acquired and analyzed. This table also contains information about each sample, including the sample locations on a plate<sup>1</sup>, sample names, quantification parameters, and recalibration parameters.

For instruments that support dual sampling (GC), an additional column **Injector Location** (with **Front** or **Back** as possible values) is displayed in the table, and the **Dual Simultaneous Injections** check box is available at the bottom:

- If you select the **Dual Simultaneous Injections** check box, the system combines runs and processes two samples simultaneously in each run. The line numbers are adjusted correspondingly. In this mode, you can sort the sequence table by **Front** or **Back** injector location.
- If you do not select this check box, one sample is processed in each run. The order of the runs is as displayed in the table. You can alternate using the front and back injector.

For a description of the columns in this table and how they interact with information stored with the method, see the online help reference.

## Creating Sequences (Sequences and Sequence Templates)

Use the sequence table to specify the samples, methods, and vials to run in the sequence. The sequence table lists each sample in the sequence in the order it will be run and contains the necessary vial number or sample position, method, calibration information, sample amount, ISTD multipliers and other data for each sample.


<sup>1</sup> New sample container types can be defined in the Instrument Configuration or imported in the Control Panel



## Choosing Columns for Display

The information displayed by the Sequence table is configurable:

- Move the columns to left or right, to get the columns most relevant to your work up front.
- Exclude columns from the view which are not needed for your work.

To change the view and content of your sequence table, click  (**Column Chooser**) in the sequence table toolbar. Select the columns that you want to show within the sequence table. Depending on the installed software packages, additional columns will be available, for example, the **Target Mass** column if an LC/MS or CE/MS is installed.

## Selection Modes

Similar to applications such as Microsoft Excel, you can select multiple cells or cell ranges:

- **Ctrl** + Click selects multiple single cells
- **Shift** + Click selects a cell range

## Copy, Cut, Paste

- *Copy*: You can copy selected cells and paste them to any other application (for example, Microsoft Excel). The copied information includes the column header tags. You can view the tags by pasting the information, for example, to Microsoft Excel. With the help of these column header tags, the values can be pasted back to a ChemStation sequence table even if the columns are in a different order.
- *Cut*: If you cut entire rows, the rows will be deleted and put into the clipboard. If you cut only some columns or cells, the rows will be kept, and only the cell values will be cleared.
- *Paste*: If an entire row is selected, paste inserts the values from the clipboard as new rows. If column header tags are available in the copied content, the values are mapped into the appropriate columns using these column header tags. If only a single column is selected, then the clipboard values are pasted from the top row down (line by line), and populate as many columns to the right as there are in the clipboard buffer. If only one single cell is selected, the cells below and to the right of the selected cell will be filled with the values from the clipboard.

## Undo, Redo

The sequence table allows you to undo or redo the last operation.

## Inserting, Appending, or Deleting Lines

To insert or append a new blank line, or to delete an existing line, use the corresponding buttons in the toolbar:



(Insert Line)




(Append Lines)




(Delete Lines)

## Using the Filldown Function

If you have many samples that use the same method, you can quickly enter these samples into the Sequence Table using the **Filldown** icon . This feature copies information from one cell into the previously selected cells or columns. For sample location, sample name, and data file name incrementation rules defined in the **Filldown Options** dialog are used. For other columns this feature simply copies the fields (for example, the method name, number of injections per vial, and if specified, the sample amount, ISTD amount, multiplier, and dilution).


Excluded from the repetition are only columns with unique values such as LIMS IDs. Also, calibration settings are not copied to samples that are not calibration standards.

With the **Filldown Options**  dialog, you can specify different fine tuned behaviors for the filldown function. This dialog allows you to set rules for the sample location and sample naming. On well plates, the direction of increment patterns can be chosen, and also whether this is to be only a sub set rectangle on the plate.

Datafile filldown is special; it takes the complete datafile name and appends a counter with the form "--001". For GC, it also appends a "F" or "B", depending on the chosen injector for the run at the time when the filldown was done.

## New Lines Wizard


This wizard allows you to efficiently create large sequence tables. You can do this in different ways:

- *Simple mode*: Fill one line with all values which you need to duplicate. Select the line, and use the **Insert/Filldown Wizard**  to repeat the line n times. You can also define a rule to insert calibrations or blank runs after a given number of samples.
- *Advanced mode*: Fill several example lines to create a pattern. Then select all these lines, and call the **Insert/Filldown Wizard**. There can be alternating calibrations, controls, blank runs and any number of sample runs, calibration levels and recalibration settings.

You can also choose, for example, to have all calibrations being run from the same vial, and increment only sample vials. Sample positions are repeated with an intelligent increment of starting positions (offset for each copied bloc), to keep all sample position distances. If you cannot set rules in the dialog, values are just duplicated downwards

Excluded from the repetition are only columns with unique values such as LIMS IDs.

## Filtering the Sequence Table


With the **Filter Options** , you can apply a set of conditions to display a subset of lines in the sequence table.

Via filtering you view the sequence table in a condensed form. You can select, for example, to show only certain sample types, methods, calibration levels, sample locations, or sample names.


This helps to quickly check for consistency, or to edit only a certain group of sequence lines by applying the filldown function to the filtered list. For example:

- Update the sample amount for all samples in a certain sample location.
- Change the vial or sample location for a specific calibration level.


## Reading Bar Codes

If your instrument supports reading of bar codes, click **Read Bar Codes**  to get the sample names. Select the sequence table row or sample location cell you want to read the barcode of. There can be one or multiple lines be selected. The barcode is placed in the cell of the sample name for each specified sample location.

## Using the Custom Fields Button

If custom fields have been set up in the method(s) used in the sequence table, select the **Custom Fields** button  in order to edit the custom fields values for each sample (sample related custom fields) or for each compound in the method of a sample (compound related custom fields).

## Previewing the Sequence

With **Sequence Preview** , a dialog opens that shows the sequence exactly as it will be executed, with all repeat calibrations, QC samples and blanks included in the correct order.

## Easy Sequence

## Overview

**Easy Sequence** is a user interface for quick and easy setup of sequences from templates. The template specifies parameters that should be viewed or edited by the user. Calibration setup provides an easy to use drag and drop interface to specify calibration types and sample positions, and displays an overview of the sequence. With **Easy Sequence** users can quickly create sequences following a certain pattern that differ in the number of samples, but are otherwise similar.

Easy Sequence Setup: C:\Chem32\2\SEQUENCE\Test Seq.est

**Method Information**

Method: DEF\_LC.M ...

Estimated Cycle Time: 10 min

**Data Information**

Data Location: C:\Chem32\2\DATA\ ...

Data File Name: Datafile\_<C> ...

☒ Reset Data File Name counter to 1 every time this sequence is run

**Sample Information**

Starting Vial Location: 1

Number of Samples: 6

Injection Volume: Use Method

Sample Name: Sample\_<C>

Import Samples... Fill Samples Clear Sample List

Vial	Sample Name	Inj Volume	Sample Info
1	Sample_0001	Use Method	
2	Sample_0002	Use Method	
3	Sample_0003	Use Method	
4	Sample_0004	Use Method	
5	Sample_0005	Use Method	
6	Sample_0006	Use Method	

Automation Engine Version: 2.05 (007)

Figure 16 Easy Sequence tab

## Using Easy Sequence Tab (Sequence)

**Easy Sequence** tab is used to create a sequence from the template created in the **Easy Sequence Setup** tab. Samples saved as a CSV format can also be imported.

### To define a Sequence

- 1 From the **Easy Sequence** tab, open a template by clicking on the **Open Easy Sequence Setup** icon.
- 2 Make updates if required. This may include sample vial locations, calibrant vial locations, data, or sequence location. Parameters available for editing depend on the template configuration.
- 3 If the pre-filled samples do not match new sample locations, click **Fill Samples** to refill the table.
- 4 Click **Preview/Print Sequence...** to preview the Sequence
- 5 Save the sequence.

#### HINT

The sequence can be edited as long as its status is **Pending** in the queue.

- 6 Click **Save and Add to Queue** to submit the Sequence to the Sequence Queue.

### To import Sample Data

Sample data set can be imported into **Easy Sequence**. Before importing samples, the CSV file must be set up and formatted properly. Refer to online help for more information on how to create a CSV sample data file.

- 1 From the **Easy Sequence** tab, open a template by clicking the **Load Easy Sequence Setup** icon.
- 2 Click **Import Samples...**
- 3 Select the CSV file you want to import.  
All valid fields are imported.

#### NOTE

To import sample data to the **Back Sample List**, make sure that the **Back Sample List** is selected and displaying before pressing the **Import Samples** button.

- 4 Verify the fields by reviewing the Sample List.

## Using Easy Sequence Setup Tab (Template)

**Easy Sequence Setup** is used to create templates which are the starting point for creating sequences. There are two panels: Samples and Calibration. The **Samples** panel specifies the method, sample, data, and sequence information. The template is also used to specify what parameters are hidden or read-only. The **Calibration** panel provides a graphical interface to configure and view calibration runs. It provides an easy-to-use drag and drop interface to specify calibration types, cyclic and bracketed, and sample positions.

### Creating an Easy Sequence template:

- 1 From the **Easy Sequence Setup** tab, select the **Samples** panel. Open an existing template or create a new template.
- 2 Select the **Method**. Dual injection options will be shown if the method's injection source is Dual. A back analysis method can be specified for the back signal. The method is the only parameter required for a template.
- 3 If desired, enter the estimated duration (in minutes) of a sample run. This is the time measured from when a sample starts to when the next sample starts. This parameter is used to estimate the total expected duration of your sequence. Leave this field blank if you do not want to use the Estimated Cycle Time feature.
- 4 Specify the **Starting Vial Location**, **Number of Samples**, and the **Sample Name**.
- 5 Select the **Data Location**
- 6 Select the **Sequence Location** and specify the **Sequence Name**.
- 7 Enter any comments for the template.
- 8 Specify which parameters are hidden or read-only. Enter a default value for **injections/vial**, **sample amount**, **ISTD amount**, **injection volume**, etc. This helps to minimize the chance for errors when creating a sequence in the **Easy Sequence** Tab.
- 9 Save the template.

**To define Calibrations:****Prerequisites**

The method used in the template should have been calibrated to the necessary levels.

- 1 From the **Easy Sequence Setup** tab, select the **Calibration** panel
- 2 Select **Cyclic**, **Bracketing**, or **Simple Calibration** from the **Calibration Mode** drop down list.
- 3 The **Sequence Diagram** has the following sections:
  - **Sequence Start**
  - **Bracketing/Cyclic**
  - **Samples/Injections**
  - **Sequence End**
- 4 In the **Samples** area for the Sequence, set the **Calibration Interval** based on number of samples or number of injections.
- 5 Setup the **Sample type**, **Blank**, **Calibrant**, or **QC Sample** by dragging the icon from the **Sample Type** area to the **Sequence Diagram** section.
- 6 Setup the parameters for each Sample type and set to **Hide** or **Read-Only**.
- 7 Verify the calibration mode in the **Easy Sequence** Overview.
- 8 Save the template.



## Working with Sequences (Sequences and Sequence Templates)

Sequences (Sequences and Sequence Templates) are accessed and created from the Sequence menu. Sequences may be created and saved in the same way as methods. When you save a sequence, a file is created with a .S extension. When you want to edit or use the sequence again, you access it by, for example, using the Load Sequence item in the Sequence menu.

### Data Acquisition of Single Runs

For single runs, the data file is saved directly into the respective subdirectory. Since only one method is employed for a single run, this method does not need to be copied into the subdirectory; all actions are performed directly with the master method. After the acquisition part of the method is completed, a copy of the acquisition parameters is saved into the file ACQ.txt. A copy of the data analysis parameters is saved into the data file directory (DA.M) after the data analysis part of the master method has been executed.

### Data Acquisition in a Sequence

In order to run a sequence, appropriate pre-defined methods must be available. These are the master methods as outlined above. Typically, master methods and sequence templates are worked on in the **Method and Run Control** view of ChemStation. For this reason, in **Method and Run Control** view, the ChemStation Explorer provides access to master methods and sequence templates.

The sequence template references these methods in the sequence table.

When you run a sequence with sequence template <sequence\_name>.S in the default execution mode, and use the master method <method\_name>.M, a new folder is created that contains all resulting files from the sequence run ("result set"). The location of this result set folder is determined by the settings in the **Sequence Parameters** dialog box (see [Figure 12](#) on page 82). The name of the result set folder and the execution mode are determined by the settings in the **Preferences** (see "[Preferences - Sequence Tab](#)" on page 113).

At the start of an acquisition sequence, the method specified in the sequence table is copied from the master methods folder into the result set. In addition, a copy of the sequence is created and placed with the sequence log and the batch (\*.b) file in the result set. All updates of the method (for example, updates of the calibration table) are written to this sequence method in the result set. If you use Intelligent Reporting, the report templates you selected in the Sequence Parameters or in the Method Properties are also copied to the result set. All necessary files are now available for future data review and reprocessing, without changes that were applied to the master method or sequence template for other sequence runs.

During acquisition, the data files are stored to the result set. Within each data file (\*.D), a copy of the sequence method is saved for this specific run. The file ACQ.txt contains the acquisition parameters of the sequence method, preserving the state of the method as it was at the time of acquisition of the specific data file. The folder DA.M contains a copy of the data analysis parameters used in the sequence method.

With these files saved in the sequence folder, all data review and reprocess activities can be performed without altering the master method or the sequence template. If needed, method changes can also be saved to the master method again.

**NOTE**

The result set must always contain the complete set of all data files (\*.D). If you delete part of the data files, uploading the result set to central data storage will cause problems. If you need to shorten a sequence, create a self-assembled result set from the reduced set of sequence lines (see ["Creating a Self-Assembled Result Set"](#) on page 108).

## Automatic Update of Master Methods

These functions allow you to select if and when to update the master methods used in the sequence. This ensures that, for example, the calibration table is kept up to date.

You can activate the functions in the **Sequence Parameters** dialog (see figure below):

- **Update data analysis parameters only:**

Select this check box if you want to update the data analysis parameters of all methods from the result set in the master methods folder at the end of the sequence.

- **Full method update during sequence acquisition (instrument and data analysis parameters):**

Mark this check box if you want to update the master method with changes to the instrument parameters at the end of each run. The data analysis parameters are updated at the same time. If the instrument parameters do not change, the data analysis parameters are updated at the end of the sequence.

The precondition for updating a master method that the corresponding master method (a method with the same name as the sequence method) still exists in the same master methods directory as at the time when it has been copied to the result set.

To change the check box setting and update master methods, you need the privileges **Save method changes** and **Edit sequence summary**. For details on user management and privileges refer to the *OpenLab ChemStation Configuration Guide: User Management and Instrument Configuration* (CDS\_CS\_configure.pdf).

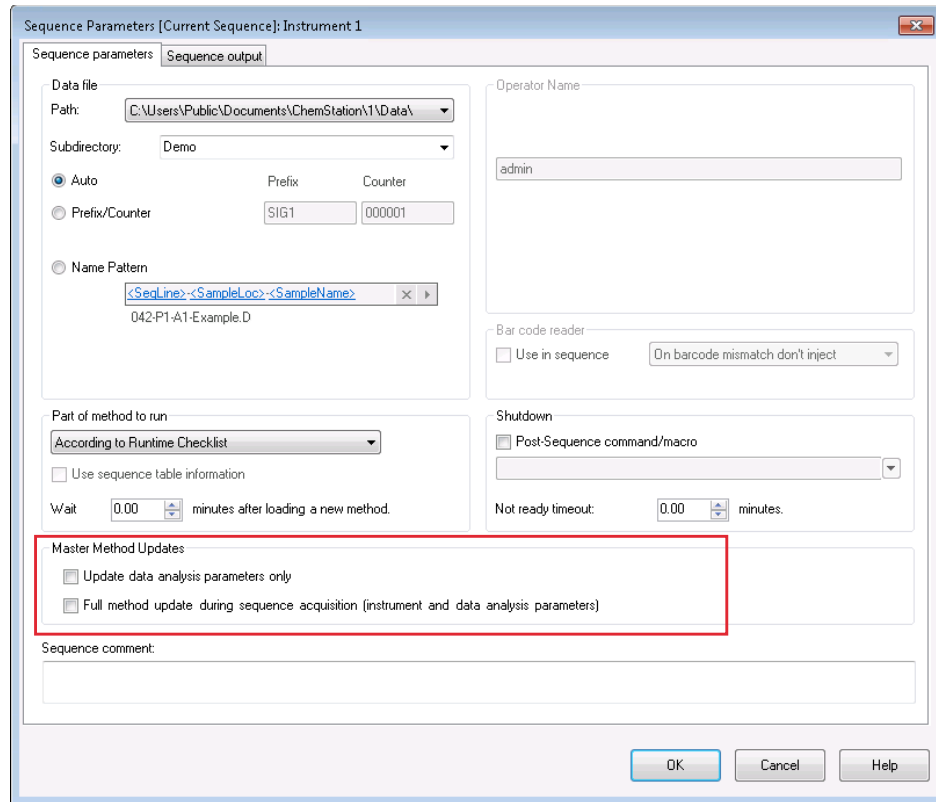


Figure 17 Update master methods option in Sequence Parameters dialog

## NOTE

As this function will cost performance, it is not advised to use it if you have sequences with hundreds of methods.

## Priority Samples

A currently running sequence can be paused after the current method is completed. The sequence can be paused to allow the analysis of a priority sample by the same or another method. The sequence can then be resumed, where the sequence continues with the sample at which the sequence was paused.

## Sequencing with Control Samples

Control samples can be specified in the Sample Type field of the sequence table. The method used to analyze the control sample must contain a calibration table where control sample limits for one of the compounds are specified. If the control sample limits you specified are exceeded, the sequence is stopped and a message is written into the logbook. If you are using one of the ChemStation report styles, the control sample limits are also printed on the reports generated for these analyses. For more information on how to define a sequence with control samples, see the How To section of the online help.

## Sequencing with Blank Reference Samples

Reference signals are required to evaluate the signal-to-noise ratio as defined by European Pharmacopeia. You can specify the reference data file in the sequence table by choosing the sample type **Blank** for the corresponding samples.

If you use multiple reference files, the order of the files is essential. ChemStation uses one reference file for all successive runs, until there is new reference file given in the sequence table. The reference file of a blank sample serves as its own reference. The following overview shows an example of a sequence containing two blank samples:

**Table 7** Example for a sequence with blank samples

	Sample	Data file	Reference file
1	Sample1	DF01.D	
2	<i>Blank1</i>	<i>DF02.D</i>	<i>DF02.D</i>
3	Sample2	DF03.D	<i>DF02.D</i>
4	Sample3	DF04.D	<i>DF02.D</i>
5	<i>Blank2</i>	<i>DF05.D</i>	<i>DF05.D</i>
6	Sample4	DF06.D	<i>DF05.D</i>
7	Sample5	DF07.D	<i>DF05.D</i>

Please refer to the Reference Guide for details on the calculation of the signal-to-noise ratio.

## Running a Sequence

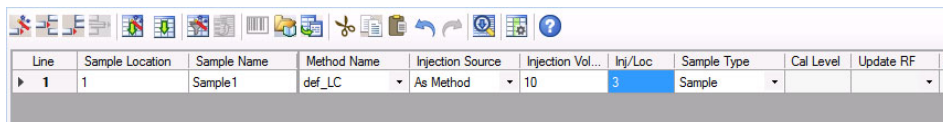
As soon as you submit a sequence to the queue, the sequence table changes to a run-by-run list. It shows the sequence exactly as it will be executed, with all repeat calibrations, QC samples and blanks included in the correct order. The generated sequence file will be stored in the result set.

Sequence lines that have already been acquired or are currently being acquired are locked. They cannot be edited anymore. With specific workflows, for example if you use a Headspace instrument or you configured Overlap injections, several pending runs are locked in addition.

### NOTE

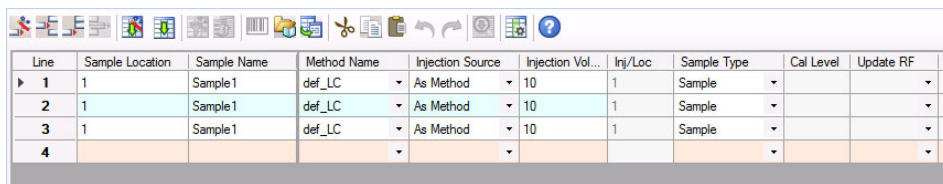
If you add sequence lines while a sequence is already under acquisition, the corresponding data file names depend on the naming scheme you selected in the Sequence Parameters. With the **Name Pattern** naming schema, the data file name is resolved at the moment the run starts, using the given tokens.

Example: Sequence With Multiple Injections



Line	Sample Location	Sample Name	Method Name	Injection Source	Injection Vol...	Inj/Loc	Sample Type	Cal Level	Update RF	
1	1	Sample1	def_LC	As Method	10	3	Sample			

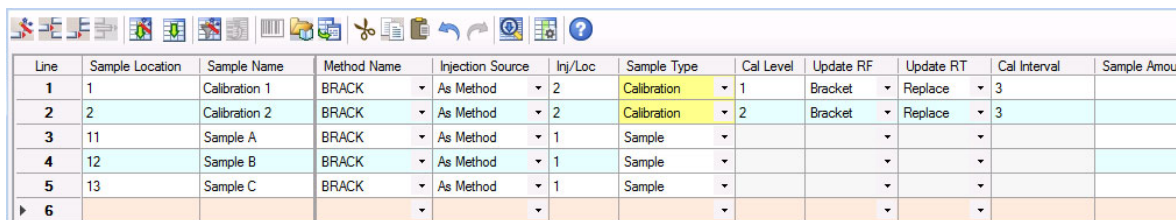
Figure 18 Sequence template before submitting to the queue, sample with 3 injections



Line	Sample Location	Sample Name	Method Name	Injection Source	Injection Vol...	Inj/Loc	Sample Type	Cal Level	Update RF	
1	1	Sample1	def_LC	As Method	10	1	Sample			
2	1	Sample1	def_LC	As Method	10	1	Sample			
3	1	Sample1	def_LC	As Method	10	1	Sample			
4										

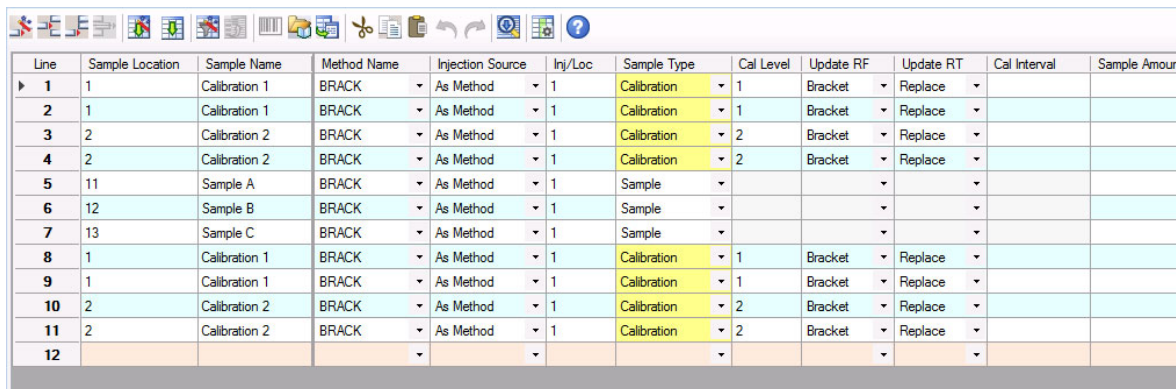
Figure 19 Sequence file after submitting to the queue, 3 separate lines

Example: Sequence With Cyclic Calibration



Line	Sample Location	Sample Name	Method Name	Injection Source	Inj/Loc	Sample Type	Cal Level	Update RF	Update RT	Cal Interval	Sample Amou
1	1	Calibration 1	BRACK	As Method	2	Calibration	1	Bracket	Replace	3	
2	2	Calibration 2	BRACK	As Method	2	Calibration	2	Bracket	Replace	3	
3	11	Sample A	BRACK	As Method	1	Sample					
4	12	Sample B	BRACK	As Method	1	Sample					
5	13	Sample C	BRACK	As Method	1	Sample					
6											

Figure 20 Sequence template before submitting to the queue, cyclic calibration with bracketing



Line	Sample Location	Sample Name	Method Name	Injection Source	Inj/Loc	Sample Type	Cal Level	Update RF	Update RT	Cal Interval	Sample Amount
1	1	Calibration 1	BRACK	As Method	1	Calibration	1	Bracket	Replace		
2	1	Calibration 1	BRACK	As Method	1	Calibration	1	Bracket	Replace		
3	2	Calibration 2	BRACK	As Method	1	Calibration	2	Bracket	Replace		
4	2	Calibration 2	BRACK	As Method	1	Calibration	2	Bracket	Replace		
5	11	Sample A	BRACK	As Method	1	Sample					
6	12	Sample B	BRACK	As Method	1	Sample					
7	13	Sample C	BRACK	As Method	1	Sample					
8	1	Calibration 1	BRACK	As Method	1	Calibration	1	Bracket	Replace		
9	1	Calibration 1	BRACK	As Method	1	Calibration	1	Bracket	Replace		
10	2	Calibration 2	BRACK	As Method	1	Calibration	2	Bracket	Replace		
11	2	Calibration 2	BRACK	As Method	1	Calibration	2	Bracket	Replace		
12											

Figure 21 Sequence file after submitting to the queue, cyclic calibration with bracketing

## Using the High-Throughput Option

Several LC and GC autosamplers offer a *High-Throughput* option to optimize the run time. With this option, the injections of a sequence overlap; the subsequent vial is prefetched and positioned by the sampler while the current acquisition is still running. This can save a considerable amount of time per run.

## Pausing a Sequence

The currently active run will be completed before the sequence pause.

During a sequence pause, the sequence table file name and the data file name cannot be changed. In the sequence table you can only change sequence lines that have not already been executed or change the vial number in the current sequence line. You can add, delete, and change sequence lines for future analyses.

For example, it may be necessary to edit an active sequence to add a new batch of samples. You can edit the sequence so these vials will be the next sample that ChemStation will process after the samples in the currently running sequence line.

## Stopping a Sequence

The currently active run will be terminated immediately. However, the data analysis will still be executed for this run. A stopped sequence can never be resumed.

If you want to finish the current run before stopping the sequence, pause the sequence, wait for the run to be finished, and then stop the sequence.

## Aborting a Sequence

The abort function terminates a currently active sequence immediately. No Data Analysis is executed. The abort function is implemented as an emergency stop and will require a restart of the current session.

## Running a Partial Sequence

### Result Set Selection for Partial Acquisition

You can choose between the following options for a partial sequence acquisition:

- acquire the partial sequence into a new result set

or

- acquire the partial sequence into an already existing result set.

Acquiring the data files from a partial sequence execution into an already existing result set may be useful in the following scenarios:

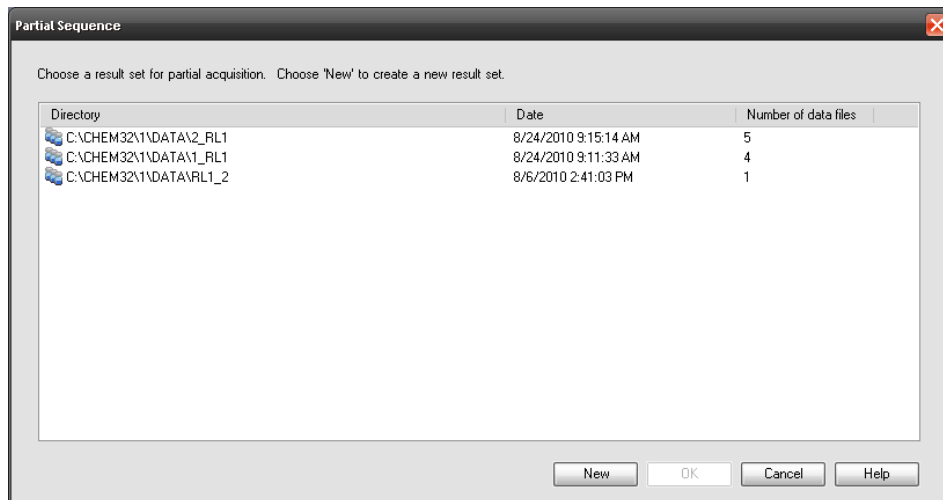
- A single data file (or several data files) has to be overwritten, for example, because an incorrect vial was used in the first place.
- Only the first part of the sequence has been executed in the first place, and the missing samples have to be added by executing partial sequence. This may occur in the case of an instrument failure during sequence acquisition.
- Additional lines have been appended to the sequence template after acquisition of the already existing lines. The additional runs are to be added to the already existing data.



**NOTE**

Deleting lines from or inserting lines into the already acquired part of the sequence template will lead to serious inconsistencies in the naming of data files.

Therefore, when you select **Partial Sequence** from the **Sequence** menu, a dialog will come up providing you the option to either select an existing result set from a list or to create a new result set.



**Figure 22** Partial Sequence dialog

However, in order to maintain consistency of the result set (so it can be completely reprocessed in **Data Analysis**), only those result sets are offered for partial acquisition that fulfill certain conditions:

- The name of the sequence template (source sequence) and the name of the sequence \*.S file in the result set (target sequence) are identical.
- Both the data path and the subdirectory have to be identical for the sequence files.
- The number of sequence lines in the source sequence must be equal or higher than the number of sequence lines in the target sequence.
- For each line in the target sequence the sample type and the number of injections must be identical to the values in the corresponding lines of the source sequence.
- The data file naming scheme must be identical for the two sequence files.

After leaving this dialog with **OK** (for selecting one of the existing result sets) or **New** (for creating a new result set), you can select the sequence lines to be executed during partial sequence.

### Selection of Sequence Lines for Partial Sequence Acquisition

The system displays the **Partial Sequence** dialog box and allows you to select individual samples from the table for analysis.

A single run is shown on each line of the **Partial Sequence** dialog box. For each run, the vial, method, data file, and sample name are given. Additionally, encoded information about the sequence table and any calibration samples is shown in the Seq Tbl and Calib:RF:RT columns. See the online help for an explanation of these codes.

#### NOTE

Partial Sequence populates the data file names at the start of the sequence. As a consequence, the file name tokens DATE and TIME will not produce the accurate date and time of the injections.

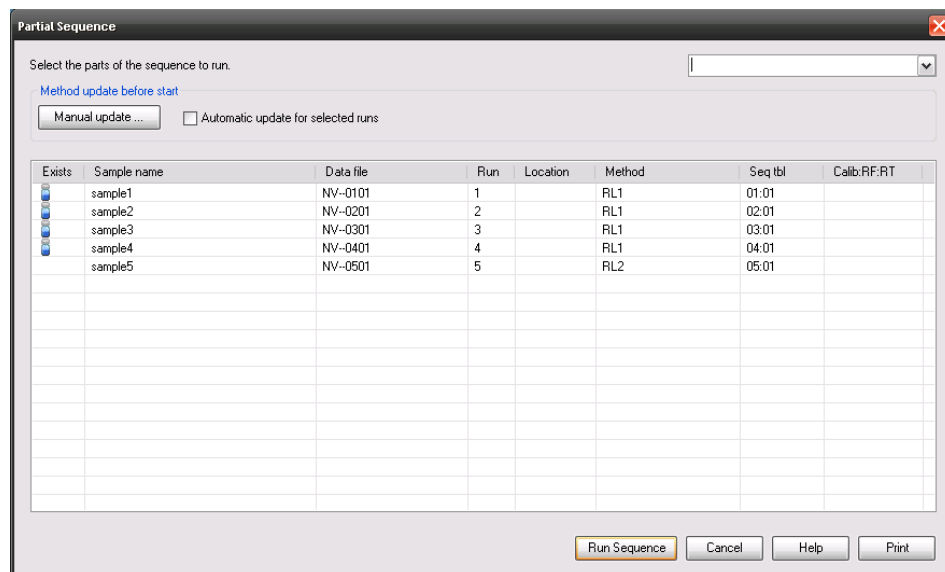
You can obtain a paper copy of the partial sequence by selecting the **Print** button.

With **Manual update ...**, you open the **Update Methods** dialog box, which allows you to manually synchronize the master methods and the methods used in the sequence template. With the **Automatic update for selected runs** option, you can update all sequence methods that are used in the selected runs with their corresponding master methods.

#### NOTE

Both acquisition and data analysis parameters are updated.

For example, the **Partial Sequence** dialog may look like the following. You can mark specific samples for processing.



**Figure 23** Partial Sequence dialog box

A running partial sequence cannot be edited.

The **Partial Sequence** dialog does not support overlapped injections (see “Using the High-Throughput Option” on page 103).


## Creating a Self-Assembled Result Set

Using the **Sequence >Create New Result Set** command in the **Data Analysis** view, you can create a new self-assembled result set from the data currently shown in the Navigation Table. Self-assembled result sets are helpful, for example, in the following scenarios:

- You want to combine single samples, sequences, or a combination of both in order to reprocess them with a specific method.
- You want to shorten a sequence.

### To assemble a new result set

- 1 Add the required data files into the Navigation Table.
- 2 In the Navigation Table, select all the data files that you want to include in your new result set.
- 3 Select **Sequence >Create New Result Set** to open the **Create New Result Set** dialog box.
- 4 Select a method to be associated with the new result set.
- 5 Specify a folder for the new result set.
- 6 Sort the samples.

The names of output data files are automatically updated. If required, you can restore the initial order of the samples using the  (**Restore initial order**) button.

Note that the position of a blank file is relevant for the evaluation of the signal-to-noise ratio as defined by European Pharmacopeia. See also ["Sequencing with Blank Reference Samples"](#) on page 101.

- 7 Confirm the settings to assemble the list of data files into a result set in the specified folder.

## Sequence Log File

A sequence log file is produced that indicates what has happened during the running of the sequence. It is useful for identifying when errors occurred if the sequence is running unattended or overnight. The name of the logbook file always has the .log extension. The logbook file is located in the directory where the data of the sequence is stored.

## What Happens When a Sequence is Run?

### Starting a Sequence

When operating in the default sequence execution mode, the system creates a result set based on the path definition in the sequence parameters and the sequence preference settings. The sequence template \*.s, all methods defined in the sequence table belonging to this particular sequence are copied to the result set. If you use Intelligent Reporting, all report templates \*.rdl that are defined in the method or in the sequence template are also copied to the result set. The system continues to work with these files during acquisition. Starting the sequence, the method of the corresponding sequence line is loaded within ChemStation from this result set.

For details on the execution modes, see [“Sequence Execution Mode”](#) on page 115.

### Further Executed Steps During Sequence Execution:

The following steps will be repeated for each executed sequence line:

- If equipped with an autosampler, the ChemStation software first locates the sample in the autosampler according to the number entered in the vial column
- The instrument is loaded with the method parameters.
- The pre-run macro is executed.
- The sample is then injected into the instrument (manually or automatically).
- The data is acquired.
- The method data evaluation is done. Integration, quantification, and reporting, including any user specified macro. The system stores an additional methods DA.M during the run.
- The post-run macro is executed.
- During the entire process, ChemStation tracks the sequence's progress in real time and produces a sequence log file.

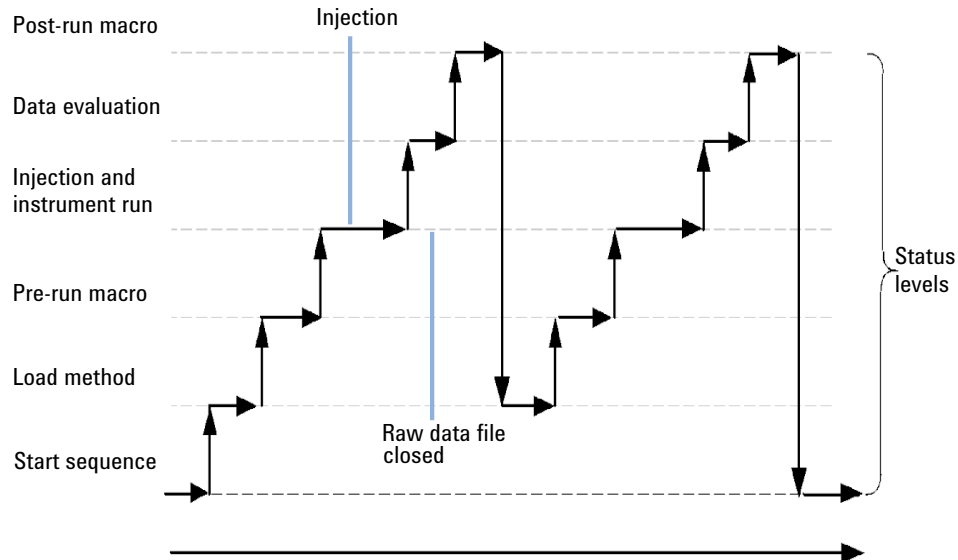
**ChemStation status**

Figure 24 Sequence Status

## Sequence Data File Structure

### Data File Structure

There is a strong link between the raw data, the method, and the result set. The result set folder contains all data files (\*.D) acquired within a sequence.

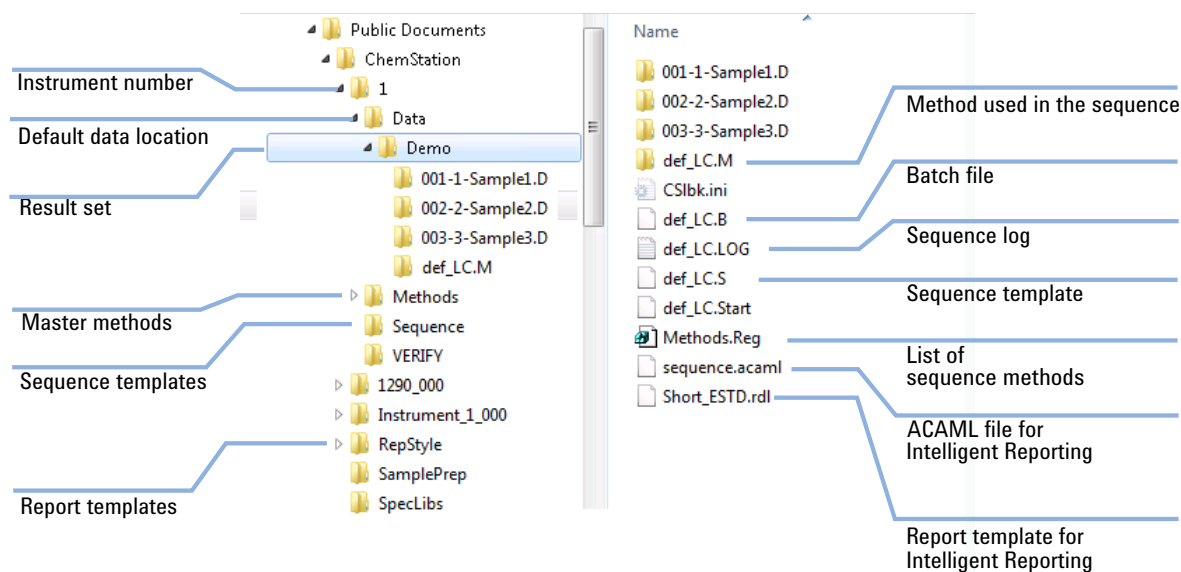


Figure 25 Sequence Data File Structure

#### NOTE

The result set must always contain the complete set of all data files (\*.D). If you delete part of the data files, uploading the result set to central data storage will cause problems. If you need to shorten a sequence, create a self-assembled result set from the reduced set of sequence lines (see ["Creating a Self-Assembled Result Set"](#) on page 108).

Each data file, whether acquired within a sequence or as a single run, has a link to the method that was used for data analysis.



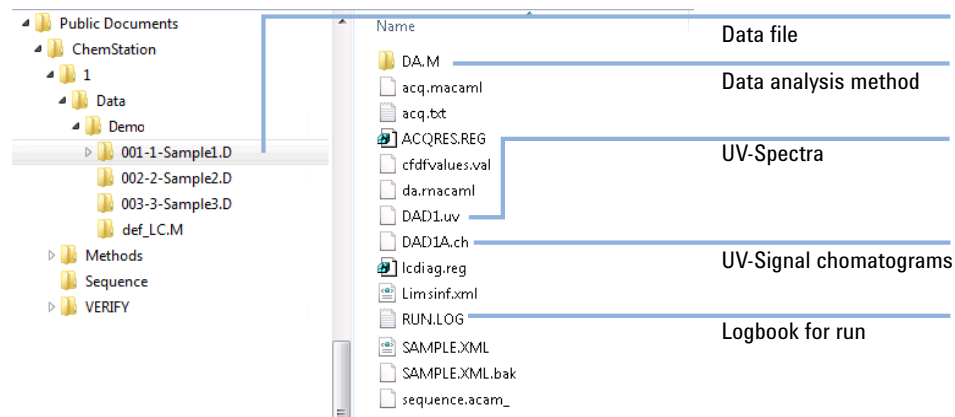


Figure 26 Data file content

## Preferences - Sequence Tab

In the **Preferences** dialog/**Sequence** tab, you define which folders and files shall be created during sequence runs.

The sequence data are stored in a result set using a unique result set name. You can specify the naming conventions (Name Pattern) for these result sets in the **Sequence** tab of the **Preferences** dialog box. If no name pattern is specified, a default sequence name pattern is used. The **Sequence** Tab is used only for data acquisition and therefore is present only for online systems.

The sequence name pattern can contain various sections. The system creates a name for your result set that is determined by the sequence name pattern sections you select. All data files, methods, the sequence logbook, the <sequence\_name>.s file and the <sequence\_name>.b file belonging to this particular sequence are stored in the result set. The result set is created when the sequence is started.

The sequence (\*.s) files are used as sequence templates, and this concept allows you to run any sequence file multiple times without overwriting existing data or changing the sequence parameters. If neither counter nor time is used in the sequence name pattern, the system introduces a counter automatically to avoid overwriting data. For the second, third and all subsequent sequences using the same sequence template, a counter is added to the result set name.

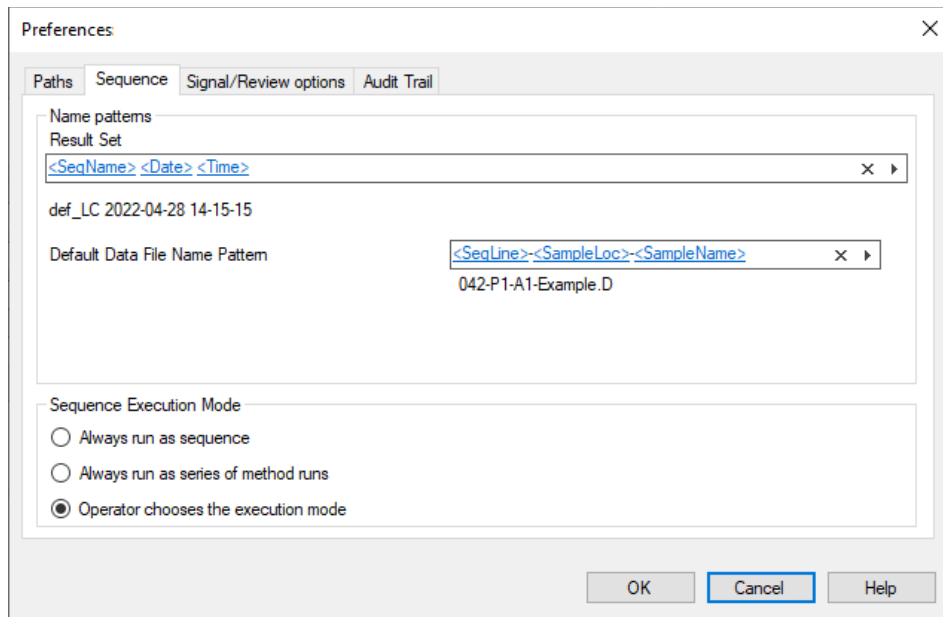


Figure 27 Preferences Dialog / Sequence Tab

## Result Set Naming

You define the name pattern of the result set folder in the **Result Set** field (see [Figure 27](#) on page 114). By default, the name is <SeqName> <Date> <Time>, but it can be configured by using tokens, or you can manually enter any name. For more information on using tokens, see [“File Names and Tokens”](#) on page 13. For the result set folder, you can use the following tokens:

- **Current date**
- **Current time**
- **User name**
- **Instrument name**
- **Sequence name**
- **Counter**
- **Computer name**

If the name pattern would not result in unique names for the result sets, ChemStation will append a counter to ensure uniqueness.

The location of the result set folder is determined by the settings in the **Sequence Parameters** dialog box (see [“Sequence Parameters”](#) on page 82).

## Default Data File Name Pattern

In the **Preferences** dialog, you define a default name pattern for data files that are created during sequence execution. This setting serves as a default value for the **Sequence Parameters** dialog (see “[Sequence Parameters](#)” on page 82). In the **Sequence Parameters** dialog, you define the actual way how data file names are created.

## Sequence Execution Mode

If you run a sequence, all data and related files are available in one single folder. The data is evaluated in the context of the entire sequence. This is required, for example, to run a bracketed calibration, or to create a sequence summary report.

Single runs, however, offer more flexibility in editing the run queue.

ChemStation allows you to run sequences as a *series of single runs*. If you use this function, each line of the rolled-out sequence is added to the run queue as a single sample. In the file system, there will be no result set folder; only the data files (.D) for single runs are generated. The data file names follow the definition that you provided in the **Default Data File Name Pattern** field.

Under **Sequence Execution Mode**, choose one of the following options:

- **Always run as sequence** (default): Running sequences will always generate result set folders.
- **Always run as a series of method runs**: Sequences will always run as a series of single runs. As long as this preference is set, you cannot create any result sets.
- **Operator chooses the execution mode**: Each time you run a sequence, you can choose to either run it **as Sequence** or **as Series of Runs**. All Run or Add to

Queue commands in the ChemStation are extended by a corresponding option. See the following examples:

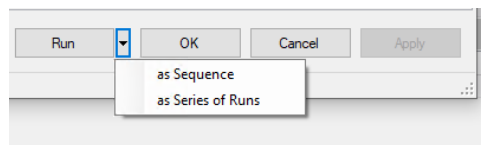


Figure 28 Run options in the sequence table

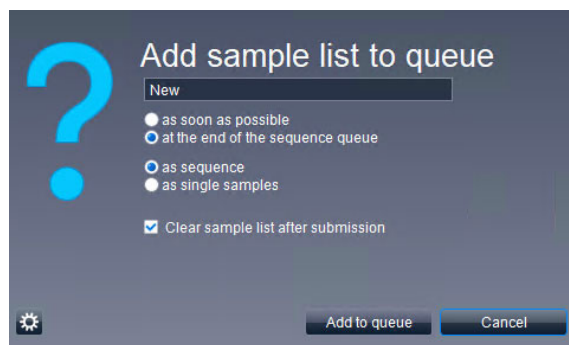


Figure 29 Queue options in the Sample Entry tab

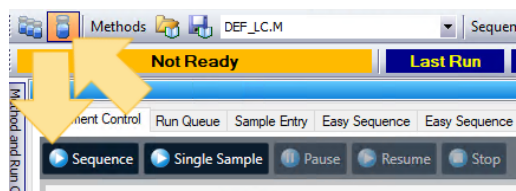


Figure 30 Sequence button in the Single Sample display to run a sequence as series of single runs

## Data File Naming

### Data File Naming in a Sequence

To define the names of the data files in a sequence, configure the sequence parameters (see “[Sequence Parameters](#)” on page 82).

Choose between the following options:

- automatic,
- manually,
- using a prefix/counter, or
- using a name pattern.

### Automatic Data File Naming in a Sequence

#### Sample Vials in Vial Trays

For example 017-0103.D

where:

- The first three digits are the vial number, for example, 017.
- The fourth digit in liquid chromatography and capillary electrophoresis is a separation hyphen (-); in gas chromatography, this will be either (F) for front or (B) for back.
- The fifth and sixth digits are the sequence line that defines the method used, for example, 01 for the first sequence line.
- The seventh and eighth digits are the injection number for this vial by the method, for example, 03 for the third injection.

#### Samples in Multisampler

For example D1F-A3-0201.D

where:

- D1F: position (here: front) of sample container in drawer (here: D1)
- A3: position of sample in sample container
- 0201: sequence line 2, first injection

### Blank Runs

For example NV--0499.D

where:

- NV stands for no vial.
- - is a separation hyphen.
- 0499 is the 99<sup>th</sup> blank run of sequence line 4.

### Entering Data File Names Manually

One of the columns in the sequence table is named **Datafile**. When it contains no entry, the data file naming scheme specified in the Sequence Parameters (automatic, prefix-counter, or name pattern) is used to create the data file name. If any text is entered into the **Datafile** column, ChemStation uses that text as the data file name for the run.

If more than one injection per vial is specified on a line with a manual data file name, ChemStation automatically truncates characters from the end of the name entered by the user and appends the injection number. This prevents the same data file name from being reused for multiple injections.

### Using a Prefix/Counter to Name Data Files

If you use the Prefix/Counter to name data files, ChemStation generates a name for each analysis. For an instrument that supports dual signal analysis such as the GC, ChemStation will generate a name for each signal.

The sequence set up allows long filenames for the prefix/counter. The data file name defined by prefix/counter can have up to fifteen characters plus .d extension, so in total seventeen characters.

Following rules apply to the prefix/counter field:

- the counter itself can have a maximum up to 6 characters
- if a prefix provides less than nine characters for prefix, the counter is automatically extended to 6 digits
- the number given in the counter is the start number being incremented

Table 8 File names

Prefix	Counter	Results in file name
long	000001	long000001
longname	000001	longname000001
testwithalongna	1	testwithalongna1

## Using a Name Pattern to Name Data Files

You can use the following tokens to create the data file names for each sequence line:

**Sample Name** The information that has been barcoded or typed into the **Sample Name** field.

### NOTE

The barcode will not be visible in the data file name. The barcode is evaluated at a point in time where the data file path and name have already been resolved.

**Sample Type** The type of sample: QC sample, calibration, sample.

**Sample Location** The vial or wellplate location of the sample.

**Method** The name of the method used for the sequence line.

**Sequence Line** The current line number of the rolled-out sequence.

**Replicate Number** The number of the injection from this vial.

**Date** The date stamp at the start of acquisition of the sample.

**Time** The time stamp at the start of acquisition of the sample.

If your instrument supports different injection locations (GC with back and front injector, for example), you can provide different patterns for each location. For example, use a prefix with an indication of the injection location:

- *F-<Sequence Line>-<Sample Location>-<Sample Name>* for front injections, and
- *B-<Sequence Line>-<Sample Location>- <Sample Name>* for back injections.

### NOTE

The data file names are not resolved until the run starts; therefore, the sequence table does not contain any data file names.

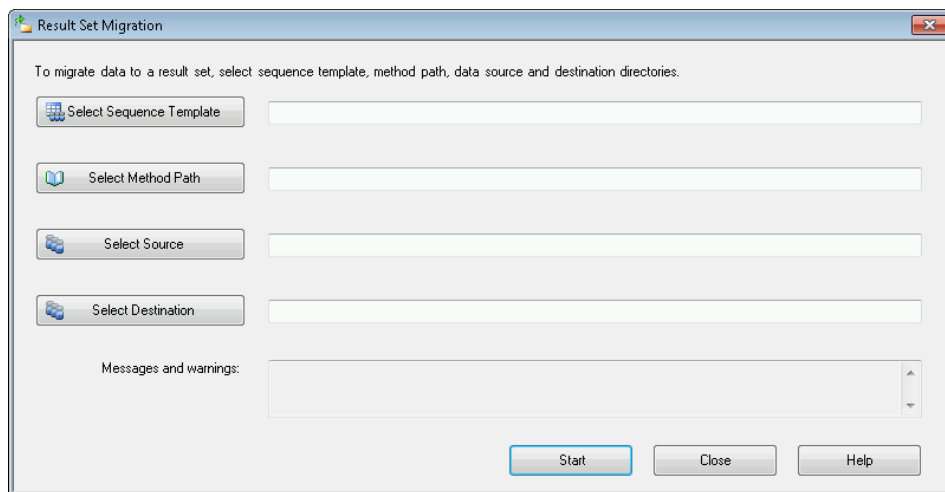
The resolved data file names are limited to 40 characters; longer file names are truncated. If a resolved file name is not unique, a counter is appended.

## Result Set Migration

ChemStation provides a tool to migrate non-result set data to result set format. To successfully perform this task, it is required that the original sequence file is still available. It must contain all the necessary sequence lines and follow the original data file naming scheme to reprocess all the data files of the sequence. In addition, all the methods in the Method column of the sequence table have to be available.

To perform migration, start the **Result Set Migration** from the **Sequence** menu in **Data Analysis** view.

Result Set Migration is not supported for data from sequences that has been run as a series of single method runs (see [“Sequence Execution Mode”](#) on page 115).



**Figure 31** Result Set Migration

Fill in the following required fields:

**Select Sequence Template:** Select the sequence file (\*.S) that contains the sequence table that matches the data set to be migrated.

**Select Method Path:** Select the directory where the methods are located that are referenced in the sequence table.



**Select Source:** Select the directory that contains the data files to be migrated.

**Select Destination:** Specify the path and name of the result set to be created. You may select an existing folder or create a new one.

When all fields are filled in, the migration can be started.

The following steps will be performed:

- The result set directory will be created.
- The sequence template will be copied to the result set. It will also be converted to a state where it is able to reprocess data files in **Data Analysis** view.
- The methods referenced in the sequence table are copied from the specified method path to the result set folder.
- The data files, the sequence logbook, and the batch file are copied from the data source directory to the destination directory.
- According to the information in the sequence table, a copy of the corresponding method is copied to each data file as DA.M.

When the result set migration is completed, a success message is displayed in the **Messages and warnings** field. Otherwise a warning message indicates any problem during migration. Details about the warning can be obtained by double-clicking the warning message.

## Postsequence Operation

You can specify what happens after a sequence has finished during normal execution or when ChemStation encounters an error during sequence operation. This is done by activating the **Post-Sequence command/macro** check box of the Sequence Parameter section **Shutdown**. You have a selection of built-in commands configured for certain instrument types, for example:

- Setting the system to a STANDBY state where all lamps, pumps, thermostat, and sample cooler are off,
- Setting the system to a LAMPOFF state where all lamps are off,
- Setting the system to a PUMPOFF state where all pumps are off, or
- Using a default SHUTDOWN macro or modifying SHUTDOWN.MAC to determine specific operation.

For example, you may want to switch off your system after your sequence has completed. Other uses of the shutdown macro could be to set your flow to zero or slowly reduce your flow. The unmodified SHUTDOWN macro will execute the STANDBY command.

For more information about available built-in commands, see "commands" in the ChemStation online help.

In the **Shutdown** Sequence Parameter section, you may specify a custom command or macro. For more information about custom commands and how to set them up, see ["Using Custom Commands or Macros in ChemStation"](#) on page 26.

## Not Ready Timeout (LC and CE only)

The Not Ready Timeout in the Sequence Parameters is the length of time the system will wait for the instrument to become ready – after this time the system will shut down.

## Wait Time (LC and CE only)

Sequence Parameters allows you to specify a wait time which is executed after loading method and before injecting with that method. This can be useful for column/capillary re-equilibration when using new analysis conditions.

## Automatic Recalibration

Calibration is often done after a change in operating conditions, for example, after changing a column or capillary. Automatic recalibration is usually done at the start of a sequence of analyses or at regular intervals during a sequence as part of a program to compensate for factors that affect the analytical performance.

While performing a recalibration, the calibration table of the used method is updated according to the defined method settings. The recalibrated methods are available within the result set. The calibration table of the sequence method is updated during that process. In addition, the DA.M method of the individual data files contains the updated calibration used for result creation.

There are two ways to specify automatic sequence recalibration:

- explicit calibration sequences, or
- cyclic calibration sequences.

It is also possible to update the calibration table of master methods when running single samples or series of single samples.

## Specifying Recalibrations

The recalibration parameters for the sequence are entered directly into the sequence table. These parameters define how the method is recalibrated during a sequence.

### Recalibration Parameters in the Sequence Table and Sample Info Dialog

The response factor (RF) and retention/migration times (RT) can be updated in several ways. The calibration level, update response factor and update retention/migration times are instructions used in the data analysis when recalibrating the calibration table.

When Calibration is entered in the SampleType column of the sample table, the following columns become active and can be edited:

- Cal Level
- Update RT
- Update RF
- Interval

The values that can be entered into each of these columns are shown in the table.

**Table 9** Recalibration Parameters in Sequence Table

CAL Level	Update RT	Update RF	Interval
Calibration table Level # (1-999)	No update	No update	Cyclic recalibration interval # (1-999)
	Average	Average	Blank
	Replace	Replace	
		Bracket	
		Delta%	

The table shows the columns in the sequence table that contain the recalibration parameters and the values that can be entered. The same parameters can be entered into the Sample Info dialog when submitting a single method run, or when modifying single method runs pending in the run queue.

#### No Update

Does not change the response factor or retention/migration time.

#### Replace

Replaces the previous retention/migration times and the response (areas or heights) with those from the current run only. The response is not changed for any peak that is not found in this recalibration run.

#### Average

Averages the retention/migration times and responses (areas or heights) for each peak based on the original calibration run and all averaged recalibrations since then. If a peak is missing in one of the recalibrations, the average response of the peak will not suffer.

#### Bracket

The samples are bracketed by pre-sample and post-sample calibrations. Evaluation is done when the last calibration sample of the closing bracket has been run. The existing calibration data is replaced by the result data of the calibration run of the opening bracket. The closing bracket calibrations are averaged to that calibration table.

#### Interval

The Interval determines how often a calibration is done during a sequence. Calibration frequency corresponds to the number of sample injections that are done before the next set of calibration injections takes place. At the start of the analysis, a calibration is done and the results (response factors) are entered into the calibration table. These results are then used in subsequent quantitative calculations. After the specified number of injections have been done, another calibration is made and the results are entered into the calibration table overwriting the results of the previous calibration run.

### Delta%

The delta% calculation allows you to compare response factors from an analysis with response factors entered manually into a calibration table. The delta% is then applied to all of the calibrated peaks in the table. You can identify several internal standards, and their measured response factors are then used to calculate new response factors for the other peaks. You identify which internal standard is to be used for the delta% calculation for each peak in the calibration table.

## Types of Sequences

When preparing a sequence, you can use the following types of sequences:

- explicit calibration sequences,
- explicit single-level calibration sequences,
- cyclic multiple-level calibration sequences,
- explicit and cyclic calibrations together in a sequence, and
- cyclic calibration sequences with bracketed calibrations.

### NOTE

After submitting the sequence to the Run Queue, all sequences (including sequences with bracketed calibrations) are transformed to explicit calibration sequences. See [“Running a Sequence”](#) on page 102.

During the run, the sequence table simply shows the injections, run by run, as they are processed by the instrument. If you add a sample during the run, all subsequent samples (including calibration samples) will move downwards in the sequence table.

## Explicit Calibration Sequences

This type of sequence recalibrates at defined intervals specified by you in the sequence table.

For explicit calibration sequences, the calibration samples are entered in the sequence without an interval entry in the sequence table. A recalibration is done once for each calibration sample entry in the sequence table.

## Cyclic Single-Level Calibration Sequences

This type of sequence uses the same vial, that is, the calibration sample at regular intervals in the sequence.

The interval entry in the sequence table determines how the recalibration is done. For example, an interval value of 2 will recalibrate after every two sample vials in the sequence.



## Cyclic Multiple-Level Calibration Sequences

This type of sequence uses different calibration samples to recalibrate a multiple-level calibrated method.

The following example describes a two-method sequence comprising method A and method B to analyze two groups of samples. Both methods are multiple-level calibration methods that will recalibrate automatically at defined intervals.

For each method the Sequence Table has three entries:

- Two calibration levels:
  - Sequence lines 1 and 2 in method A.
  - Sequence lines 8 and 9 in method B.
- Five entries for the samples:
  - Sequence line 3 through 7 in method A.
  - Sequence line 10 through 14 for method B.

The calibrations are specified at regular intervals by the recalibration interval entry in the Sequence Recalibration Table.

- Method A will recalibrate after every two samples.
- Method B will recalibrate after every three samples.

The Sequence Table below is truncated to simplify the example.

**Table 10** Sequence Table for Method A and Method B

Line	Sample Location	Method Name	Inj/Loc	Sample Type	Cal Level	Update RF	Update RT	Cal Interval
1	1	Method A	1	Calibration	1	Average	No update	2
2	2	Method A	1	Calibration	2	Average	No update	2
3	10	Method A	1					
4	11	Method A	1					
5	12	Method A	1					
6	13	Method A	1					
7	14	Method A	1					
8	3	Method B	1	Calibration	1	Average	No update	3
9	5	Method B	2	Calibration	2	Average	No update	3
10	20	Method B	1					

Table 10 Sequence Table for Method A and Method B

Line	Sample Location	Method Name	Inj/Loc	Sample Type	Cal Level	Update RF	Update RT	Cal Interval
11	21	Method B	1					
12	22	Method B	1					
13	23	Method B	1					
14	24	Method B	1					

### Method A Analysis Order

Method A is the first part of the two-method sequence.

Table 11 Method A Analysis Order

Inj No.	Method	Vial	Operation
1	Method A	1	Calibration level 1 and report
2	Method A	2	Calibration level 2 and report
3	Method A	10	Sample analysis and report
4	Method A	11	Sample analysis and report
5	Method A	1	Calibration level 1 and report
6	Method A	2	Calibration level 2 and report
7	Method A	12	Sample analysis and report
8	Method A	13	Sample analysis and report
9	Method A	1	Calibration level 1 and report
10	Method A	2	Calibration level 2 and report
11	Method A	14	Sample analysis and report

## Method B Analysis Order

Method B is the second part of the two-method sequence. Method B differs from Method A in that there are two injections per vial for calibration level 2. The Interval entry is set to 3.

**Table 12** Method B Analysis Order

Inj No.	Method	Vial	Operation
12	Method B	3	Calibration level 1 and report
13	Method B	5	Calibration level 2 and report
14	Method B	5	Calibration level 2 and report
15	Method B	20	Sample analysis and report
16	Method B	21	Sample analysis and report
17	Method B	22	Sample analysis and report
18	Method B	3	Calibration level 1 and report
19	Method B	5	Calibration level 2 and report
20	Method B	5	Calibration level 2 and report
21	Method B	23	Sample analysis and report
22	Method B	24	Sample analysis and report

Note that the results shown in [Table 11](#) on page 130 and [Table 12](#) on page 131 can be obtained by using the Preview button in the Sequence Table.

## Explicit and Cyclic Calibrations Together

This type of sequence comprises explicit and cyclic calibrations in the same sequence.

This feature allows you to recalibrate the method completely at the beginning of a sequence (*explicit recalibration*) and then update the calibration (*cyclic recalibration*) during the sequence.

- Two calibration lines for each calibration level in the Sequence table must be specified. One calibration line is for the explicit recalibration entry and the other for the cyclic recalibration entry.
- The sequence table *must* have entries for each calibration line and all cyclic recalibration vials *must* appear before both the explicit recalibration and sample entries.

### Example

The sequence table below illustrates a single-level calibrated method called SimpReg. It is truncated to simplify the example.

**Table 13** Sequence Table for SIMPREG

Line	Sample Location	Method Name	Inj/Loc	Sample Type	Cal Level	Update RF	Update RT	Cal Interval
1	1	SimpReg	1	Calibration	1	Average	Average	3
2	1	SimpReg	1	Calibration	1	Replace	Replace	
3	2	SimpReg	1					
4	3	SimpReg	1					
5	4	SimpReg	1					
6	5	SimpReg	1					
7	6	SimpReg	1					

There are two entries for the single calibration level.

- The first calibration line is for the same level but averages the calibration parameters. The interval entry specifies that the recalibration is done after every three samples.
- The second entry replaces all the recalibration parameters, that is, a complete recalibration is done. It has *no* recalibration interval.

**Sequence Table**

The sequence table comprises seven lines. The first line specifies the cyclic recalibration sample. The second line specifies the explicit recalibration that is done only once at the beginning of the sequence. The third through seventh lines specify the samples to be analyzed.

The order of the entries into the sequence table is very important. All cyclic recalibration vial entries specifying cyclic calibration *must* appear *before* the sample entries or any explicit recalibration entries for the method.

**SimpReg Analysis Order**

The table below describes the analysis order for the SimpReg method.

**Table 14** SimpReg Analysis Order

Seq Line	Inj No.	Method	Vial	Operation
2	1	SimpReg	1	Simple calibration
1	2	SimpReg	1	Regular calibration
3	3	SimpReg	2	Sample analysis
3	4	SimpReg	3	Sample analysis
4	5	SimpReg	4	Sample analysis
5	6	SimpReg	1	Regular calibration
6	7	SimpReg	5	Sample analysis
7	8	SimpReg	6	Sample analysis

## Cyclic Calibration Sequences with Bracketing

In a cyclic calibrated sequence with bracketing, the calibration table used to calculate the unknown quantitative results is generated by averaging the results of the current calibration with those of the previous calibration. This new calibration table is a more accurate representation of the instrument response at the time the sample was analyzed.

### Example

Consider the following situation:

- The instrument response is drifting.
- Three injections of an identical two-component mixture are specified.
- Two injections are specified as calibration samples, and one is specified as a sample.
- The first and third are calibration samples.
- The second injection is a sample.

To obtain a precise quantitative result for injection two (the sample), an interpolation must be made between the two calibration samples; see the figure. This process is known as bracketing.

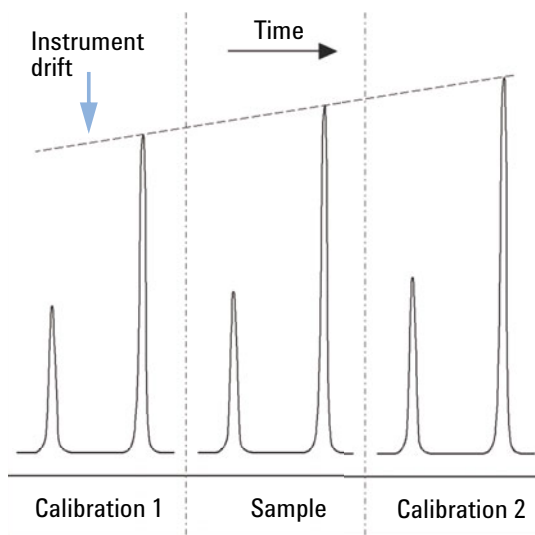


Figure 32 Bracketing

### Bracketed Sequence Operation

- The first calibration vials are analyzed.
- The sample vials are analyzed.
- The next calibration vials are analyzed.
- The calibration table is produced by replacing the existing response factors by new ones and averaging the following calibration runs into a new calibration table.
- The sample vial data files are evaluated, and reports are generated.
- The sequence returns to step 2 if there are more sample vials to be analyzed.

### Example

This section describes a sequence bracketing example comprising one method called Brack.M. The Brack.M method is a two-level internal standard method using cyclic calibration.

#### Sequence Table

The sequence table of Brack.M (next page) is truncated to simplify the example. It consists of seven lines. The first two lines define the recalibration conditions for each level. The remaining lines define the samples to be analyzed.

More specifically, the sequence table of Brack.M method has:

- A Bracket entry in the Update Response Factor column that specifies bracketing of samples with calibration samples.
- A Replace entry in the Update Retention/Migration Times column which specifies a replacement of the retention/migration times.
- An entry of 3 in the Recalib Interval column that specifies recalibration after every three samples.

Table 15 Sequence Table for BRACK-M

Line	Sample Location	Method Name	Inj/Loc	Sample Type	Cal Level	Update RF	Update RT	Cal Interval
1	1	BRACK-M	2	Calibration	1	Bracket	Replace	3
2	2	BRACK-M	2	Calibration	2	Bracket	Replace	3
3	10	BRACK-M	1					
4	11	BRACK-M	1					
5	12	BRACK-M	1					
6	13	BRACK-M	1					
7	14	BRACK-M	1					



Run No.	Method Name	Vial No.	Inj No.	DataFile Name	Lvl No.	Upd RF	Upd Ret	Operation
1	Brack.M	1	1	c1-03001.d	1	R	R	Report for Calibration Run No.1
2	Brack.M	1	2	c1-03002.d	1	A	R	Report for Calibration Run No.2
3	Brack.M	2	1	c2-03001.d	2	R	R	Report for Calibration Run No.3
4	Brack.M	2	2	c2-03002.d	2	A	R	Report for Calibration Run No.4
5	Brack.M	10	1	010-0301.d				Print Calibration Table
6	Brack.M	11	1	011-0301.d				Sample Analysis, no report
7	Brack.M	12	1	012-0301.d				Sample Analysis, no report
8	Brack.M	1	1	c1-03003.d	1	A	R	Calibration Analysis, no report
9	Brack.M	1	2	c1-03004.d	1	A	R	Calibration Analysis, no report
10	Brack.M	2	1	c2-03003.d	2	A	R	Calibration Analysis, no report
11	Brack.M	2	2	c2-03004.d	2	A	R	Calibration Analysis, no report
				010-0301.d				Print Calibration Table
				011-0301.d				Report for Sample Run No.5
				012-0301.d				Report for Sample Run No.6
				c1-03003.d	1	R		Report for Sample Run No.7
				c1-03004.d	1	A		Report for Calibration Run No.8
				c2-03003.d	2	R		Report for Calibration Run No.9
				c2-03004.d	2	A		Report for Calibration Run No.10
12	Brack.M	13	1	013-0301.d				Report for Calibration Run No.11
13	Brack.M	14	1	014-0301.d				Sample Analysis, no report
14	Brack.M	1	1	c1-03005.d	1	A	R	Sample Analysis, no report
15	Brack.M	1	2	c1-03006.d	1	A	R	Calibration Analysis, no report
16	Brack.M	2	1	c2-03005.d	2	A	R	Calibration Analysis, no report
17	Brack.M	2	2	c2-03006.d	2	A	R	Calibration Analysis, no report
				013-0301.d				Print Calibration Table
				014-0301.d				Report for Sample Run No.12
				c1-03005.d	1	R		Report for Sample Run No.13
				c1-03006.d	1	A		Report for Calibration Run No.14
				c2-03005.d	2	R		Report for Calibration Run No.15
				c2-03006.d	2	A		Report for Calibration Run No.16
								Report for Calibration Run No.17

Where A = average

R = replace

Figure 33 Bracketed Sequence Analysis Order

## Cyclic Recalibration Sequences with Multiple Vials Containing the Same Dilution of a Standard

### Cyclic Recalibration Sequence with “Round-Robin” Calibration Vial Usage

When running a large sequence that performs cyclic recalibrations, that is, performs an automatic recalibration after a fixed number of sample injections, there is a potential risk of emptying the volume of calibration vial during the course of the sequence. The ChemStation sequence table provides a means of using a series of vials that contain the same dilution of a standard to be used in a *round-robin* fashion.

With this capability, large sequences can be defined with automatic recalibrations at fixed intervals using multiple calibration vials for each level and each calibration vial would be consumed to the same extent.

By defining an appropriate number of calibration vials, it is even possible to guarantee that each calibration vial is only used once. This is an important requirement in cases where a fresh calibration vial is required for every recalibration, for example, because the analyte evaporates once the septum is punctured or starts degrading after getting in contact with the steel needle. The following section describes how the ChemStation sequence table needs to be set up to fulfill these requirements.

Determine the total number of calibration vials for each level based on the estimated calibrant usage throughout the sequence.

Set up a separate cyclic recalibration line for each calibration vial. Lines defined for the same calibration level must be in adjacent sequence lines and the defined vial positions must be adjacent, too. Choose an identical recalibration interval for all calibration lines. For example, if your sequence should recalibrate after every 6 sample injections, set the recalibration interval to 6.

**Table 16** Cyclic Recalibration Sequence with 3 Vials Defined for Each Level

Vial No.	Sample Name	Sample Type	Method Name	No. of Inj.	Lvl	Upd RT	Upd RF	Interval
1	Cal1a	Calib	MethodA	1	1	Avg	Avg	6
2	Cal1b	Calib	MethodA	1	1	Avg	Avg	6
3	Cal1c	Calib	MethodA	1	1	Avg	Avg	6
5	Cal2a	Calib	MethodA	1	2	Avg	Avg	6
6	Cal2b	Calib	MethodA	1	2	Avg	Avg	6
7	Cal2c	Calib	MethodA	1	2	Avg	Avg	6
10	Sample10	Sample	MethodA	6				
11	Sample11	Sample	MethodA	6				
12	Sample12	Sample	MethodA	6				
13	Sample13	Sample	MethodA	6				
14	Sample14	Sample	MethodA	6				

The execution order is:

- Vial 1 (Cal1a)
- Vial 5 (Cal2a)
- 6 injections out of vial 10 (Sample10)
- Vial 2 (Cal1b)
- Vial 6 (Cal2b)
- 6 injections out of vial 11 (Sample11)
- Vial 3 (Cal1c)
- Vial 7 (Cal2c)
- 6 injections out of vial 12 (Sample12)
- Vial 1 (Cal1a)
- Vial 5 (Cal2a)
- 6 injections out of vial 13 (Sample13)
- Vial 2 (Cal1b)
- Vial 6 (Cal2b)
- etc.

### Cyclic Recalibrations Where Each Calibration Uses a Different Vial

To ensure that every calibration vial be injected only once, the sequence must define a sufficient number of different calibration vials, so that the *round-robin* order described in the previous example is not applied. For example, if the sequence processes 80 sample vials with recalibrations required after every 10 samples, the sequence table must contain  $80/10 + 1 = 9$  calibration lines for each level.

As in the previous example, the calibration lines must be adjacent sequence lines that reference adjacent vial positions.

### Bracketing Sequence that Uses Different Vials for Opening and Closing Bracket

The same capability is available for bracketing sequences. By defining the appropriate vial range of calibration vials, a bracketing sequence can be defined so that different calibration vials are used for the opening and closing brackets. In this case, too, calibration lines in the sequence must be adjacent just like the vial positions of the calibration vials.

Whether or not the bracketing calibration vials are used in round-robin mode or for one single injection only simply depends on the total number of calibration vials for each level and the number of recalibrations required by the sequence.

The following example defines 3 sample injections that are bracketed by calibrations. The opening bracket uses a different calibration vial than the closing bracket. Recalibrations are required after every sample injection. so the recalibration interval has to be 1. The number of calibration lines per level is the number of samples plus one.

**Table 17** Different Vials Used for Opening and Closing Brackets

Vial No.	Sample Name	Sample Type	Method Name	No. of Inj.	Lvl	Upd RT	Upd RF	Interval
1	Cal1a	Calib	MethodA	1	1	Brkt	Brkt	1
2	Cal1b	Calib	MethodA	1	1	Brkt	Brkt	1
3	Cal1c	Calib	MethodA	1	1	Brkt	Brkt	1
4	Cal1d	Calib	MethodA	1	1	Brkt	Brkt	1
10	Sample10	Sample	MethodA	1				
11	Sample11	Sample	MethodA	1				
12	Sample12	Sample	MethodA	1				

The execution order for this sequence is:

- Vial 1 (Cal1a), Opening Bracket 1
- Vial 10 (Sample10)
- Vial 2 (Cal1b), Closing Bracket 1 and Opening Bracket 2
- Vial 11 (Sample11)
- Vial 3 (Cal1c), Closing Bracket 2 and Opening Bracket 3
- Vial 12 (Sample 12)
- Vial 4 (Cal1d), Closing Bracket 3

# 5

## Run Control

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This chapter explains the concepts of Run Queue and Queue Planner. It explains how to add single samples, sequences, pauses, or commands to the Run Queue. It also describes the Command Scheduler in which you can schedule events to make your everyday lab work easier.

## About the Run Queue

The Run Queue is very useful when numerous samples (single samples or sequences) for an instrument have to be analyzed in a short time. All single samples or sequences created for the instrument are displayed in the Run Queue tab. You can add pauses or custom instrument commands to the queue (for examples about built-in instrument control commands, see [“Postsequence Operation”](#) on page 122). In this way, you can automate time-consuming tasks such as night or weekend jobs.

While the instrument is processing the workload displayed in the **Run Queue** tab, you can still modify the workload, such as:

- Change the position of the queued items, or add a pause (see [“Pauses in the Run Queue”](#) on page 147).
- Add a series of single samples and sequences to the queue (see [“Single Samples and Sequences in the Run Queue”](#) on page 146).
- Edit an already existing item in the Run Queue (see [“To edit an existing item in the Run Queue”](#) on page 147).
- Run a single sample or sequence immediately (see [“Run a single sample or a sequence”](#) on page 147).
- Add a built-in or custom command, for example, to shut down the system after the run (see [“Commands in the Run Queue”](#) on page 148).
- Add a Queue Plan with a predefined set of sequences that was created with the **Queue Planner** (see [“Add a Queue Plan with a predefined set of sequences”](#) on page 149).

The ChemStation status bar shows the status of the Run Queue, which can be **Resumed**, **Paused**, or **Blocked** (if the method or sequence has unsaved changes that would be overwritten if the run were to be started).

The **History Queue** of the Run Queue tab shows you which runs have been already executed on the current instrument.

Run Queue and Queue Planner are only available in online ChemStation sessions in the **Method and Run Control** view.

## Run Control

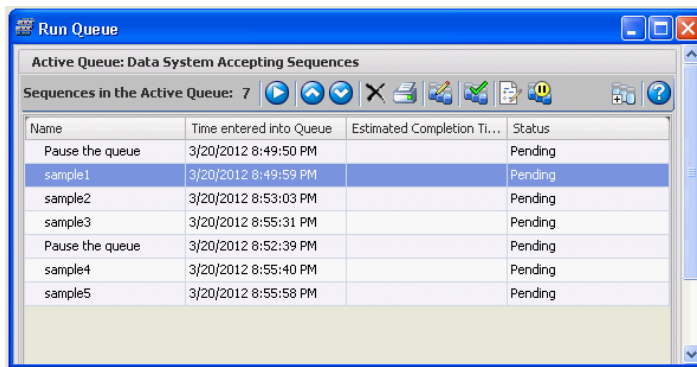
### About the Run Queue

Since the Run Queue allows long-term jobs, it is very likely that sessions will be taken over by other users on the same instrument while the Run Queue is being processed. The individual users who take over the session are noted in your report. The report displays the **Acquisition Operator** who is logged on as the current user and the **Sample Operator** who submitted the single sample or sequence to the Run Queue.




## Using the Run Queue

The Run Queue is available both from the **Instrument Control** tab or the **Run Queue** tab. In the Instrument Control tab, you can show or hide the Run Queue with the **View >Run Queue** command.



**Figure 34** Run Queue dialog

You can add an item to the front or to the back of the queue. As long as the status of the items in the queue is pending, you can change both the execution order and the properties of the item. Depending on the **Active Queue Options** , the first item in the queue either starts when the data system is ready or when you resume the queue.

The Run Queue supports single samples, Easy Sequence templates, and classic ChemStation sequences. The only items that cannot be added to the Run Queue are Partial Sequences, Priority Samples, and Runs that are started directly from the instrument.

For more information on Easy Sequence, see the online help system. **Easy Sequence Setup** tutorials are available in online help.

## Single Samples and Sequences in the Run Queue

To queue a single sample

- 1 Select **RunControl >Queue Method...**
- 2 In the **Queue Method** dialog, edit the sample parameters.
- 3 Add the sample to the queue.

The first item added to the queue starts when the data system is ready, unless it is paused from the queue.

To queue a sequence or a series of single samples


- 1 Select **RunControl >Queue Sequence...**
- 2 Select a classic ChemStation sequence template or an Easy Sequence template.
- 3 Edit or review the sequence table and the sequence parameters. You can modify the sequence table and sequence parameters without changing the currently loaded sequence.
- 4 Save the settings. In the **Finish Queue Sequence** dialog, you can choose whether you want to add the sequence to the queue or save it as a new sequence template. Depending on the preference settings (see [“Sequence Execution Mode”](#) on page 115), you can also submit the sequences as a series of single method runs.

The **Finish Queue Sequence** dialog also contains the check box **Delete temporary Sequence Template after completion**. ChemStation always keeps a copy of the queued sequence template in a temporary directory. This temporary sequence template will be used to run the sequence from the queue. As the same sequence may be queued several times using different parameters, ChemStation needs a separate copy for each queued item. Depending on the status of the check box, this temporary sequence template will be kept or deleted when the queue continues with the next item.

The **Delete temporary Sequence Template after completion** check box is selected by default. All information required for reprocessing is already available in the result set, therefore you do not need a copy of the temporary sequence template. However, if you select the check box, a copy is saved by default under **C:\Users\Public\Documents\ChemStation\<instrument>\TEMP\AESQ**.

To edit an existing item in the Run Queue

You can edit an already existing item in the Run Queue, for example, you can assign a different vial position to the single sample or the samples in the sequence, or assign a different method with modified parameters.

- 1 In the Run Queue, select the single sample or the sequence you want to edit.
- 2 In the toolbar of the Run Queue, select  **Edit Selection....**  
Depending on whether you edit a single sample or a sequence, the **Queue Method** dialog or the **Sequence Table** opens.
- 3 Edit the parameters and confirm your entries.  
Your settings will be applied to the item in the Run Queue.

Run a single sample or a sequence

To run a single sample or a sequence immediately, select the **RunControl >Run Method** or **RunControl >Run Sequence** command.

The single sample or sequence is first added to the Run Queue and is then immediately started.

If the Run Queue is currently paused, it is automatically enabled so that the item runs immediately. The instrument returns to the paused state after the run has finished.

## Pauses in the Run Queue

To schedule a pause to the queue, click **Add Pause to Queue** in the Run Queue toolbar. In these pauses, ChemStation shows a customizable message and waits for a user confirmation.

## Commands in the Run Queue

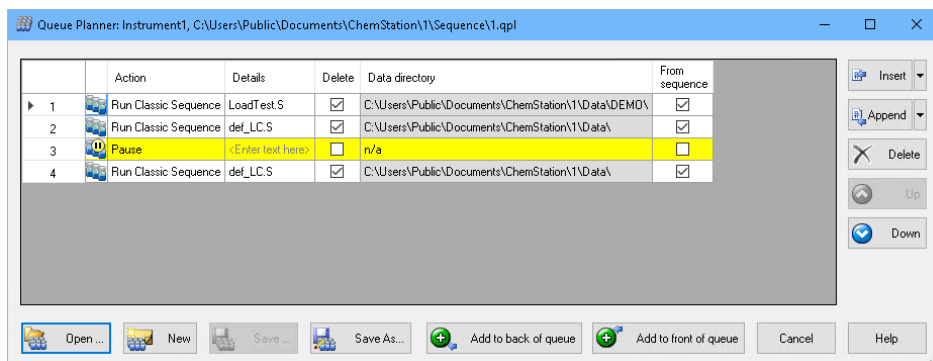
To add built-in or custom commands to the Run Queue, use the menu **Run Control >Queue Command....** Alternatively, configure a custom command in the **Active Queue Options** that will be executed when the instrument is idle.

All commands assigned to this instrument are displayed in the drop-down list. Select a command from the list, or set up your own command. To set up custom commands, you need the privilege **Command Line**.

For more information about where you can use commands, see ["Using Custom Commands or Macros in ChemStation"](#) on page 26.

## Using the Queue Planner

With the Queue Planner, you can prepare an ordered set of sequences (ChemStation sequence templates \*.s or Easy Sequence template \*.es), pauses, or commands. The entire Queue Plan can be added either to the back or to the front of the Run Queue.



**Figure 35** Queue Planner

Add a Queue Plan with a predefined set of sequences

With the Queue Planner you can create Queue Plans for sequences to be run and also integrate pauses and commands in between. To prepare a Queue Plan:

- 1 Select the **RunControl >Queue Planner...** command.
- 2 Prepare your queue plan and insert sequences.
- 3 As in the Run Queue, you can add a pause and provide your own message in the **Details** column. When the Queue reaches the pause, ChemStation stops, and displays the given message. A user must confirm the message before the queue can be resumed.
- 4 Save the queue plan. The queue plan is saved as a \*.qpl file.
- 5 At the time when you want to run the Queue Plan, open the Queue Planner, load the Queue Plan, and add it to the Run Queue.

For more information on the user interface, see the online help system.

## Schedule Commands

Use the Command Scheduler to set up your ChemStation to automatically execute commands for time-based events such as:

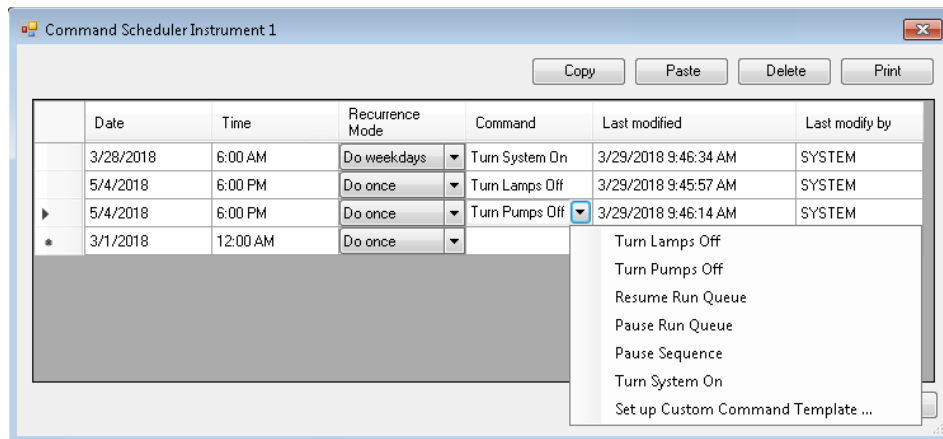
- Turning the system on
- Resuming a paused queue to prepare an instrument for the day
- Running an MS Autotune
- Adjusting the detector offset
- Loading a method or sequence
- Starting a sequence or Run Queue

The Command Scheduler allows you to schedule these events at a specific date and time, and to set a recurrence interval. The following intervals are supported:

- Do once
- Do daily
- Do weekdays
- Do weekly (on the same day)
- Do monthly (on the same day)

### Schedule an Event

Events are scheduled in the Command Scheduler interface. In the table, you must specify the command as well as the corresponding date, time, and recurrence mode.



The **Command** field offers you built-in commands in a drop-down list. The list of commands can be extended by user-defined commands. To set up custom command templates, you need the privilege **Command Line**. For more information, see ["Using Custom Commands or Macros in ChemStation"](#) on page 26. Non-privileged users can only select commands from the drop-down list.

For more information about built-in commands and macros, see "commands" and "macros" in the ChemStation online help.

## Scheduler Operating Mode

The scheduler scans for existing commands every minute. Executed macros are displayed in the instrument logbook and in the OpenLab activity log. Tasks with an execution date more than two weeks ago, and configured as **Do once** are automatically deleted.

The execution of tasks may be delayed if ChemStation is busy at the scheduled time. The execution is performed when ChemStation is ready. A prerequisite for execution of recurring tasks is that the instrument must be running.

### NOTE

Tasks are instrument-specific and are associated with the instrument name. If an instrument is renamed, all scheduled tasks for that instrument are deleted.

## 6

# Data Analysis and Review Concepts

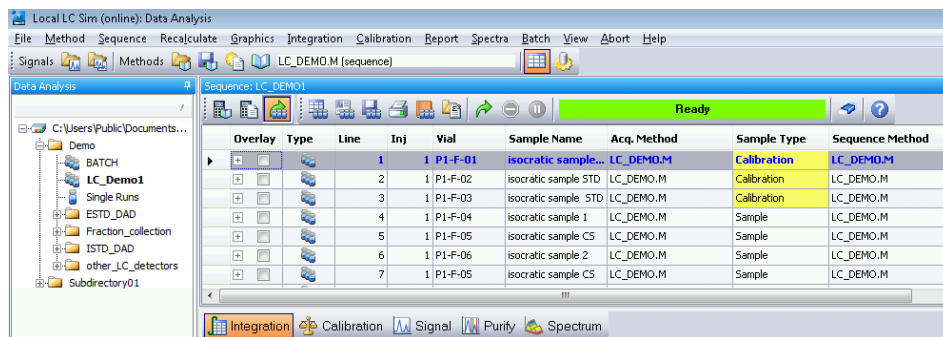
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You can analyze and review your data with ChemStation. This chapter outlines the ChemStation data analysis and data review options.



## Data Analysis

Once the data has been acquired, it can be analyzed in **ChemStation Data Analysis** view. When selecting the **Data** tab of the ChemStation Explorer, you can load all the runs of a sequence or all single runs in a specific folder by double-clicking the corresponding symbol. The corresponding data set is then available in the Navigation Table.



**Figure 36** Loading a sequence from the ChemStation Explorer into the Navigation Table

The main body of the Navigation Table consists of a list of all runs of the set. You can load a run into ChemStation memory by double-clicking the relevant line in the Navigation Table. Additionally, right-clicking on a run offers several options, for example, to load or overlay specific signals from the file, to export the data, or to view the acquisition method parameters.

*Sequence runs* are (in the Reprocessing mode) loaded with the sequence method that has been used during acquisition or reprocessing. The name of this method is shown in the toolbar, and also in the **Sequence Method** column in the Navigation Table. The acquisition method name is shown in the **Acq Method** column.

*Single runs* are loaded with their associated analysis method. The name of this method is shown in the **Analysis Method** in the Navigation Table and in the Run Details. If the method is not available at the original path, an error is shown.

The acquisition method name is shown in the **Acq Method** column.

ChemStation allows you to specify default actions that are performed automatically when a data file is loaded from the Navigation Table. These include data analysis tasks like integrating the chromatogram directly after loading,

viewing a report for each single injection, or integrating and printing in one single step (see figure below).

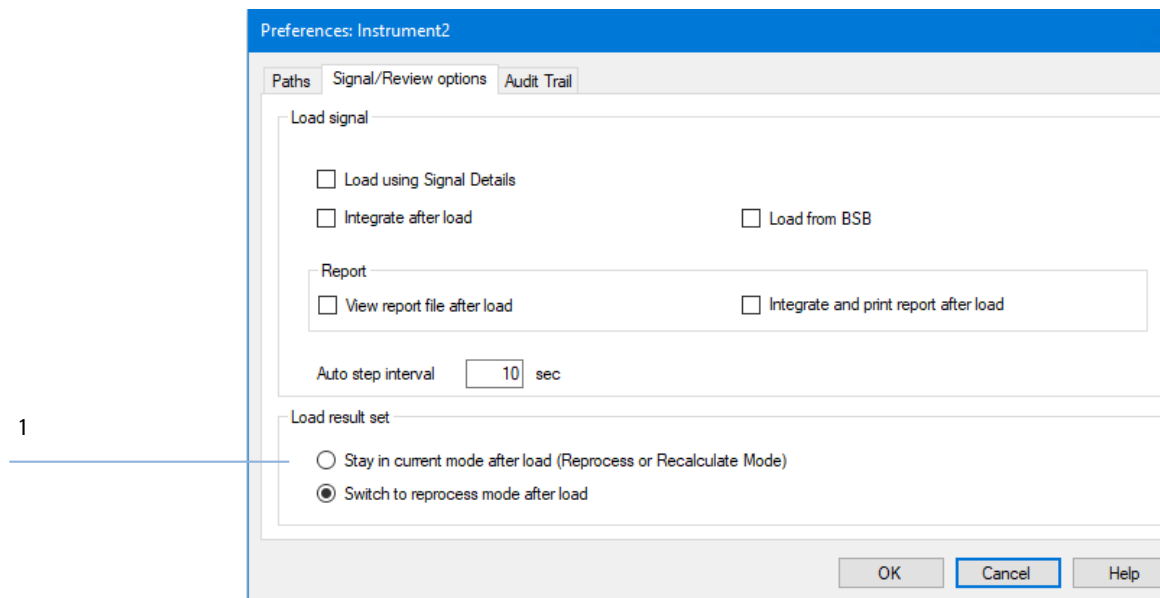


Figure 37 Signal/Review options tab of the Preferences dialog

## Navigation Table Configuration

The Navigation table includes standard table configuration features, such as sorting and drag-and-drop options to move columns to different places. It is also possible to select the columns that are displayed in the Navigation Table.

In addition, column-specific grouping is possible, for example, single runs of a particular operator can be displayed by grouping the loaded files by the column **operator**.

The Navigation table offers right mouse click functions to load a signal, overlay a signal, export data, print reports, view the acquisition method parameters etc. Each Navigation Table line can be expanded by clicking the + (plus) sign at the left of the line to configure signal-specific options:

- **Signal:** Lists the acquired signals and allows you to specify the signals to be loaded. The signal display selection is applied to each run individually.
- **General Info:** Lists the header details about the run.
- **Instrument curves:** Allows you to select the instrument data curves to be displayed along with the chromatogram/electropherogram on screen and in the printout.

## Data Analysis Modes

You can choose between the following Data Analysis modes:

- Recalculation mode
- Last Result mode
- Reprocessing mode

These modes are accessible either via the **View** menu or via the tool set (see figure below).



**Figure 38** Mode selection

For each of the modes, the tool set contains specific functions. The modes and the respective functions are described in the following sections. In the **Signal/Review Options** tab of the **Preferences** dialog box, you can choose which mode should be active by default when you load a result set (see [Figure 37](#) on page 154, marker 1).

## Recalculation Mode

Once the run is loaded, you can review it, that is, adjust data analysis parameters, integrate the signals and finally print a report. In this case you analyze the run as a single run without taking the sequence context into account or using the features of the sequence table. The Navigation Table for this type of data analysis provides the toolset shown in the figure below.



**Figure 39** Recalculation toolset of the Navigation Table

With this toolset, you can jump to the beginning or end of the navigation table, step on to the next or previous run, automatically step through the runs, stop automatic stepping, recalculate a run using a specific method, or clear the Navigation Table.

Recalculation means analyzing on a run-per-run base. Only the runs shown in the Navigation Table are analyzed. If you applied a filter to the Navigation Table, only those runs actually shown in the table are recalculated. The sorting of the Navigation Table is also taken into account.

You can use recalculation in the following workflows, for example:

- You want to review the data files of a result set with a different method that is not currently in the result set, for example, a master method not used for acquisition, because your workflow employs separate acquisition and data analysis methods.
- You have edited a sequence method and want to review only specific runs using this method in order to check how well these parameters apply for different runs.
- You want to review a single run with a specific analysis method. In Recalculate mode, no analysis method is loaded along with a single data file.

### Recalculate With Specific Method

With this function, you can recalculate the runs shown in the Navigation Table using a specific master method. You specify the required master method in the **Recalculate With Method** dialog (see figure below). If the selected master method uses Intelligent Reporting (see ["Reporting"](#) on page 189), you can also specify the report template that will be used for the single injection reports.

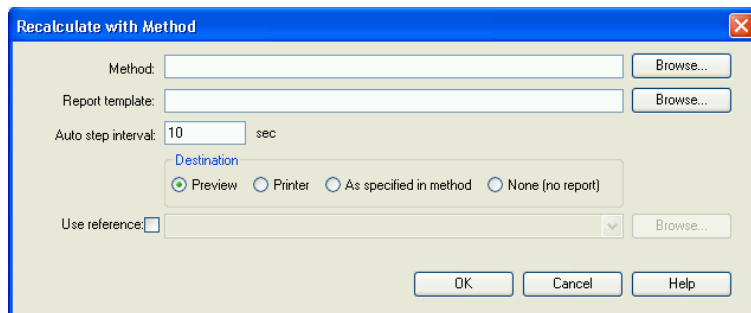


Figure 40 Recalculate With Method dialog

The **Browse for methods in master paths** dialog and **Browse for templates in master paths** dialog offer all file locations that you specified in the Preferences.

#### NOTE

In previous revisions of ChemStation you have been able to recalculate with a specific method by choosing **Use current method**, **Use method from data file**, or **Use sequence method** in the toolbar.

If you select the **Use reference** check box, you can select a data file containing a reference signal. ChemStation uses this signal to calculate the signal-to-noise ratio as defined by European Pharmacopeia. The drop-down list offers the data files that you used during the current session. With the **Browse** button, you can select any data file that is also present in the Navigation Table. If want to use a different reference file, you must first add it to the Navigation Table.

The new reference overwrites the previous one and will be used from now on in signal-to-noise calculations in every report. If you select the **Use reference** check box, but do not select any file, the references are cleared for all recalculated data files, and no signal-to-noise values will be calculated from now on.

Each time you recalculate a sample or generate a report, the data file method (DA.M) is automatically updated with the data analysis parameters of the used method. The path to the specific method is saved as a reference in the data file.

## Last Result Mode



Figure 41 Last Result Mode toolset of the Navigation Table

In this mode, the data file method (DA.M) for each run is loaded. DA.M is an exact copy of the method which was used for the last data analysis (during acquisition, reprocessing, or recalculation). So even if the sequence method has been changed in the meantime, you can reproduce the last result with the method originally used. In that way you can, for example, track changes done to the method in successive recalibration steps in a result set.

The method name in the toolbar shows DA.M, which indicates that the data file method is loaded. When you move the mouse pointer over this field, a tool tip additionally displays the full path and name of the method. In addition, the name of the method last used for data analysis (which was copied to DA.M) is shown in the **Analysis Method** column in the Navigation Table. The tool tip of this column shows the full path of this method.

### NOTE

The DA.M is normally read-only. You cannot manually load it, it is only loaded by ChemStation in the Last Result Mode for recalculation. You can edit it, but you cannot manually save it.

If you have changed the method, and you want to print report, a message box will ask you for confirmation, as this action will generate new results. If confirmed, the changes are saved to the last used data analysis method. A corresponding entry is added to the method audit trail.

In Last Result Mode, you can update the loaded master method or any master method with the current data analysis parameters from the DA.M, or save a changed DA.M method as an entirely new master method. For example, you loaded a data set analyzed a few weeks or months ago, and you find the data analysis parameters stored in the DA.M useful for your current work. You can then transfer the settings to a master method of your choice. For more information, refer to [“Adminstrating Methods”](#) on page 55.

## Reprocessing Mode

## Reprocess Mode for sequences

A different way to analyze your data is to **Reprocess** a complete sequence. In contrast to recalculation, all runs are reanalyzed in the sequence context, i.e. the calibration tables of the sequence methods are updated in the case of calibration runs, and multipliers, amounts etc. can be changed in the sequence table.

The result set includes all files needed for reprocessing: the data files, a copy of the sequence file, all the sequence methods and all the report templates originally employed with the acquisition. Thus, in order to reprocess a sequence you simply have to load it into the Navigation Table and select the reprocessing tool set.

If it becomes necessary to propagate changes in the sequence method to the corresponding master method as input for all future acquisition runs, you can achieve this conveniently by using the **Update Master Method** functionality (see [“Updating DA Parameters in the Master Method”](#) on page 58).

The DA.M is automatically updated each time you reprocess a data file.

For reprocessing sequences, the navigation table provides the following toolset:



**Figure 42** Sequence Reprocessing Toolset of the Navigation Table

With this toolset, you can edit the sequence table, edit the sequence parameters, save the current sequence, print the current sequence, show or hide the sequence logbook, view the saved sequence summary report file(s), start sequence reprocessing, or stop the sequence.

Note that the reprocessing icons in the Navigation Table are available only for result sets generated with ChemStation B.02.01 and higher. Reprocessing in **Data Analysis** is not accessible for data generated prior to B.02.01, and for data acquired in the legacy non-unique folders mode. Such sequences need to be reprocessed in **Method and Run Control**, defining the sequence parameter **Part of method to run** as **Reprocess Only**. For sequences generated with ChemStation B.02.01 and higher, the reprocessing option in **Method and Run Control** has been removed, and the navigation table offers reprocessing as a **Data Analysis Task**.

Another alternative is to add such samples or sequences to a new self-assembled result set. There you also assign sequence methods, and you can reprocess the entire sequence afterwards (see “Self-Assembled Result Set” on page 162).

Note the following rules with regard to reprocessing:

- When loading a result set into the Navigation Table, ChemStation also automatically loads the sequence file (\*.S) that is located in this result set. This sequence file contains all the sequence lines that are related to any data file belonging to this result set.
- All actions are performed on the sequence methods. If changed analysis parameters are to be applied, you have to change the sequence methods.
- During reprocessing, the Batch (\*.b) file, the sequence/single run log (\*.log), and the Navigation Table are updated. The individual data analysis method (DA.M) of each processed data file is overwritten with the sequence method.
- To add new methods from one of the master method directories to the sequence table, use the ChemStation Explorer to copy the master method to the result set, or click **Method >Update Methods...** You can then select the new sequence method in the sequence table. It is not possible to add or remove lines in the sequence table.
- In the Sequence Parameters dialog, only the sequence comment and the usage of sequence table information can be changed. All other fields have to be set during data acquisition or do not apply to reprocessing.

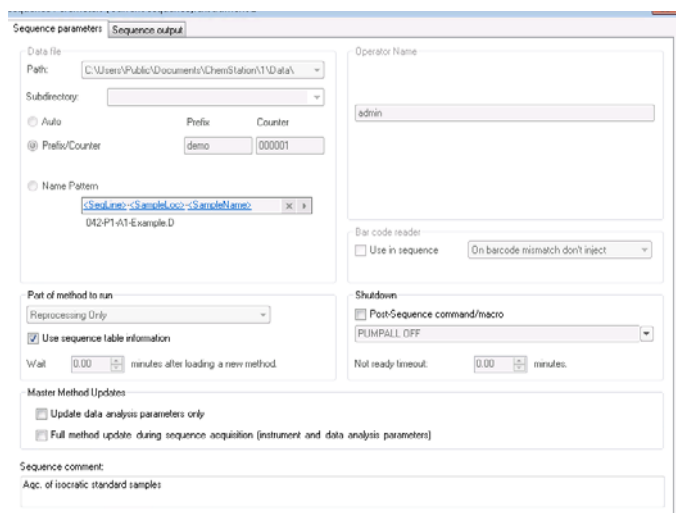


Figure 43 Sequence Parameters in Data Analysis



## Reprocess Mode for single runs

When loading a single run into the Navigation Table, ChemStation loads the associated analysis method. The name of this method is shown in the **Analysis Method** column. The full path can be shown via the context menu (**View Run Details**).

If the analysis method is not available at its original path, an error is shown. In acquisition only runs, where no analysis method was used, the acquisition method is loaded and used as analysis method.

For reprocessing single runs, the navigation table provides the following toolset:



Figure 44 Single run Reprocessing Toolset of the Navigation Table

With this toolset, you can step through the runs, and reprocess them with their associated analysis methods. In combination with the View **report file after load** option (see Figure 37 on page 154), this mode allows an easy review of multiple single run results without any data modification.

**NOTE**

Calibration data stored in the method will not update on reprocessing, even if the single run is a calibration sample. To recalibrate, see [“Recalibration”](#) on page 186.

**Treatment of Manual Integration Events**

Manual integration events, for example, a manually drawn baseline, are even more data file specific than timed integration events. In case of complicated chromatograms, it is highly desirable to be able to use these events for reprocessing.

Therefore, in ChemStation B.04.01 and higher, manual integration events can be stored directly in the data file instead of the method. Whenever the data file is reviewed or reprocessed, the manual events in the data file are automatically applied. A run containing manual integration events is marked in the Navigation Table in the corresponding column.

In addition to the tools for drawing a baseline and deleting a peak manually, three other tools are available in the user interface to:

- save manual events of the currently shown chromatograms into the data file,
- remove all events from the currently shown chromatograms
- undo the last manual integration events (this is available until the event is saved)

When continuing to the next data file during review in the Navigation Table, ChemStation will check for unsaved manual integration events and ask the user whether he wants to save the events.

Manual events stored in the data file during review in the Navigation Table do not interfere with manual integration events stored during review in the **Batch** mode. These two ways of review are completely separated with regard to the manual events of a data file.

In ChemStation revisions prior to B.04.01, manual integration events could only be stored in the method. In B.04.01, this workflow can still be used. The **Integration** menu in **Data Analysis** view provides the following items in order to handle manual integration events with the method:

**Update Manual Events of Method:** Save newly drawn manual events to the method.

**Apply Manual Events from Method:** Apply the manual events currently saved in the method to the currently loaded data file.

**Remove Manual Events from Method:** Delete the manual events from the method.

In order to convert manual events stored in a method to storage in the data file, apply the events from the method and store the results in the data file. If required, remove the events from the method.

If the **Manual Events** checkbox of the **Integration Events Table** of a method is selected, the manual events of the method are always applied when loading a data file using this method. If the data file contains additional manual events, the events in the data file are used. When the **Manual Events** checkbox is selected, the user is never asked to save the events to the data file.

### Self-Assembled Result Set

In the **Data Analysis** view, the Navigation Table shows the contents of the single run or sequence that is loaded. You can load, unload, or add data files to the Navigation Table. Using the **Sequence > Create New Result Set** command, you can create a new self-assembled result set from the data currently shown in the

Navigation Table (see [“To assemble a new result set”](#) on page 108). Self-assembled result sets can be reprocessed the same way as automatically created result sets.

### **Unload Current Dataset**

Using the **Unload Current Dataset** command from the context menu of the Navigation Table, you can revert the Navigation Table to the original empty state, as it is directly after launching ChemStation. If there is unsaved data, you are asked to save it.

### **Delete Selected Data File**

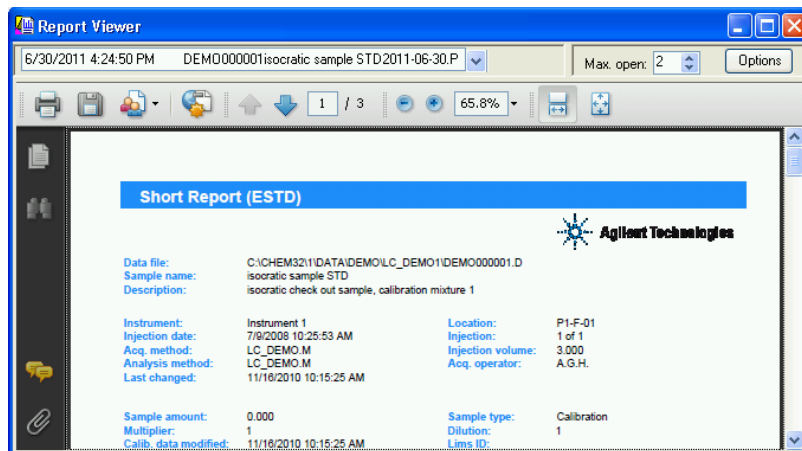
Using the **Remove selected Data Files** command from the context menu of the Navigation Table, you can remove the selected lines from the Navigation Table. This only removes the reference in the Navigation Table, it does not delete the physical data file from the loaded result set or single run on the file system. It is only possible to delete the references of added/overlaid files.

## **Updating Methods**

In the **Data Analysis** view, you have several options to copy methods between the master method directories and the result sets. For more information, refer to [“Administrating Methods”](#) on page 55.

## **Report Viewer for Data Analysis**

Depending on the configuration, ChemStation automatically saves the single injection reports and sequence summary reports to the file system at a certain point in time. With the Report Viewer, you can easily view the saved report files in order to check the results from data acquisition, reprocessing or recalculation.



**Figure 45** Report Viewer

Using the Report Viewer has the following advantages:

- You can directly open the report files from ChemStation. You do not need to search for the files in the file system.
- Each report opens in a separate floating window. Therefore, you can easily compare different reports by placing the windows side by side.
- You can use the full screen to view the report file.
- You can use the features from Adobe Reader to view .pdf reports.
- You can search for specific text in .txt reports as well as .pdf reports.
- When you reprocess a sequence, you do not have to wait until the entire sequence reprocessing is completed. You can open the saved report files for those sequence samples that are already completed.

## Starting the Report Viewer

You can open the Report Viewer via the menu, via toolbar icons, or via the context menu of the Navigation Table. There are different items for sequence summary reports and single injection reports.

To view single injection reports:

- Select the menu **Report >View Report File** to view the report file or files of the loaded signal.

- Select the **View Saved Report File(s)** command from the context menu of a specific sample in the Navigation Table. With this command you can load the report file or files of any signal, even if it is currently not loaded.
- Click the **View saved Report File(s)** icon from the Workspace Toolbar to view the report file or files of the loaded signal.



To view sequence summary reports:

- Select the menu **Sequence >View Summary Report File**.
- Click the **View Saved Sequence Summary Report File(s)** icon from the Navigation Toolbar (in reprocessing mode).



## Configuring the Report Viewer Windows

You can configure several aspects of the Report Viewer behavior. All of these settings are accessible via the **Options** button in the Report Viewer window.

You can define the maximum number of Report Viewer windows that will be open in parallel. The windows are cyclically reused. When you view more report files than the maximum number of Report Viewer windows, the first opened windows are the first to change their content.

### NOTE

If you do not need to compare multiple reports, we recommend to limit the number of Report Viewer windows to 1.

For comparing multiple reports, it may also be helpful to adjust the title bar of the Report Viewer windows. Various tokens are available for Report Viewer windows displaying sequence summary reports, single injection reports for sequence samples, or single injection reports for single runs. These tokens help you to distinguish the single Report Viewer windows.

The Report Viewer windows are always displayed on top of the ChemStation application. In order to work with ChemStation and the Report Viewer at the same time, you can resize and position both windows in such a way that you can see them both. When you close ChemStation, the windows' size and positions are saved. When you launch ChemStation the next time, the same settings will be used again.

## Arranging the Report Viewer Windows

The Report Viewer windows are always displayed on top of the ChemStation application. In order to work with ChemStation and the Report Viewer at the same time, you can resize and position both windows in such a way that you can see them both and can work conveniently.

When you close ChemStation, the windows size and positions are saved. When you launch ChemStation the next time, the same settings will be used again.

## Working with the Report Viewer

You can use the Report Viewer, for example, in the following workflows:

- You set up the method and the sequence to save PDF reports to the file system. After completing the sequence run, you open the report files (sequence summary report or single injection reports) directly from the ChemStation in the Report Viewer. Use the Adobe Reader features such as zooming or searching to check the report in detail.
- You download a sequence that already contains report files from central data storage.
  - To look at the final result, you select the relevant sample in the Navigation Table and open the report file directly from the ChemStation in the Report Viewer.
  - If required, you can change the method and reprocess the sequence. While the reprocessing is ongoing, you start viewing the reports of the already completed samples.

In the Report Viewer, you can select both old and new report from the list at the top left corner. You can distinguish the reports by their creation date, which is shown as a part of the list entry. Depending on the transfer settings, the data - including the new report files - may be automatically uploaded to central data storage after reprocessing has finished.

- You run a sequence that saves only TXT report files. You can check these report files as well in the Report Viewer.
- You review different reports on the same sequence samples, based on different report styles or templates.

First, you create a sequence with an extended performance report. You run or reprocess the sequence to obtain the report file. If you are satisfied with the results displayed in this report, you change the sequence method to create a shorter report (for example, select a different report template or the classic report style **Short**). Then you reprocess the sequence to obtain the shorter reports. When you view a report with the Report Viewer, you can switch

between the two different reports by selecting them from the list in the top left corner. The creation date of each file is shown as part of the list entry.

## Batch Review

### What is Batch Review?

Batch review is a capability within data analysis designed to help an analyst perform a “first-pass” review of the results of a sequence or a selection of runs quickly and easily. It will save time especially when reprocessing large numbers of samples. Whenever a sequence is run, a batch file (with a .b extension) is automatically generated and placed in the data directory along with the data files. This batch file contains pointers to the data files in the batch review itself. Upon loading a batch, the analyst need only select the method to use for the batch, and then individually select the desired data files to analyze in the batch. One can check the calibration accuracy, instrument performance and individual integrations before approving the results. Any chromatogram specific integration parameters which are modified can be stored with the data file for data traceability. This interactive environment provides complete access to all other data analysis capabilities, such as peak purity, library searching, etc., as well.

Batch review uses the same data analysis registers (ChromReg and ChromRes) as the standard data analysis and should therefore not be used in an online session that is currently performing analyses.

### Batch Configuration

A batch is a user-selected series of data files that is processed using a user-defined method. All data files in the batch are processed using the same method. The processing steps carried out each time a new sample is loaded for review can be selected (integration, identification/quantitation, reporting).

All calibration runs in the batch are used to produce a single calibration table, using averaged response factors, which is then used for quantification.

### Batch Table

Runs are displayed in a user-configurable batch table:

- the number and content of the table's columns can be specified;
- the runs can be sorted by
  - run index (the order in which the runs were acquired) independent of any other criteria,
  - sample type (control samples first, then calibration samples, then normal samples) then by run index within each sample type,
  - method (if more than one method was used to acquire the runs) then by run index within each method;
- samples, calibration samples and control samples can be displayed in the table or hidden.

Each selected run occupies a line in the batch table. You can exclude a run in the batch table (e.g. from calibration) by changing its sample type to Removed.

### Compound Table

The compound results are displayed in a user-configurable compounds table, but contents of the compounds table depends on the type of samples in the batch table:

- the compound list contains all compounds found in the method that was loaded for batch review.
- if calibration samples only are displayed in the batch table (samples and control samples are hidden), the compound table shows additional columns for calibration-related information (expected amount, relative error and absolute error).
- if control runs only are displayed in the batch table (samples and calibration samples are hidden), the compound table shows additional columns for any defined control limits.

For columns containing compound-specific information, you can include the name of the compound in the table title by adding %s to the column specification.

### Batch Report

The batch report contains two tables that are generally analogous to the batch table and the compound table; these tables are also user-configurable.

For columns containing compound-specific information, you can include the name of the compound in the table title by adding %s to the column specification.



Multi-line headers are allowed; you insert the character ']' at the point where you want the line to break.

### User Interface

Batch review provides a choice of two user interfaces:

- the standard interface includes a button bar, with buttons mirroring most of the Batch menu items, together with the batch table and compound table;
- a minimal interface provides a button bar similar to the standard interface, but replaces the batch table and compound table with a combo box that contains only the information specified for the batch table. The minimal interface button bar does not contain batch table-related or compound table-related buttons.

### Review Functions

Data files can be displayed in one of two ways:

- manually, by selecting a run to display from the table,
- automatically, with a predefined interval between each data file. During automatic display, only those sample types displayed in the table are displayed; the runs are displayed in the order in which they appear in the table. The automatic review can be paused and later resumed, or stopped.

The standard functions provided by the ChemStation are available with batch review. This includes calibration, manual manipulation of chromatograms, for example by smoothing or manual integration. Any changes made to a data file can be marked and saved with the batch file. Chromatograms that have been reviewed are marked with an asterisk in the batch table. You can also discard changes made to either the current chromatogram only, or all changes to all chromatograms in the batch.

#### NOTE

Batch Review allows you to save manual integration events per run. It is also possible to save manual events with the data file outside of Batch Review. To avoid conflicts with two sets of manual integrations, any manual events that have been stored with the data file will not be applied in Batch Review.

When a run is loaded, the selected processing options are performed; if the run has already been processed and the changes saved, the processed run is loaded. This is a faster process than loading the unprocessed run, because no processing needs to be done.

### Calibration in Batch Review

Calibration in batch review works independently from the recalibration settings in the sequence table. The first step in batch calibration always replaces both response and retention time entries in the calibration table. For the following calibration standards, both response and retention time values are averaged.

Clicking on the batch review toolbar causes the system to recalibrate with all calibration runs in the batch, creating a recalibrated calibration table. Clicking on the Batch Review toolbar then recalculates amounts for each calibrated compound. The amounts for all samples are calculated from the recalibrated calibration table.

### Batch Reporting

The user-configurable “Batch Table” on page 168, can be printed directly on the printer, displayed on the screen or printed to a file with a user-specified prefix in one of the following formats:

- UNICODE text file with the extension .TXT
- Data Interchange Format with the extension .DIF
- Comma-Separated Values format with the extension .CSV
- Microsoft Excel format with the extension .XLS.

The reporting options also give the possibility of sorting the samples (by Run Index, Sample Type or Method) independent of the sort method in the batch table. The sort priorities are as for the “Batch Table” on page 168.

### Batch History

Batch review maintains a log of all actions relating to the current batch. Any action that changes the batch (for example changing the displayed chromatogram, changing the sample type, loading and saving the batch) adds a line to the batch history with a date and time stamp, the current operator name and a description of the event.

You can also add your own comments to the batch history. Existing batch history entries cannot be edited, and the history list cannot be accessed except through the Batch History menu item.

## Review

In ChemStation, a view is available that covers the pure data review workflows of Data Analysis. In this **Review** view, you can generate reports for either an entire sequence, a subset of a sequence, or any selection of data files from different sequences or single samples.

In the **Review** view, you do not load any methods and you do not create any new results as in recalculation or reprocessing. The reports that you generate in the **Review** view only display the results that have already been calculated.

You can select a report template and apply it to specific selection of data files. The combination of template and data file selection determines the output of the generated report.

Since the **Review** view only provides a view on existing results, it is used in compliant workflows to present existing results without generating a new result version.

### NOTE

The **Review** view is only available if you activated Intelligent Reporting in the Instrument Configuration in the OpenLab Control Panel.

## Requirements for Intelligent Reporting

ChemStation generates the result data in a specific format (\*.ACAML) that is used by Intelligent Reporting. If you want to create reports for data acquired with a ChemStation Version A or B, you must first regenerate results using OpenLab ChemStation rev. LTS 01.11 (for example, recalculate the data or generate single injection reports in the Data Analysis view). If the results are not available in the required format, the generated reports in the Review view will not contain any data.

## Data File Selection

You can select the required data files by loading the sequences or single runs from the Navigation Tree in the ChemStation Explorer. All available data files are then shown in the Navigation Table. In the Navigation table, you select the specific data files for which you want to see the results in the report.

## Loading Data Files

You can load all data files from an entire sequence or Single Runs folder. In the **Data** tab of the ChemStation Explorer, you can either double-click the sequence or use the **Load** command from the context menu to load all included data files.

When you load the data files, the Navigation Table is automatically cleared before the new data files are shown. You can therefore prepare the data for either a *Single Sample Report* or for a *Sequence Summary Report*.

## Adding Data Files

If you want to compare the results from different sequences, you can first load one sequence, and then add the required data files from another sequence. In the **Data** tab of the ChemStation Explorer, use the **Add Data Files...** command from the context menu to add only specific data files to the selection already loaded. A dialog opens in which you can select the required data files.

When you add data files, the Navigation Table appends the data files to the list of data files already loaded. You can therefore prepare the data, for example, for *Cross-Sequence Reports*.

## Selecting Data Files for Reporting

The Navigation Table shows all data files from the sequence or single sample collection that you double-clicked in the ChemStation Explorer. In the Navigation Table, you select those data files for which you want to create the report. Only the selected lines will be included when you generate a report.

## Report Template Selection

You can select the required report templates from the **Report Templates** tab in the ChemStation Explorer. The Navigation Tree shows all report templates in the REPSTYLE directory.

By default, the REPSTYLE directory is located under C:\Users\Public\Documents\ChemStation. This path is defined during installation.

Use ChemStation menu **File >Open Windows Explorer...** to open the path for the current instrument (for example, C:\Users\Public\Documents\ChemStation\1). Alternatively, use the shortcut to **Instrument Data** in the Start menu.

## Report Preview

The resulting report is always determined by both the data selection and the report template. Therefore, ChemStation generates the corresponding report and displays the report preview once you have selected one or more data files and loaded a report template.

You can send the report to a printer or save it as a file (.PDF, .XLSX, .DOCX, .TXT, or .CSV). If you use a central data storage system, you can also upload the report directly to the central repository.

## Possible Review Workflows

You can use the **Review** view for example in the following workflows:

- You load a sequence and select all data files of the sequence. You load a report template and generate a *sequence summary report*.
- After generating a sequence summary report, you load a different report template. You review the same data using a *different report layout*.
- You load a sequence and select only a subset of data files. You load a report template and generate a sequence summary report for *only part of the sequence*.
- After loading a subset of data files, you add other data files (from a sequence or from a collection of single samples). You load a report template and generate a *cross-sample or cross-sequence report*.

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This chapter explains the concepts of calibration.

## Definition of Terms

<b>Calibration</b>	Calibration is the process of determining response factors used to calculate absolute component concentrations by injecting specially prepared calibration samples. The calibration table is also used for identification.
<b>Compound</b>	A chemical compound can comprise several peaks, in a multiple signal calibration, typically one per signal. In a single signal calibration a compound refers to one peak.
<b>Calibration Level</b>	A calibration level comprises the calibration points for one calibration sample concentration. In a multisignal calibration the different compounds can be calibrated using different signals.
<b>Calibration Point</b>	A calibration point refers to an amount/response ratio for a peak on the calibration curve.
<b>Calibration Sample</b>	A calibration sample, also referred to as a calibration standard or a standard mixture, is a sample containing a known amount of the compound to quantify. In the software the calibration sample is referred to as an injection from the calibration sample vial.

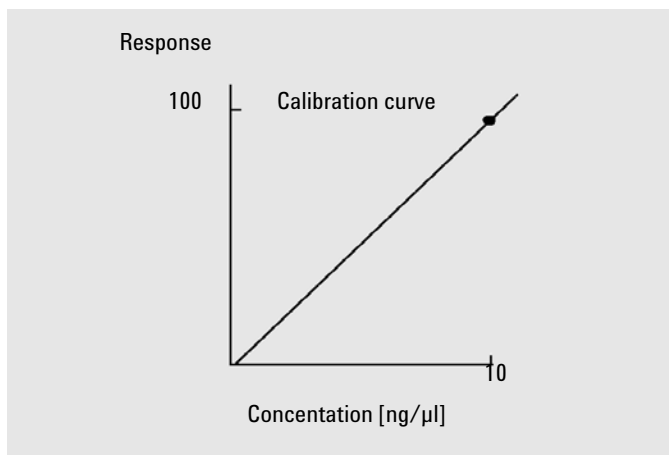
Calibration samples may be purchased from chemical suppliers or they may be prepared using an accurately measured amount of the pure compound. The amount of the compound in the calibration sample is usually expressed as a concentration, typically in ng/μl units.

## Types of Calibration

ChemStation offers two types of calibrations, single-level and multilevel calibrations.

### Single-Level Calibration

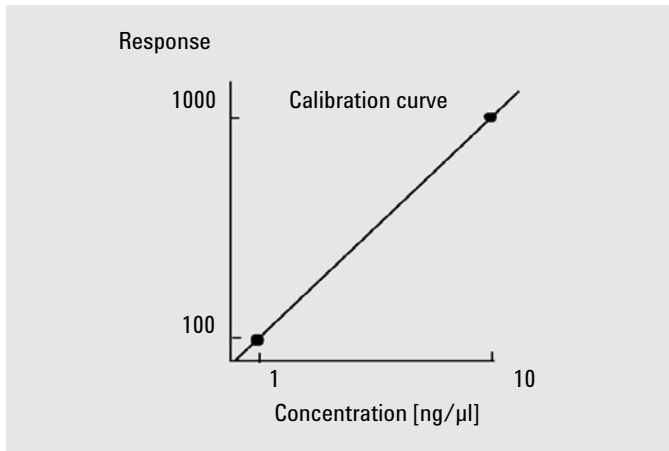
The calibration curve shown in [Figure 46](#) on page 176 contains one point, that is, one level. For the single-level calibration curve, the response of the detector is assumed to be linear over the working range of concentrations for the samples of interest. The response factor for a given component peak is given by the inverse of the slope of the calibration curve line through the point and the origin. A disadvantage of single-level calibration is that the detector response to the sample concentration is assumed to be linear and pass through the origin on a concentration versus response plot. This is not always true and can lead to inaccurate results.



**Figure 46** Single-level calibration curve

To obtain accurate quantitative results, a calibration curve should have at least two levels. These levels should bracket the amounts expected to be found in the unknown samples.





**Figure 47** Two-level calibration curve

For example, if you want to quantify a compound, and the unknown samples are expected to range from 1 – 10 ng/μl, then a calibration curve should have at least the two levels as shown in [Figure 47](#) on page 177.

### Amount Limits

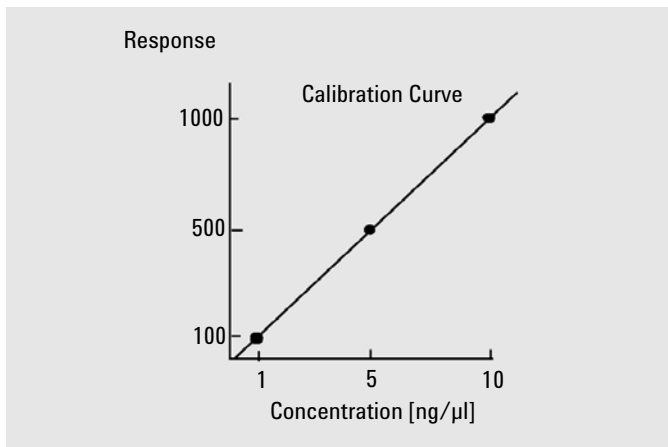
ChemStation allows you to define the valid quantification ranges in terms of absolute amounts for each component.

## Multilevel Calibration

Multilevel calibration can be used when it is not sufficiently accurate to assume that a component shows a linear response or to confirm linearity of the calibration range. Each calibration level corresponds to a calibration sample with a particular concentration of components. Calibration samples should be prepared so that the concentration of each component varies across the range of concentrations expected in the unknown samples. In this way it is possible to allow for a change in detector response with concentration and calculate response factors accordingly.

This multilevel calibration curve has three levels and shows a linear fit through the origin. This method of linear fit through the origin is similar to the single-point method calibration. The detector response to concentration is assumed to be linear. The difference between the two calibration types is that, with linear fit, the

slope of the detector response can be determined by a best fit through a number of points, one for each level.



**Figure 48** Multi-level calibration curve with three levels

The corresponding calibration table, which is the tabulation of the information used to generate this curve, might look similar to the one shown in [Table 18](#) on page 178.

**Table 18** Calibration Table

Level	Amount (ng/μl)	Response (area counts)
1	1	100
2	5	500
3	10	1000

In this example, the calibration samples that were used to generate the three levels had been identified as 1, 2 and 3.

## Calibration Ranges

Each multilevel calibration is valid over the range of concentrations used in the calibration samples. Extrapolation of a calibration curve, especially if it is non-linear, is at best an approximation. The valid calibration range for each compound may be defined in the **Compound Details** dialog box. Each entry for

that compound can be expressed as lower and upper limits. If these limits are exceeded, the report is annotated.

## Calibration Curve Fits

Various curve-fit calculations are available for use with multilevel calibration.

- Piecewise Linear
- Linear
- Log
- Power
- Exponent
- Quadratic
- Cubic
- Average (Response/Amount)

### Non-Linear Fit

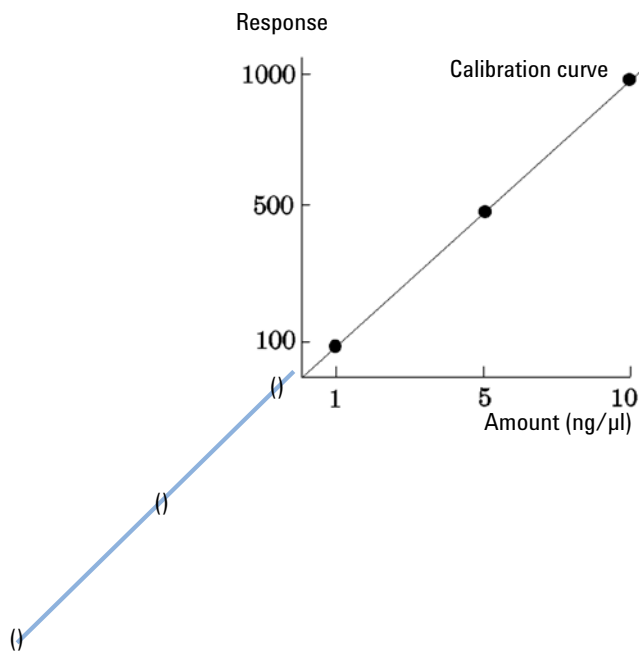
In some cases, the detector response to changes in sample concentration is not linear. For these types of analyses, a linear regression calibration method is not appropriate and a multilevel calibration calculation should be used.

## Origin Treatment

There are four ways to treat the origin when the response curve is plotted:

- ignore the origin,
- include the origin,
- force the origin, or
- connect the origin.

To force the origin to be included in the calibration curve the calibration points are mirrored about the origin from the first quadrant into the third quadrant. Using all points for the regression calculation ensures that the resulting calibration curve passes through the origin. This is also explained in [Figure 49](#) on page 180.



**Figure 49** Forcing the origin to be included

For further information about calibration curve fits and origin treatment, see the [online help](#) file.

### Calibration Point Weighting

When setting up your default calibration curve, you can specify the relative weighting (or importance) of the various calibration points used to generate the curve.

The following weighting options can be selected:

Weight	Description
Equal	All calibration points have equal weight in the curve.
Linear (Amnt)	A calibration point with the amount $x$ has the weighting $1/x$ normalized to the smallest amount so that the largest weight factor is 1. Normalization is done by multiplying the weight with the smallest amount. For example the weight of a calibration point with the amount $x$ is $(1/x) \times a$ where $a$ is the smallest amount of the calibrated compound prepared in the calibration standards. If the origin is included it is assigned the mean of the weightings of the other calibration points.

## Calibration

### Types of Calibration

Weight	Description
Linear (Resp)	A calibration point with the response $y$ has the weighting $1/y$ normalized to the smallest response so that the largest weight factor is 1. Normalization is done by multiplying the weight with the smallest response. For example the weight of a calibration point with the amount $y$ is $(1/y) \times b$ where $b$ is the response corresponding to the smallest amount of the calibrated compound prepared in the calibration standards. If the origin is included it is assigned the mean of the weightings of the other calibration points.
Quadratic (Amnt)	A calibration point with the amount $x$ has the weighting $1/x^2$ normalized to the smallest amount so that the largest weight factor is 1. Normalization is done by multiplying the weight with the smallest amount. For example the weight of a calibration point with the amount $x$ is $(1/x^2) \times a^2$ where $a$ is the smallest amount of the calibrated compound prepared in the calibration standards.
Quadratic (Resp)	A calibration point with the response $y$ has the weighting $1/y^2$ normalized to the smallest response so that the largest weight factor is 1. Normalization is done by multiplying the weight with the smallest response. For example the weight of a calibration point with the response $y$ is $(1/y^2) \times b^2$ where $b$ is the response corresponding to the smallest amount of the calibrated compound prepared in the calibration standards.
# Calibrations	A calibration point is weighted according to the number of recalibrations of the point. No normalization is done.

Quadratic calibration point weightings, for example, can be used to adjust for a spread in calibration points. It makes sure that calibration points closer to the origin, which can normally be measured more accurately, get a higher weight than calibration points further away from the origin, which may be spread.

You should base your decision, which kind of calibration point weighting to use, on your method requirements.

## Calibration Table

The calibration table specifies conversions of peak areas or heights into the units you choose according to the calculation procedure you select. It contains a list of retention/migration times from a calibration run. These retention/migration times are compared with retention/migration times of peaks from a sample run. Where a match occurs, the peak in the sample is assumed to represent the same component as that in the calibration table. During an analysis or while a report is being generated, the amounts entered for each peak are used to calculate the amounts for the calculation procedure selected for the report. The type and amount of information required for creating a calibration table varies with the type of calculation procedure desired.

The following information is needed to create a calibration table:

- the retention/migration time for each calibration mixture component peak, and
- the amount of each component used in making the calibration mixture, expressed in consistent units.

## Peak Summing

The peak sum table is provided for certain applications in the petrochemical and pharmaceutical industries. Typical applications are reporting of the total impurities or decomposition products, or summing the areas of uncalibrated peaks that lie within a specific range.

The peak sum table is similar to, but distinct from the standard calibration table. Like the calibration table, it is associated with the current method. Peak Summing is not designed for multi-signal data files.

The summed up areas from a specific time range can be expressed as amounts by using the calibration curve of a compound from the calibration table. It is also possible to use a fixed response factor.

**NOTE**

You must create a calibration table for an analysis before you can create the peak sum table.

## Compound Groups

Compound groups allow individual compounds from the calibration table to be grouped for reporting purposes. A compound can only be part of one single group. You create the groups in the calibration table. The calibration table contains only a number for each group; in a separate box, you assign a group name to the number and add one or more compounds. It is possible to perform a group amount calibration, where a total amount is assigned to the group. The amounts of the compounds in the group are calculated according to the response contribution to the total response. A common example is a mix of isomers where only the total amount is known, but the detector response of the isomers is identical.



## Unknown Samples

An unknown sample is a sample containing an unknown amount of the compound to be quantified.

To find out how much of the compound is in the unknown sample, you must:

- create a calibration curve for the compound,
- inject an aliquot of your unknown sample and run the analysis in exactly the same way as for the calibration sample,
- determine from the signal the response, which is the area or height of the peak due to the unknown amount of the compound, and
- use the calibration curve to calculate the amount of the compound in the unknown sample.

For example, if the area of peak in the unknown sample is 500, you can determine that the amount in the unknown is 5 ng/ $\mu$ l, by using the calibration curve shown in Figure 50 on page 185.

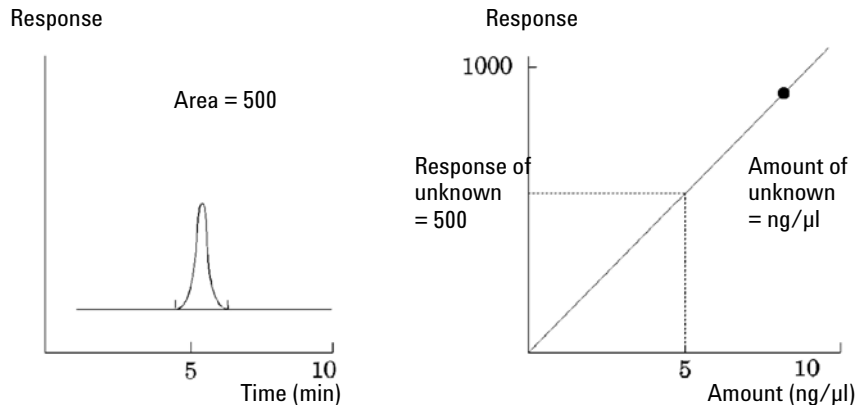


Figure 50 Signal from Unknown Sample and Calibration Curve

## Recalibration

### What is Recalibration?

Recalibration is the process used when you want to update a level on a calibration curve. When you recalibrate you run another sample that contains the same calibration compounds as the original, and most important, the same amount of these compounds. When you run the calibration sample, you obtain updated response factors and retention/migration times. You may also choose to average the response factors over a number of calibration runs so that response factors are weighted equally.

### Why Recalibrate?

Most calibrations have a limited lifetime, due to changes in chromatography. Recalibration is necessary to maintain the accuracy of the analysis. For example, assume you have created a calibration table for the compound caffeine which you use whenever you are required to quantify samples containing caffeine. At some point you will need to replace the column/capillary. Although the column/capillary is replaced with exactly the same type, it will not behave in exactly the same way as the previous column/capillary when you first created the calibration table for caffeine. Therefore, to ensure consistency you should recalibrate the levels in the calibration table before using the new column/capillary to analyze samples containing unknown amounts of caffeine. By doing this you are quantifying samples analyzed under the same system conditions.

### Manual Recalibration

You can enter peak calibration information manually and normalize the calibration table using the Manual Setup option button in the New Calibration Table dialog box. Typically, a new calibration method is produced by running a calibration standard mixture, creating a calibration table, and entering the amounts of all calibrated peaks to obtain response factors. This approach is useful for some applications, such as found in the petrochemical industry, where

the same compounds have been analyzed for many years and the response factors for various compounds and detectors are readily available.

You create the calibration table manually by entering peaks and their response factors into the calibration table, recalibrating the method using a standard that contains at least one response reference peak, and selecting Delta% update.

To reference to a specific peak for the calculation of retention time ratios, you can set this peak as a retention time ratio reference peak. All peaks with the same RT Ratio Ref # are then referenced to this peak.

## Recalibrations with Peak Summing

When a recalibration is performed, the retention/migration time ranges in the Peaksum Table of the method will be updated before the actual recalibration is done. Peak Sum recalibrations are performed in this way to ensure the delta is incorporated into the time calculations.

## Ways to Recalibrate

Recalibration can be done in two ways using the ChemStation software. You can recalibrate interactively or automatically during a sequence of automated analyses. Interactive recalibration is when you directly go through the process of recalibration using the ChemStation software after injecting one or more calibration samples. Recalibration using a sequence is where you specify when the recalibration occurs, but the automation software does the recalibration. For more information refer to [“Automatic Recalibration”](#) on page 124.

For information on how to perform recalibration using the software, see the How To part of the help system.

## Recalibration in Case of Missing Peaks

There are three ways to recalibrate unidentified peaks.

### No Recalibration

If a compound in the calibration table cannot be identified in the integration results, the calibration is aborted. If this occurs in a sequence, the sequence is also aborted.

### Partial Recalibration

This feature allows the recalibration of only the identified peaks. If peaks are missing, the calibration is not aborted but the report and the run log are annotated that peaks are missing.

### Recalibration of all Retention/Migration Times

This feature allows the retention/migration time recalibration of all identified and unidentified peaks. This is done by using the retention/migration times of the identified compounds. There is no update of response factors for unidentified peaks.

## Recalibration in Batch Review

The recalibration methodology in Batch Review differs from the recalibration in the original sequence.

Clicking the **Update Calibration** button on the batch review toolbar causes the system to recalibrate with all calibration runs in the batch, creating a recalibrated calibration table. Clicking the **Start** button on the Batch Review toolbar will then recalculate amounts for each calibrated compound. The amounts for all samples will be calculated from the recalibrated calibration table.

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This chapter describes the concepts of Intelligent Reporting and Classic Reporting.

## What Is a Report?

A report can comprise quantitative and qualitative information of the sample you analyze. The report can be a hardcopy printout, a display on the screen or an electronic file. The report can include details of the peaks detected during the run and plots of the signals that were acquired.

### Reports for different purposes

You can specify reports that serve different purposes during data acquisition and data review:

- The *sequence summary report* is defined in the **Sequence Output** tab of the **Sequence Parameters** dialog. This report is automatically created by ChemStation after completing a sequence acquisition or reprocessing a sequence.
- The *single injection report* is defined in the **Specify Report** dialog. This report is created for each single sample during a sequence acquisition or sequence reprocessing.

With Intelligent Reporting, you create templates for different report types, depending on the purpose of a report. For more information, see [“Report Types”](#) on page 197.

### Report destination

A report can be sent to the following destinations:

- **Screen**  
The report (including text and graphics) is displayed on the screen in the report preview window, from which it can be printed.
- **Printer**  
The report comprising text and graphics is printed on the currently selected printer.
- **File**  
The report is saved to a file, for example, an Adobe PDF file.

## Consideration of time zones

When you acquire data, you can see the injection date at different places in ChemStation and in your results. Depending on your local time zone and your regional settings in Windows, the displayed injection date may be adapted to the local time zone or date/time formats:

- in the logbook:  
This date is always shown in the local time of where data was acquired. It is not adapted when viewed in a different time zone, nor when printed on reports.
- in the **File Information** window of the data file:  
This date is always shown in the local time of where data was acquired. It is not adapted when viewed in a different time zone, nor when printed on reports.
- in reports:  
This field is adapted to local time zone and time format of the region in the world where the report is generated.

If data acquisition and report generation occur in the same time zone, all dates (logbook, data file, report) show the same time, only in different printed formats.

If you generate reports in a different time zone than the one where the data has been acquired: The reports will show the time of acquisition converted to the local time of the region.



The following example demonstrates how the acquisition date would be displayed at the different places in ChemStation, depending on the local time zone and regional Windows settings.

**Table 19** Example: Time representations for data acquired at Coordinated Universal Time (UTC) 2021-07-30 15:00:00

Event	Acquisition date/time converted to local format	Time format in the local Windows settings	Displayed acquisition date
Data acquisition and report generation in New York time zone UTC-05:00	2021-07-30 10:00:00	MM/dd/yyyy HH:mm:ss tt	Logbook: 2021-07-30 10:00:00 AM Data file: 2021-07-30 10:00:00 AM Classic report: 07/30/2021 10:00:00 AM Intelligent report: 2021-07-30 10:00:00+05:00
Report regeneration in Zurich (UTC+01:00).	2021-07-30 16:00:00	dd.MM.yyyy HH:mm:ss	Logbook: 2021-07-30 10:00:00 AM Data file: 2021-07-30 10:00:00 AM <b>Classic report: 30.07.2021 16:00:00</b> <b>Intelligent report: 2021-07-30 16:00:00+01:00</b>
Second report generation in New York (UTC-05:00)	2021-07-30 10:00:00	yyyy-MM-dd HH:mm:ss	Logbook: 2021-07-30 10:00:00 AM Data file: 2021-07-30 10:00:00 AM Classic report: 2021-07-30 10:00:00 Intelligent report: 2021-07-30 10:00:00 +05:00

## Reporting Results

Two types of reports are available:

- an uncalibrated report which does not correct for detector response, and
- a calibrated report that shows results corrected for the difference in the detector response to various components of the sample.

### Uncalibrated Reports

The uncalibrated reports include the **Area%** and **Height%** reports. These reports are mainly used in the preparation of calibrated reports. They may be of value as a final report if the amounts of compound required to produce a unit area or height response for the compounds of interest are similar.

### Calibrated Reports

Calibrated reports correct for the difference in the detector response to the reported compounds. One or more calibration samples containing known amounts of the reported compounds must be run under the same conditions used for the unknown sample. The integration data from these calibration sample(s) are used to prepare a calibration table. This is a list of



retention/migration times, amounts and responses which is used in the generation of the report. The calibrated reports are based on two calibration procedures called external standard and internal standard.

### External Standard Report

The ESTD report lists the results with the units of your choice or with each compound as a percentage of all the compounds present. One amount is used for all compounds in the calibration table and for the sample amount. The external standard procedure requires that the relative injected volume of both the calibration and unknown samples must be known accurately. The reliability of the external standard report is limited by the reproducibility of the injection and any other factors that might change from sample to sample.

### Internal Standard Report

The limitations of the external standard procedure can be overcome by using the internal standard approach. An accurately known amount (not necessarily the same amount) of the internal standard is added to both the calibration sample(s) and unknown sample. The response of each compound of interest is divided by the response of the internal standard to give a response ratio. The calibration curves are a plot of this response ratio versus the amount ratio and this information is used in the calculation of the reported results. In this way inadvertent errors in injection volume or slight changes in the chromatographic/electropherographic system that affect all compounds similarly are cancelled out. The ISTD report lists the results with units of your choice.

### Control Charts Report

The Control Charts Report tracks a single result from multiple runs for a specific calibrated compound. The **Control Chart** feature is installed after ChemStation is operational. Methods that use this feature pass the tracked result to a Microsoft Excel work sheet after each run. Excel is then used to print the report.

## Quantitative Results

The report type is identified by the name of the calculation method used to prepare it, for example, an ISTD report. Each type is briefly described below.

**Area%** provides the simplest report and requires no calibration data since no correction is made for the difference in detector response of sample

components. The Area% report is particularly useful in developing a calibration table for use with the other report options. This report is suitable for analyses in which the difference in detector response of the components is not significant.

**Height%** gives a report similar to the Area% report except that peak height is used for the calculations instead of peak area.

**Norm%** gives a report in which each component is reported as an amount percentage of all the components present.

**ESTD** produces a report of the actual amount of each substance. Amounts are calculated using a previously established calibration table. The use of an external standard requires that the injected volume of the calibration mixture be known.

**ESTD%** produces a report of the relative amount of each substance as a percentage of the injected sample amount. Amounts are calculated using a previously established calibration table. The use of an external standard requires that the injected volume of the calibration mixture be known.

**ISTD** produces a report of the actual amount of each substance. Amounts are calculated using a previously established calibration curve. The use of an internal standard in both the sample and the calibration mixture eliminates the need to know and control the volume of the sample injected. This also corrects for any variation in instrument performance between runs.

**ISTD%** produces a report of the relative amount of each substance as a percentage of the injected sample amount. The use of an internal standard in both the sample and the calibration mixture eliminates the need to know and control the volume of sample injected. This also corrects for any variation in instrument performance between runs.

## Classic and Intelligent Reporting

With ChemStation, you can choose the type of reporting you want to use: *Classic ChemStation Reporting* that is unchanged compared to ChemStation B reporting, or *Intelligent Reporting* (which is shared with OpenLab CDS).

The following sections describe the two types of reporting.

### Consequences of Activating Intelligent Reporting

If you want to use Intelligent Reporting, you need to enable Intelligent Reporting in the Instrument Configuration in the OpenLab Control Panel.

Activating Intelligent Reporting has the following consequences for ChemStation:

- The **Report Layout** view shows the Report Template Editor for Intelligent Reporting. Instead of classic report templates, you can now edit report templates for Intelligent Reporting in this view.
- The **Review** view is visible.
- In the **Sequence Parameters** and **Specify Report** dialogs, you can choose between Classic and Intelligent Reporting. You can still use the settings for Classic Reporting and use "classic" report templates that already exist for the instrument.

## Intelligent Reporting

### Advantages of Intelligent Reporting

Intelligent Reporting offers you the following advantages:

- You can use the **Review** view.
- Most of the functionality that is available in different settings and several dialogs for Classic Reporting is now part of the report templates. You can create or edit report templates using the **Report Layout** view, which contains the new Report Template Editor for Intelligent Reporting. The Report Template Editor offers several powerful functions:
  - You can access all result data generated by ChemStation by selecting the corresponding data field.
  - You can create your own expressions in order to make calculations with the data fields. You can use any valid Microsoft Visual Basic expression.
  - You can create expressions where you make calculations with the ChemStation Custom Fields.
  - Result Flagging: You can provide expressions to highlight specific results depending on their value.
  - Snippets: The Report Template Editor provides preconfigured report items, also referred to as *snippets*, that you can insert into your report template via drag and drop.
- You can use the Report Template Documentation Tool to create descriptions of your report templates.
- You can report the following values as defined by European Pharmacopeia (the peak-to-valley ratio is also available with Classic Reporting; for details on the required fields, refer to the *Reference Guide*):
  - Signal-to-noise ratio
  - Relative retention
  - Relative retention time

## Limitations of Intelligent Reporting

The reports generated with Intelligent Reporting are always based on the raw signals. Modified signals, where blank subtraction, smoothing, signal alignment, or background subtraction have been applied, cannot be reported.

## Report Template Editor (RTE) for Intelligent Reporting

### Report Types

You can create different types of reports. Depending on the report type, different data fields are available in a report template, and the report items are grouped differently.

The following report types are available

- **Single Injection**

The generated report shows the report items from the template separately for each injection in the current data scope. You can show the data per injection, but you cannot compare results from different injections in one table or matrix.

- **Single Sequence Summary**

The generated report shows the report items from the template separately for each of the sequences in the current data scope. You can compare results from different injections in one table or matrix, but not the results from different sequences.

- **Cross-Sequence Summary**

With this report type, the data is *not* automatically grouped. Therefore, you must pay more attention to the grouping of your report items, but in return you can create report items that compare data from different sequences.

### Template Format

All report templates are based on the Report Definition Language (RDL), which is a standardized XML format provided by Microsoft.

*RTE* provides an easy-to-use interface that helps you create report templates in a few steps. It supports all types of report items and most of the respective configuration options.

## Data Fields

You can access all result data generated by ChemStation during an acquisition. For each value you can select the respective data field in which the value is stored. You can arrange the data fields in the report template according to your requirements. The available data fields are arranged in the following categories:

- Sequence
- Sample
- Injection
- Signal
- Compound
- Peak
- Calibration Curve
- Instrument
- File
- Project

## Report Items

You can add various report items to a report template, depending on your requirements. For each report item you can configure several properties such as the font format, background color, expressions, etc. The following report items are available:

- Text Fields
- Data Fields
- Tables
- Matrices
- Composite Groups
- Images
- Chromatograms
- Calibration curves
- Spectra
- Charts
- Method Information

## Snippets

The Report Template Editor provides snippets, multiple preconfigured report items or groups of report items, which you can insert into your report template via drag and drop.

These snippets are, for example, preconfigured tables for compound results or system suitability, chromatograms for a single signal plot or multi signal plot, or control charts for calibration accuracy or retention time stability. You can use the snippets as a starting point and adjust them according to your requirements.

## Custom Calculation

In the Report Template Editor, you can either display the values of the data fields as they were generated by ChemStation, or you can calculate new values for different purposes. You can create expressions using the existing data fields and also using the custom fields.

You can store the values as variables and access these variables from a subsequent report item in the template.

The Report Template Editor provides an Expression Editor that helps you to create valid expressions. All expressions are based on Microsoft Visual Basic.

## Conditional Formatting

You can configure certain properties of a field or cell, depending on the values resulting from the expression. For example, if the compound amount is shown, you can create a condition for a red background if the amount exceeds a certain value.

## Demo Data

When you develop a new report template in the Report Layout view, ChemStation provides the demo data that is shown in the Report Template Editor when you edit or preview a template. The demo data corresponds to the data set (sequence or single runs) that is currently selected in the Navigation Table of the **Data Analysis** view. If you develop a template for a sequence summary report, you need to load a sequence in the Data Analysis view and select a subset of samples. If you develop a template for a single injection report, it is sufficient if you select only one sample in the Data Analysis view.

## Storage of Report Templates

ChemStation provides a number of predefined report templates. These default templates are located in the public documents folder in the REPSTYLE directory.

By default, the REPSTYLE directory is located under C:\Users\Public\Documents\ChemStation. This path is defined during installation. Use ChemStation menu **File >Open Windows Explorer...** to open the path in your system (for example, C:\Users\Public\Documents\ChemStation\1). Alternatively, use the shortcut to **Instrument Data** in the Start menu.

For sequences, the report templates used for sequence summary reports and single injection reports are located in the result set on the same level as the sequence methods. No report templates are stored on the data file level of a sequence.

### Browse Templates Dialog

If you browse for report templates in the **Sequence Parameters** dialog or in the **Specify Report** dialog, you can synchronize the templates in the Default Templates directory and in the result set.



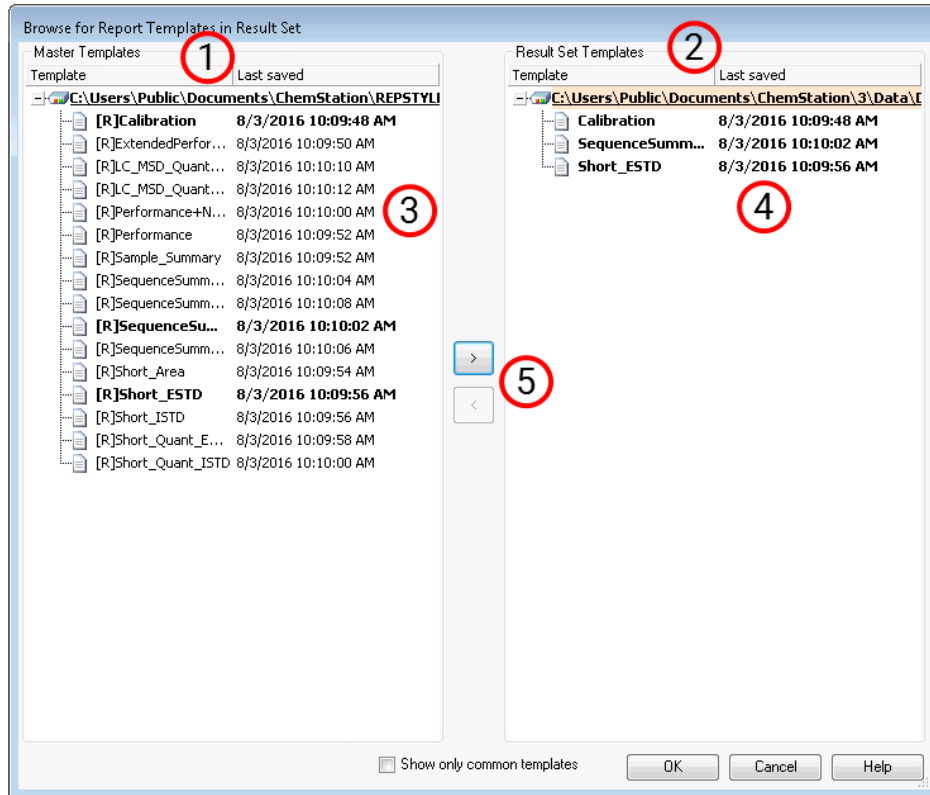


Figure 51 Browse for Report Templates in Result Set dialog

- 1 On the left side, you see the templates in the Default Templates directory (defined during installation).
- 2 On the right side, you see the templates in the currently loaded result set.
- 3 For each template, you see the date when it was last saved. The tooltip of the date shows the template's last history entry.
- 4 Templates that are common for the result set and the Default Methods directory are shown in bold. The templates are matched only by name.
- 5 You can copy templates from the Default Templates Directory to the result set either by using Drag&Drop or by using the > button.

## Storage of Generated Reports

### File Naming for Single Injection Reports

When you provide a file name for the single injection report in the **Specify Report** dialog, you can use the following tokens:

- <Date> current date
- <Time> current time
- <SeqName> sequence file name (will be "\_" for a single sample)
- <ResultSet> name of result set (will be "\_" for a single sample)
- <SampleName> sample name
- <LimsID> LimsID
- <InjDateTime> injection date & time
- <DataFile> data file name
- <SampleLoc> sample location

### File Naming for Sequence Summary Reports

When you provide a file name for the sequence summary report in the **Sequence Output** tab of the **Sequence Parameters** dialog, you can use the following tokens:

- <Date> current date
- <Time> current time
- <SeqName> sequence file name
- <ResultSet> name of result set
- <LimsID> LimsID

## Report Templates in Central Data Storage

If you use a central data storage system, report templates are treated as a separate document type. You can upload templates to central data storage, download templates from central data storage, or update all local report templates with the latest version from central data storage.

## Classic Reporting

### Reporting Custom Field Values

The values of the custom fields attached to a certain sample according to its acquisition method can be added to the report. Sample custom fields are listed at the end of the report header that contains the general sample information. Compound custom fields appear at the end of the report.

### Report Styles

You choose to add a signal to any of the classic report styles by checking the appropriate box in the Specify Report dialog box.

The following report styles are available:

- **None** - No text will be reported. The chromatogram will be reported only if the Add Chromatogram Output option is selected.
- **Short** - Comprises quantitative text results.
- **Detail** - Comprises header, quantitative results, and calibration curves. The header is stored in a file called RPTHEAD.TXT in the method directory. You can change the header using a text editor to include a method specific text.
- **Header + Short** - Comprises file header and quantitative text results. The header is stored in a file called RPTHEAD.TXT in the method directory. You can change the header using a text editor to include a method specific text.
- **GLP + Short** - Comprises header, sample information, instrument conditions, logbook, signal, and quantitative results. The header is stored in a file called RPTHEAD.TXT in the method directory. You can change the header using a text editor to include a method specific text.
- **GLP + Detail** - Comprises header, sample information, instrument conditions, logbook, signal, quantitative results, and calibration curves. The header is stored in a file called RPTHEAD.TXT in the method directory. You can change the header using a text editor to include a method specific text.
- **Full** - Comprises header, sample information, instrument conditions, logbook, signals, and quantitative results. The header is stored in a file called RPTHEAD.TXT in the method directory. You can change the header using a

text editor to include a method specific text. For data files containing spectra the apex spectrum for each peak is also reported.

- **Performance** - Produces a report according to the limits specified in the Edit Performance Limits dialog box of the System Suitability menu.

For uncalibrated methods, the report parameters include the peak number, retention/migration time, peak area, peak height, signal description, true half-height peak-width (please refer to *True Peak Width W<sub>x</sub> [min]* in the Reference Guide), symmetry, k', efficiency (plates) and resolution for each peak.

For calibrated methods, the report parameters include the peak number, retention/migration time, compound name, amount, signal description, true half-height peak-width, symmetry, k', efficiency (plates) and resolution for each peak.

The half-height peak calculation is not the same as the more complex peak width formula used by the integrator. The values of efficiency and resolution are based on this calculated peak width. The report header consists of all method relevant information, including instrument, column/capillary, sample, and acquisition parameters. The signal is also plotted.

- **Performance + Noise** - Combines the Performance report style with the noise calculations for the noise ranges defined in the Edit Noise Range dialog box of the System Suitability menu. In addition, the noise, given as six times the standard deviation, as peak-to-peak, and as ASTM noise. The drift and wander is also determined.
- **Performance + Extended** - Produces an extended report with all the parameters from the peak performance calculations and individual plots of each peak. The plots include the baseline, the tangents, and the peak widths at defined heights. This report type includes only calibrated peaks.

In addition to the parameters printed for the Performance report style, more Peak Performance Parameters are determined for calibrated peaks: the peak start and end peak times, skew, excess, peak width, USP tailing factor, time interval between data points, number of data points, statistical moments, plates, plates per meter, selectivity and resolution of each peak are printed. The peak width, plates, plates per meter, selectivity, and resolution are calculated by the true half height, 5 sigma, tangent and tailing methods (please refer to *Performance Test Definitions* in the Reference Guide for details).

The report header consists of all method relevant information such as instrument, column/capillary, sample and acquisition parameters and a plot of the signal. For a complete list of the peak performance parameter

algorithms refer to *Performance Test Definitions* in the Reference Guide for details.

The spectral report styles (**Short + Spectrum**, **Detail + Spectrum**, **Performance + Library Search**) are described in *Understanding Your Spectra Module*.

### Adding a Customized Report to Report Styles

You can add a custom report template that you have created in the Report Layout view of ChemStation to the list of available report styles.

#### NOTE

All reports apart from the performance reports list the peakwidths calculated with a more complex formula by the integrator (for details on the peakWidth calculation please refer to *Peak Width* in the Reference Guide).

## Other Report Style Parameters

### Summed Peaks Table

When the report is generated, ChemStation uses the peak sum table to produce a peak sum report that is printed after the standard report calculations.

### Report Layout for Uncalibrated Peaks

To change the report layout for uncalibrated peaks, choose one of the following in the Specify Report dialog box.

- Separately to report the uncalibrated peaks in a separate table if sorting by retention/migration time is selected, or separate tables if sorting by signal is selected.
- With Calibrated Peaks to report the uncalibrated peaks together with the calibrated peaks.
- Do Not Report to suppress the reporting of uncalibrated peaks.

## Sequence Summary Reporting

### Overview

ChemStation can print a variety of standard reports for individual sample analyses. Sequence summary reporting is an additional way of reporting, that allows you to calculate and report parameters across a number of different analyses. It is useful, for example, to test the stability of an instrument or the robustness of a new method.

A sequence summary report may include:

- a title page,
- instrument configuration, including the revision numbers of the instrument and details of the analytical column/capillary being used,
- sequence table listings which describe what the automated sequence of analyses should have done,
- logbook descriptions of what the sequence actually did and any unexpected events which occurred during the sequence,
- method listings,
- individual reports on each sample,
- statistics on the analyses based on selected criteria—*statistics are calculated only for calibrated compounds*, and
- a table of contents with page number references to the detailed sections of the report.

### Setting up a Sequence Summary Report

When setting up a sequence summary report, you can select any combination of the following nine categories by activating the appropriate check boxes and, where appropriate, selecting a report style from the template selections. Each template specifies the contents and layout of that particular section of the whole sequence summary report.

You can choose one of the following sequence summary report styles:

#### One Page Header

The GLP template prints GLP in large letters as a title page for the following report. It also includes the date and a place for a signature.

## Configuration

Select **Configuration** if you want to include the instrument configuration and analytical column/capillary specifications in the report.

## Sequence Table

Select **Sequence Table** to include a list of the samples, sample quantification parameters and method names in the report. This list shows what the system should have run.

## Logbook

Select **Logbook** for a listing of the analyses the system ran, including instrument conditions and any unusual events that occurred while the samples were being analyzed.

## Methods

Select **Methods** to list all the analytical methods used in the series of automated analyses.

## Analysis Reports

Select **Analysis Reports** to get individual analysis reports according to the report style set up for the method.

Individual analytical reports may be printed after each analysis according to the report style specified for the method in question, in addition to the report sections specified in **Sequence Summary Reporting**. See "Sequence Output" below.

## Statistics for Calibrated and Sample Runs

Selecting the Statistics cal. runs will produce statistical trend analyses for calibration samples. Selecting the **Statistics** sample runs will produce statistical trend analyses for sample (unknown) analyses. Both selections have Standard Statistic and Extended Statistic template styles. **Extended Statistics** prints the statistical trends of the analyses as graphs, whereas the **Standard Statistics** selection prints only text. The selections that you make in the **Items and Limits for Extended Statistics** dialog box are used only when you choose the **Extended Statistic** option(s) in the **Sequence Summary Parameters** dialog box.

If you choose the **Standard Statistic** option(s) in the **Sequence Summary Parameters** dialog box, then the statistics reported are:

- retention/migration time,
- area,
- height,
- amount,
- peak width (based on the report style, see ["Report Styles"](#) on page 203)
- symmetry.

The statistic calculation does not distinguish between different calibration levels in a sequence that uses multilevel calibration methods. This means that the concentration-dependent items, for example, Area, Height, Amount (see the dialog box for Items and Limits for Extended Statistics) are all taken together, regardless of the calibration level. The **Statistics for Calibration Runs** values are therefore not useful for multilevel calibration methods in sequences.

### Summary

The **Summary** selection will print an overview of the series of samples analyzed and the methods used. If the Summary choice is selected together with other Sequence Summary selections, page numbers referring to the other parts of the sequence summary report are included. Two Summary styles are available:

The **Sample Summary** tabulates details of the sample analyses run in the sequence, with some sample information such as the sample name, data file name, method and vial number.

The **Compound Summary** tabulates the sample analyses with basic quantification results for each calibrated compound, or each peak, depending on the type of report specified in the method.

### Sequence Output

In the **Sequence Output** dialog box you can define where the sequence summary report should be printed.

Select **Report to file** and enter a file name to print the report to the specified file. The default setting is that data are saved to the file GLPrpt.txt. In GC systems with dual injection the data are saved in GLPrptF.txt and GLPrptB.txt for the front injector and back injector respectively.

Select **Report to PDF** to save the report as a PDF document. The report is saved in the sequence folder with the name GLPrpt.PDF



Select **Report to HTM** to print the report in HTML format. The report is saved into an HTM directory in the data subdirectory or sequence container directory. The HTML report consists of an index file (index.htm) and at least two other files, a contents file (contents.htm) and a GIF (Graphics Interchange Format) file for each page of the report (e.g. page1.gif). To view the html report, open the index file using your browser.

Select **Report to printer** to print the report on the system's printer. Print individual reports for each run also activates printing of sample reports after each analysis. These reports are printed in addition to the reports specified for the sequence summary report which are produced at the end of the entire sequence. You can specify a new destination for these reports in the **Sequence Output** dialog or use the destination specified in the individual methods.

## Report File Formats

A report can be saved in different formats. Each format has a specific extension. It is possible to select more than one format for a report.

- .TXT** The report text is printed as a UNICODE text file.
- .EMF** Each report graphic (signal or calibration curve) is saved in a Microsoft Windows metafile (WMF). Several .WMF files for one report are possible. The generated file format adheres to the Microsoft standard metafile format as defined in the Windows software development documentation. These files are compatible with the Aldus Placeable Metafile (APM) format used by a number of proprietary software packages.
- .DIF** The tabular report data is saved in Data Interchange Format (DIF). This format is accepted by spreadsheet programs, for example, Microsoft Windows EXCEL. Independent from the report style selected, only the information contained in the report style Short will be saved.

### NOTE

DIF files are not generated for performance reports.

- .CSV** The report is in Comma Separated Values (CSV) format. This is a very simple format for tabular data that is accepted by many spreadsheet programs and databases. Independent from the report style selected, only the information contained in the report style "Short" will be saved.

There can be several .DIF and .CSV files for a single report. For each report block, the first file, for example, REPORT00.CSV, contains the report header information. Subsequent files contain the tabular results.

If the results are sorted by retention/migration time, only one file is required for the complete table, for example, REPORT01.CSV.

If the results are sorted by signal, a separate table is required for each signal. In this case, the files are named Report01.CSV through ReportNN.CSV, where NN is the number of the signal.

**NOTE**

CSV files are not generated for performance reports.

- .XLSX** The report is exported to a Microsoft Excel spreadsheet in (.XLSX ) format. The data generally requires additional processing.
- .PDF** The report is printed to a .pdf file. While any ChemStation session is running, a ChemStation PDF printer will be listed in the **Start Menu/Device and Printers**. The option **Unique pdf file name** allows you to store the .pdf reports independent of the reports, with file names <sequence\_container\_name>\_<data\_file\_name>.pdf

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This chapter is relevant only if you use ChemStation to control CE instruments.

## CE Agilent ChemStation Specific Functions in Method and Run Control View

### Vial Table

#### NOTE

The **Vial Table** functionality is available in the online ChemStation session only.

The **Vial Table** is a table that associates vials in the vial tray with samples, and, more importantly, with task specific vials such as buffers, flush vial, clean tubes vial, and the waste. The **Vial Table** is linked to the Sequence Table. When a sequence is loaded, the information from the Sequence Table is copied into the Vial Table. However, Vial Table entries are not transferred back into the Sequence Table. The **Vial Table Advanced Settings** dialog box is displayed when you choose the **Advanced** button in the **Vial Table**. It allows you to enable warnings of conflicts between the **Vial Table** and the method or sequence and the use of symbolic names. You must select **Enable vial table checks and warnings** to check for conflicts between the **Vial Table** and the method and sequence.

When a method or a sequence is loaded, a consistency check is made between the vial allocations in the **Vial Table** and those in the method or sequence. If there are any vial conflicts they can easily be resolved by using the **Conflict** tables.

#### NOTE

Position 49 in the vial tray is used for the needle wash vial and position 50 is left empty to allow the vial lift to return. These positions are not available in the **Vial Table**.

The **Used in** column of the Vial Table enables the usage of the vial to be specified. There are five valid entries for the **Used in** fields:

<b>Don't Care</b>	No consistency check is made
<b>Method</b>	The vial is referenced in the method
<b>Sequence</b>	The vial is referenced in the Sequence Table
<b>System</b>	<p>This is a special vial belonging to the system configuration. The <b>Name</b> must be one of the following symbolic names:</p> <ul style="list-style-type: none"> <li>• <b>@INLET</b> the inlet vial</li> <li>• <b>@OUTLET</b> the outlet vial</li> <li>• <b>@FLUSH</b> the flush vial</li> <li>• <b>@WASTE</b> the waste vial</li> <li>• <b>@clean tubes</b> the vial used for cleaning the replenishment tubes</li> <li>• <b>@USER X</b> (where as X can be 1 to 10) the sequence placeholder</li> </ul> <p>This option allows the specification of individual vial numbers for the symbolic names used in the method. This enables the user to specify different vials for Inlet Home, Outlet Home, Replenishment, Preconditioning, Postconditioning, etc. for each line in the sequence.</p>
<b>Not Used</b>	There is no vial in this position

## Method Conflict Table

The **Method Conflict Table** is displayed when you load a method that has vials defined that conflict with the vials defined in the Vial Table. The **Method Conflict Table** has two sides; the left half contains an image of the **Vial Table**; the right half shows the conflicting vials.

To resolve the conflicts you can select to either replace (single arrow) or to move the vial from the method to the next free position in the **Vial Table** (double arrow). This can be done for each conflicting vial in the table.

When user-defined vials (with symbolic names @User1, @User2, etc.) are used the conflict test cannot be performed on these vials, because without the sequence information it cannot be decided whether a conflict exists or not.



## Sequence Conflict Table

The **Sequence Conflict Table** is displayed when you set up or load a sequence that has vials defined that conflict with the vials defined in the Vial Table. The **Sequence Conflict Table** has two sides; the left half contains an image of the **Vial Table**; the right half shows the conflicting vials.

To resolve the conflicts you can select to overwrite the **Vial Table** information with the information from the **Sequence Table**, or if the conflict is caused by a system entry it cannot be overwritten. You can select to close the **Sequence Conflict Table** without resolving the conflicts.

When user-defined vials (in the columns User1, User2, etc.) are used the conflict test cannot be performed on these vials, because without the method information it cannot be decided whether a conflict exists or not.

## Peak Top Type

Unlike LC, GC, or MS peaks, it is quite normal for CE peaks to be asymmetrical. Because of this, it is very important to have the ability to select integration parameters that will yield the highest level of accuracy and reproducibility in your quantitation results.

The following peak top types are available when selecting **Peak Top Type** in the **Integration** drop-down menu:

### Highest Point

- select when the peak is triangular, and
- when you work with different concentrations

### Parabolic Interpolation

- use for tailing, unseparated peaks

### Center of Gravity

- provides more accurate calculations with triangular shaped peaks
- samples with similar concentrations

### Gauss Fit

- use for symmetric peaks

## Calibration Types

Standard Calibration is based on peak area or peak height. When you select **Standard Calibration** you have the option to **Calculate Signals Separately** or **Calculate with Corrected Areas**.

Calculate Signals Separately is selected when you want to ensure that, in the calculation of Norm% reports, the amount percent of separately reported signals add up to 100% for each signal. When **Calculate signals separately** is deselected, the amount percent of all signals add up to 100%. Selecting **Calculate signals separately** is a prerequisite for sorting by signal in the calibration table.

Select **Calculate with Corrected Areas** to make a correction to the peak area based on the migration time. In this mode, the area is divided by the migration time which can improve reproducibility in quantitative analysis when migration times are unstable.

In addition to the Standard Calibration, there are 3 capillary electrophoresis specific calibrations that are migration time based one signal.

The following calibrations types are available in the drop-down list for your Calibration Table:

- **Standard Calibration**
- **Protein Molecular Weight Calibration**
- **DNA Base-Pair Calibration**
- **Capillary Isoelectric Focusing Calibration**

For more information on the capillary electrophoresis specific calibrations, refer to *OpenLab ChemStation Data Analysis Reference* (CDS\_CS\_Reference.pdf).

## Migration Time Based Calibrations

Using Migration Time Based Calibrations in a Sequence

Migration time-based calibrations and recalibrations can be included in a sequence, but only explicit calibrations and cyclic recalibrations are supported; bracketed recalibration is not supported. There is no Sequence Summary report with migration time-based calibrations.



## Report Styles for Migration Time Based Calibrations

The report styles available for migration time based calibrations are limited to **Short** (quantitative text results) and **Full** (header, sample information, instrument conditions, logbook, quantitative results and peak purity plot).

## Calibration using Mobility Correction

Slight changes in buffer composition, run temperature or viscosity, as well as adsorption to the capillary wall, can influence the Electro Osmotic Flow (EOF) and cause it to be unstable. The resulting change in the EOF can create a rather high standard deviation of migration times. Corrections for mobility can significantly reduce the effect of run-to-run migration time shifts by monitoring the migration time of a mobility reference peak and in turn significantly increasing the migration time reproducibility.

The mobility reference peak should be chosen with the following priorities:

- Select peak with the highest signal
- Select the most isolated peak
- The EOF marker or internal standard can also be used as the mobility reference peak
- Enlarge the search window to always find the mobility reference peak
- If several peaks fall in the search window, the peak with the highest signal is automatically chosen as the mobility reference peak.

There are two mobility correction types available:

**Effective  
Mobility  
Correction**

**Effective Mobility Correction** uses the effective mobilities of all peaks and requires the availability of the voltage ramp data together with the electropherogram. In addition, working with effective mobility correction allows the true effective mobilities for all sample components to be determined.

**Relative  
Mobility  
Correction**

**Relative Mobility Correction** can operate in the absence of voltage data and would then assume a constant voltage for all measurements.

## CE-MS

## Background Subtraction

When you select the **Subtract Background** (BSB) menu item, the most recently selected mass spectrum is subtracted from each point in the current electropherogram. The resulting data is saved in the same directory and with the same name as the original data file; however, the file extension is changed to .BSB.

The new data file becomes the current data file and the background subtracted electropherogram is displayed. A record of the number of background subtractions that have been performed is kept in the Operator item of the data file header.

If you view a tabular listing of BSB data, you may observe differences due to the precision of data representation.

**NOTE**

The HELP text files in the LC/MS refer only to LC parameters and not CE. Some features that are available in the LC/MS software are either not available or not applicable to CE/MS applications but are used in LC. The function **peak matching** is not applicable for CE-MS and is therefore not active. In CE-MS, UV and MS detection occurs at different effective lengths of the separation capillary. Because of the different resolution at different effective lengths, peak matching is not possible.

## Method Subdirectories for different CE Modes

Methods in CE are dependent on CE mode selected. Therefore they are stored in different subdirectories in the Method subdirectory:

- CE** Stores methods for CE mode
- CEC** Stores methods for the CEC mode
- CEp** Stores methods for the CE plus pressure mode
- CEMS** Stores methods for the CE MS mode.
- CEMSp** Stores methods for the CE MS plus pressure mode.

## In This Book

This guide describes various concepts of Agilent OpenLab ChemStation. It is intended to increase your understanding of how ChemStation works. It contains information on the following subjects:

- Basic Concepts
- Data Acquisition
- Automation/Sequences
- Run Control
- Data Analysis and Review Concepts
- Calibration
- Reporting
- CE specific Concepts and Functions





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