Agilent ChemStation Plus

Getting Started Guide

Agilent Technologies

Notices

Manual Part Number

G2181-90017

Edition

02/08

Printed in Germany

Agilent Technologies
Hewlett-Packard-Strasse 8
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Software Revision

This guide is valid for B.04.xx revisions of the Agilent ChemStation Plus software, where xx refers to minor revisions of the software that do not affect the technical accuracy of this guide.

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In This Guide...

This guide provides detailed exercises and instructions for the workflow with your ChemStation Plus. This guide particularly describes the new functions made available through the integration of ChemStore into ChemStation. The guide is organized as follows:

1 Introduction

This chapter introduces you to the concept of ChemStation Plus. It visualizes and explains the workflow of the software suite. In addition, you learn how to start and prepare the ChemStation Plus for operation.

2 Setting up a sequence

In this chapter you learn how to set up and run a sequence. You also learn how to assign a study to your sequence and how to work with custom field data.

3 Finding results in ChemStation Plus

In this chapter you learn how to set up a query and retrieve data in the ChemStore Review Client.

4 Reviewing results with the ChemStore Review Client

In this chapter you learn how to customize the user interface of the ChemStore Review Client. In addition you learn how to view and evaluate results.

5 Reporting results

In this chapter you learn how to obtain and filter your data and how to report your results in the ChemStore Review Client.

6 Batch Reprocessing

In this chapter you learn how to select a transfer process for batch review, how to transfer the batch to ChemStation Plus, and how to edit the results in ChemStation Plus.

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1 Introduction

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This chapter introduces you to the concept of ChemStation Plus. It visualizes and explains the workflow of the software suite. In addition, you learn how to start and prepare the ChemStation Plus for operation.

Concept of ChemStation Plus

ChemStation Plus is an integrated networking data system (NDS). ChemStation Plus is operating in a client/server environment as well as a stand-alone solution. The software's main objective is to support a laboratory to meet the FDA's requirement for electronic records and signatures in regulation 21 CFR Part 11. ChemStation Plus can be purchased in several combinations and installed with several configuration options.

ChemStation Plus reflects the workflow of a chemical laboratory from the development of methods, to data acquisition, data processing, data storage, data review, and reporting.

ChemStation Plus consist of a suite of programs. Each program within the suite has specific capabilities.

ChemStation

ChemStation controls a variety of Agilent analytical instruments. ChemStation is designed to acquire 2 and 3D chromatographic data, and to provide a comprehensive set of software tools for qualitative and quantitative data analysis.

ChemStore

ChemStore manages ChemStation results. Using a database, all related data can be retrieved, reviewed and reported.

Security Pack

Security Pack provides the security and traceability functions needed for regulatory compliance and secure record keeping.

Workflow with ChemStation Plus

ChemStation Plus reflects the workflow of a analytical laboratory. ChemStation and ChemStore cover together the operational tasks required. Some tasks require a higher permission level and are executed on a less frequent base. These tasks are highlighted by the *(admin)* bracket.

Typical workflow

Initial set up of the ChemStation Plus.

a Set up necessary custom fields *(admin)*

b Create a study. A study is a folder in which the data is stored after a run. *(admin)*

1 Perform the analyses and acquire data in ChemStation view **Method and Run Control**.

a Set up a sequence.

b Assign a study and fill in custom field data.

c Run the sequence.

2 Execute a pre-defined query or set up a query in ChemStore *(admin)*.

3 Review data in the ChemStore Review Client.

a Reject, approve, or mark runs for reprocessing.

b Create a batch file.

4 Reprocess runs in ChemStation view **Data Analysis**.

a Load ChemStore batch file.

b Reprocess batch file.

c Correct processing method.

5 Define and print reports and charts.

The following diagram visualizes this typical workflow for ChemStation Plus. The grey colored tasks are typical ChemStore manager's tasks, while the white boxes represent a typical operator's workflow. This guide makes use of a ChemStore **Chemist** account who has sufficient administrative permissions to proceed with the examples.

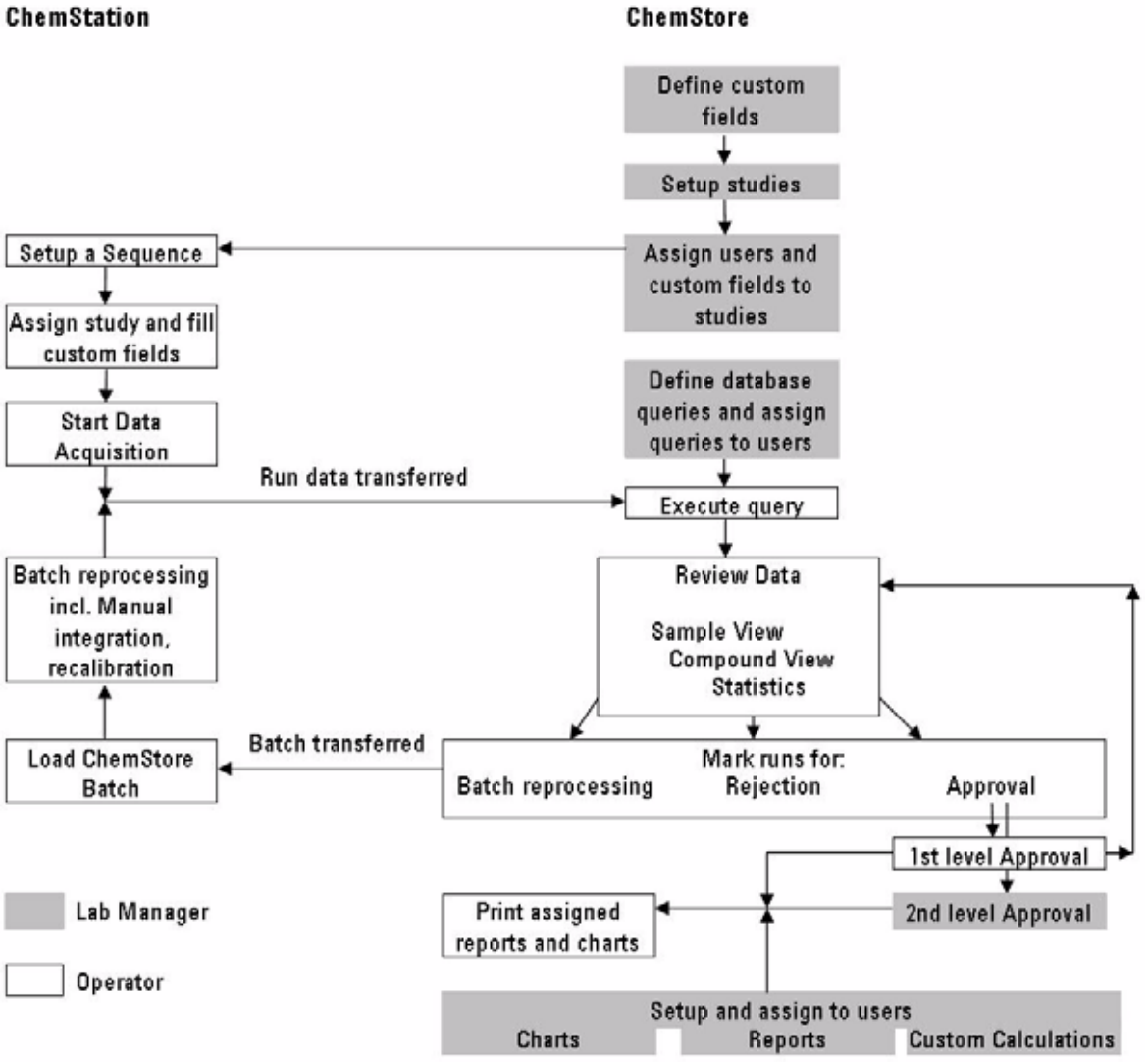

Figure 1 Workflow ChemStation Plus

Starting ChemStation Plus

Before you start

- Your administrator has:
  - installed all the necessary software packages for ChemStation Plus.
  - configured instruments.
  - set up the database to be used as the demo database delivered with ChemStore (ChemStoreDemo).
  - created studies and custom fields.

Please refer to the Installation Guide for the proper procedure.

Log on to ChemStation

1 Select **Start > Program > ChemStations > Instrument 1 Offline**.

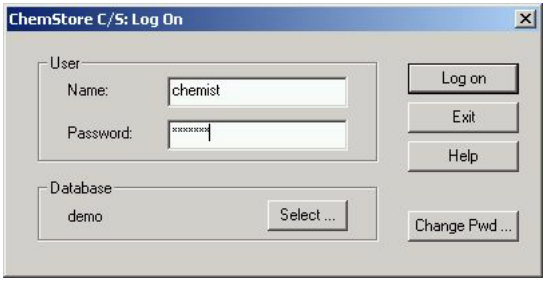

Figure 2 Log on

a Enter in the field **Name** `chemist`.

b Enter in the field **Password** `chemist`.

c Click on the button **Log on**.

2 A message informs you, that your password has expired.

Figure 3 Password expired

a Acknowledge the message by clicking **OK**.

3 The **Change User Password** dialog opens.

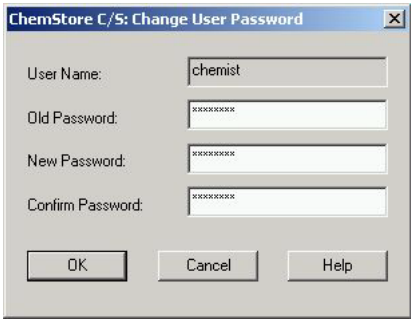

Figure 4 Changing password

a Enter in the field **Old Password** Chemist.

b Enter in the field **New Password** e.g. `12345678`.

c Enter in the field **Confirm Password** e.g. `12345678`.

d Click on the button **OK** to change your password.

4 If the **ChemStore Single Run Setup** dialog opens during startup, select **Part 11 demo** as the default study for single runs and all new sequences. This default selection might be changed later on.

5 The ChemStation Plus user interface opens in the view **Method and Run Control**. Note the presence of the ChemStore study information and ChemStore Lock and Review Client icon.

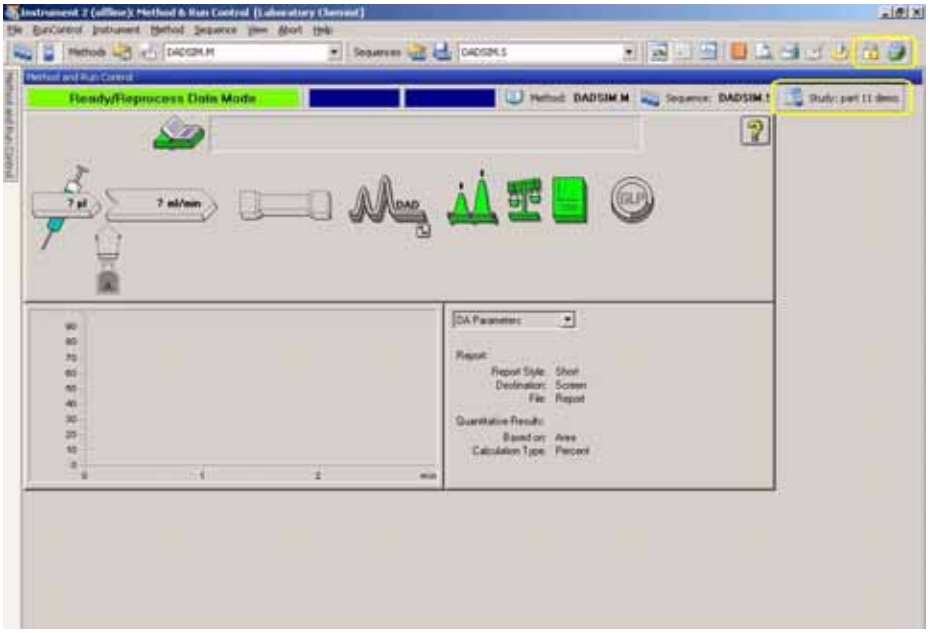

Figure 5 ChemStation Plus user interface with ChemStore study information

6 To start the ChemStore Review Client hit the Review Client icon.

2
Setting up a sequence

Selecting a sequence 16
Assigning a study and custom fields 17
Running a sequence 20

In this chapter you learn how to set up and run a sequence. You also learn how to assign a study to your sequence and how to work with custom field data.

Selecting a sequence

A sequence is a series of instructions that automate the analyses of samples. A sequence can automatically inject each sample, acquire and analyze the data according to a specific method, and print a report for each sample. A summary report may be generated for all samples with statistics. Each sample can use a different method, therefore different sets of instruments conditions and evaluation parameters may apply from sample to sample.

Before you start

- Log on to the ChemStation, off-line instrument
- During the start-up select **part11 demo** as the default study

Loading a sequence

1. Select the view **Data Analysis view** in ChemStation. The following example describes the process of sequence reprocessing, rather than acquisition of new samples. This does not require a running instrument and reduces the time for execution. Typically, you would work in ChemStation's **Method and Run Control** view where you would execute equivalent steps.
2. Load the demo sequence **DEMO_Sequence-2006-02-24-1** by double-clicking the name under the demo node in the ChemStation Explorer.
3. Navigate to **Sequence > Sequence table**. The sequence table opens and the default study gets assigned to all samples if the demo sequence was not used before. In case of an acquisition sequence you would edit the sequence table by adding samples to the table.

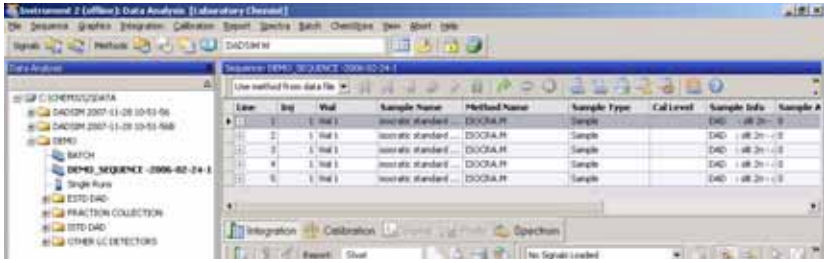

Figure 6 Loading a sequence in ChemStation's Data Analysis view

Assigning a study and custom fields

1 The ChemStation sequence table allows you to specify an individual ChemStore study per sequence line. You can only select studies that had been assigned to you. In order to select a single study for the entire sequence, you may use ChemStation's **Insert/Fill Down Wizard.** Processing a sequence table without a study selected is not possible.

In the current example change the study selection to **Procaine Decay** for one or two sequence lines. This study has a mandatory custom field assigned to it and you cannot close the sequence table with filling in some custom field values.

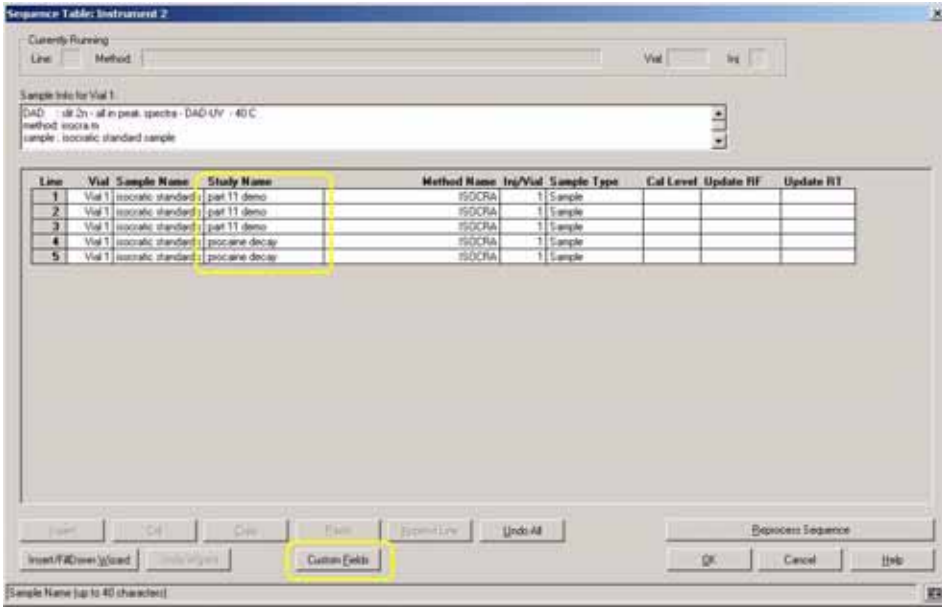

Figure 7 ChemStore study column in ChemStation sequence table

Assign custom fields

2 Click in the **Sequence Table** dialog on the button **Custom Fields**.

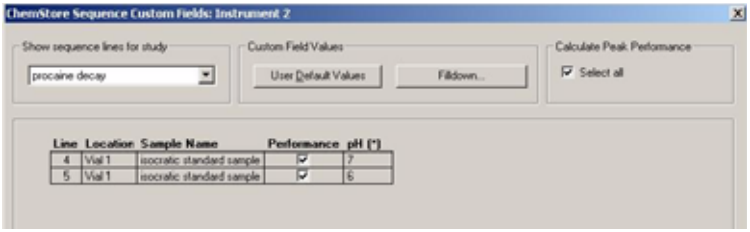

Figure 8 Custom field values

a Optional: Select the option **Select all** in the field **Calculated Peak Performance**. It will force the calculation of peak performance parameters, even if no performance report is specified in the ChemStation method.

b Enter the pH value for the lines **4** and **5**. e.g. 7 and 6.

c Click on **OK** and close the sequence table.

Transfer Settings

Transfer settings

3 Go to menu **Sequence \ Sequence Parameters**

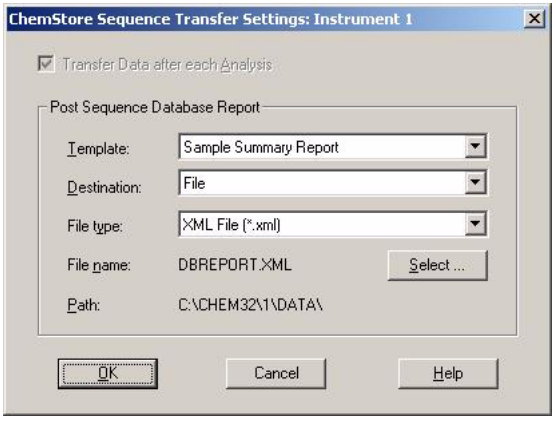

Figure 9 Transfer settings

4 Click on the button **Transfer Settings**

   a Select in the drop-down list **Template > Analysis Results Report**.

   b Select in the drop-down list **Destination > File**.

   c Select in the drop-down list **File type > XML file (*htm)**.

NOTE If Security Pack is not installed, you can select not to transfer the data after data acquisition.

5 Click on the button **Select**.

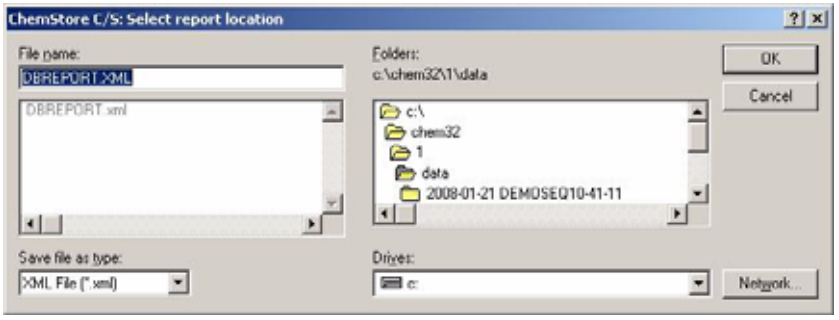

Figure 10 Select report location

6 Click on **OK**.

7 Exit the dialog **Transfer Settings** with **OK**.

8 Exit the **Sequence Parameters** dialog.

Running a sequence

1 Start the sequence from menu **Sequence > Start Reprocessing** or by pressing hot key **F6.**

In case of an acquisition sequence you would follow the equivalent procedure in the **Method and Run Control** view.

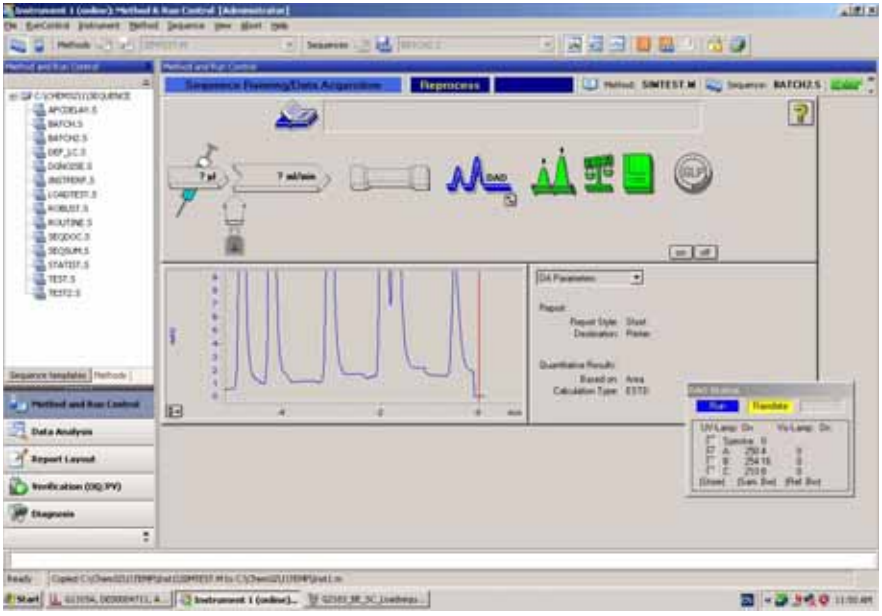

Figure 11 Running an acquisition sequence in Method and Run Control View

ChemStation Plus runs the sequence according to the selected method and stores the data in the defined studies.

3
Finding results in ChemStation Plus

Building a query 22

In this chapter you learn how to set up a query and retrieve data in the ChemStore Review Client.

Building a query

A query is the means to find the results in ChemStore after the data transfer and the data acquisition are complete in ChemStation. You can build simple and advanced queries. With the function advanced query you have additional search criteria available.

In this section we will search for the data transferred by the sequence that you just ran in the previous section.

Before you start

- Log on to the ChemStore Review Client.

Creating a simple query

1 Select in the ChemStore Review Client **File > Create Query > Simple**.

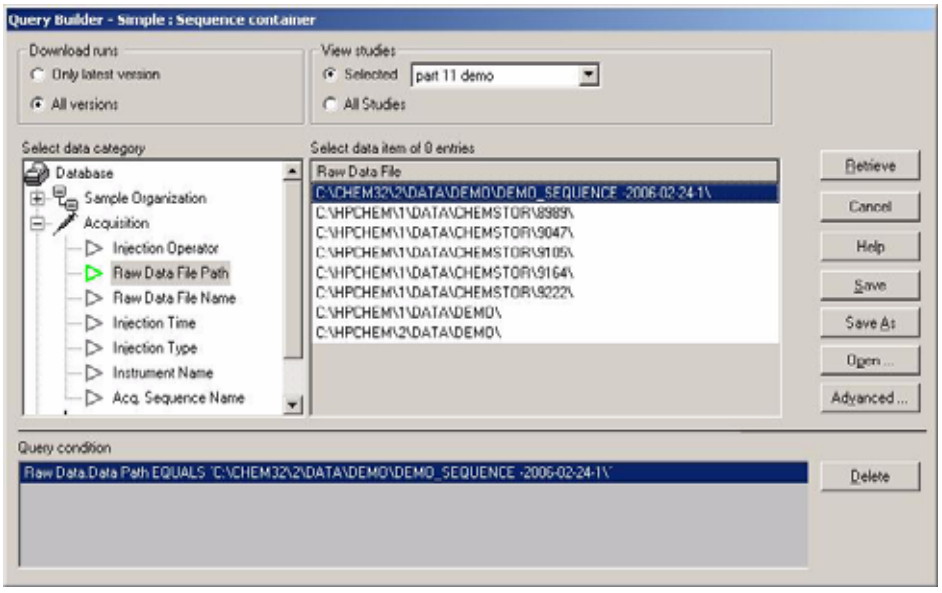

Figure 12 Create query

Select search criteria

1 In the **Download Runs** area select **All versions**

2 In the **View Studies** area select the study **part 11 demo**. This step is recommended as it shrinks down the number of selectable data items to a convenient degree

3 Select in the field **Select data category > Acquisition > Raw Data File Path**

   a Select in the 'data items' list the path name of the sequence container used during the previous step

b The selected query condition is marked in the field **Query condition**.

4 You may add a 2nd sequence container name in order to generate a cross-sequence report later on. Data items of the same data category are combined with a logical OR statement.

5 This is a very special query you may not want to use a second time. Nevertheless, it is recommend to save this query so can quickly create a similar one just by editing the saved query.

Saving a query

6 Click on the button **Save** in the dialog **Query Builder**.

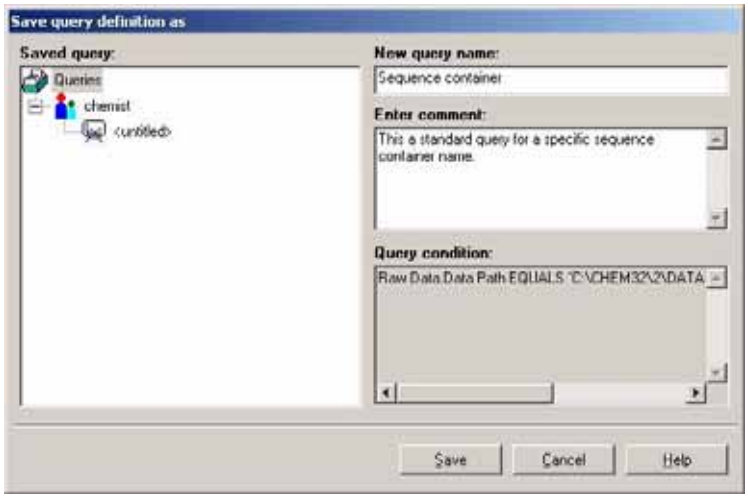

Figure 13 Save query

a Enter in the field **New query name** `sequence container`.

b enter in the field **Enter comment** e.g. `Is used most often`.

c Click on the button **Save** in the dialog **Save query definition as**.

d The query is now saved and can be selected under **File > Run Query > Sequence container**

Run a query

1 To run the just created query **sequence container**, click on the button **Retrieve**.

4 Reviewing results with the ChemStore Review Client

Layout of the user interface 28
Editing the layout of the user interface 30

In this chapter you learn how to customize the user interface of the ChemStore Review Client. In addition you learn how to view and evaluate results.

Layout of the user interface

When you open the ChemStore Review Client for the first time no user interface is defined and the screen shows no data. Although all data is available, none is displayed until you define a user interface and select some results for viewing.

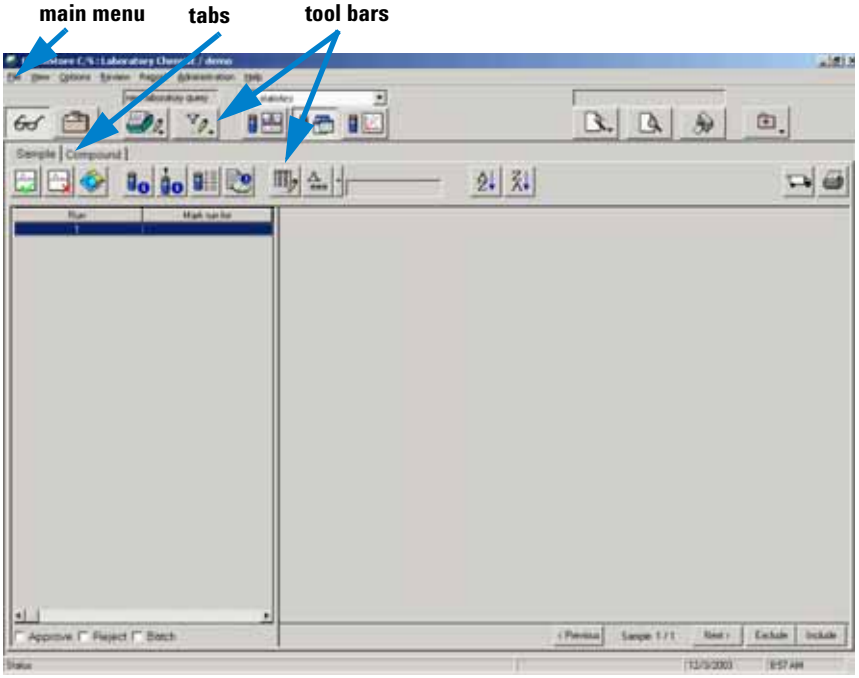

Figure 14 Empty user interface

The screen layout contains a main menu bar, a main tool bar, and the two tabs **Sample** and **Compound**.

Main menu

The following functions are available in the main menu:

- run and edit queries
- choose the different viewing options for results

- create charts and tables
- create and edit filters for data
- create and edit the user interface
- create, review and process a batch of runs for ChemStation
- create and edit a report
- change your password

Tool bars The tool bar contains icons for the most often used functions of the menu. To see the function of an icon move your cursor over the icon, a pop-up help names the function. Please refer to page 31 in the Concept Guide of ChemStation Plus for further information on the tool bars.

Tab Sample Use the sample view to see each injection (sample name and injection time) separate. This view is best for a typical sample-by-sample review workflow.

Tab Compound Use the compound view to see several compound related results in a series of injection. For example: amount, retention time, or area. This view is best for a compound-by-compound review on calibrated peaks.

Editing the layout of the user interface

You can edit the user interface to reflect your preferences. Edit the layout depending upon which type of results you want to view and how you want to visualize them. You can save your preferred layout.

Before you start

1 Select and run a query for the results you want to see, e.g. the previously defined query **Sequence container**

When working with the ChemStore Demo database you can load one of the pre-defined user interface definitions:

2 Select the menu **Options > Change User Interface Setting > Quality Control**, or click in the tool bar on the icon **User Interface Menu**  and select **Quality Control**.

3 Try the following layout options.

Layout options

NOTE All the data is available for viewing. With the layout option you select which type of data you would like to view.

Table 1 Sample tab

Icon	Description
	In the **Review Layout** you can view: • the sample information on the left of the screen • the chromatograph of the result in top right half of the screen • the selected type of results table on the bottom right half of the screen This layout represents an equivalent to a typical single run peak table. You would typically display data items like retention time, peak area, area%, compound name, amount etc.
	In the **Table Layout** you can view: • the sample information on the left of the screen • the selected type of results table on the right of the screen This layout can be used to mimic the ChemStation's sequence table or sample lists in general. You would typically display data items like sequence line, sample name, acquisition method, raw data file name, injection time etc.
	In the **Chart Layout** you can view: • the sample information on the left of the screen • a created chart on the right half of the screen

Table 2 Compound tab

Icon	Description
	In the **Review Layout** you can view: • the compound information on the left of the screen • the chromatogram and UV- or mass-spectrum of the calibrated compound in top right half of the screen • the selected type of results table on the bottom right half of the screen This layout represents a compound table equivalent to a compound specific sequence summary report. You would typically display data items like sample name, retention time, peak area, area%, amount etc.
	In the **Table Layout** you can view: • the compound information on the left of the screen • the selected type of results table on the right of the screen This layout represents a compound table equivalent to a compound specific sequence summary report. You would typically display summary or regression satistics of data items like retention time, peak area, area%, amount etc.
	In the **Chart Layout** you can view: • the compound information on the left of the screen • a created chart on the right half of the screen This layout can be used to plot various results, like amount, area, retention time etc. against injection time, run number or other numeric results. This results in a typical control chart or degregation plot.

Selecting results for viewing

You can select from a large variety of data types to view in the results table.

1 Go to **Options > Change User Interface settings >** select **Quality Control**

2 Switch to the Sample View/Table layout by using the menu **View > Sample > Table**

3 To edit the view of the result table select the menu **Options > Columns > Define...**, or click on the icon table  .

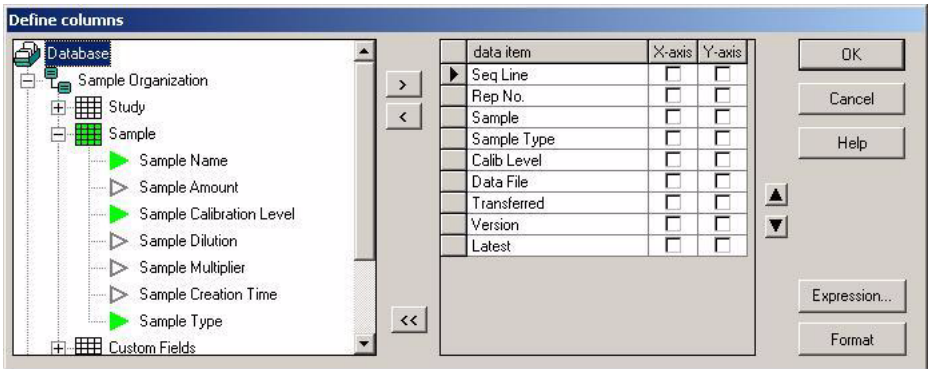

Figure 15 Define data items and display format in the Define Columns screen

4 This view is ideal for displaying a sample list. Select in the tree view the type of data you want to see, e.g. **Acquisition > Sequence > Acq. Sequence line**.

   a Click on the arrow pointing to the right to add this data category to your result table.

   b Select other typical items like **Acq. Sequence Repetition** (in case of multiple injections), **Sample Type** (under the Sample Organization > Sample node)**, Sample Calibration level, Raw Data File** (under the Acquisition > Raw Data node)**, Result Transfer Timestamp** (under the Results node)**, Result Version, Last Reprocessed Run Flag.**

5 Click on **OK** to add this data type to your results table.

6 Adjust the column width according to your needs before saving the user interface settings. Note: You may edit the column header description to your needs. Click the **Format** button in the **Define Columns** screen.

Saving your defined user interface

1 Select menu **Option > Save User Interface Setting...**.

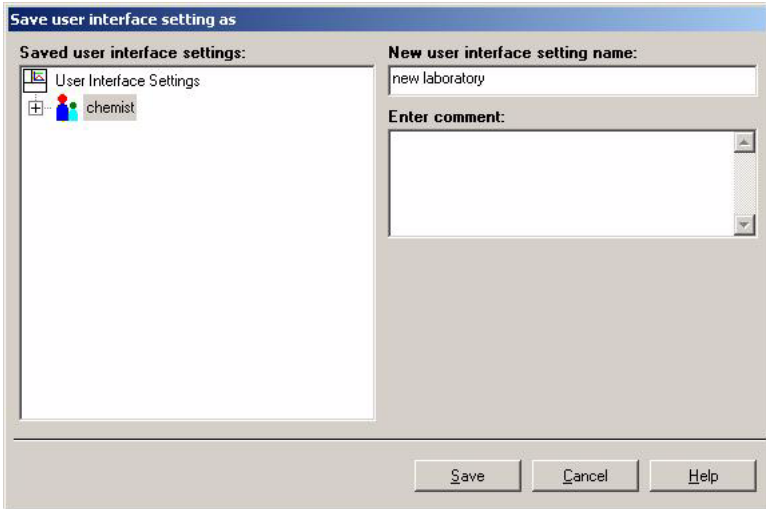

Figure 16 Save user interface setting

a Enter a name in the field **New user interface setting name**.

b Enter a comment (optional).

c Click on **Save** to save the new user interface.

d You can select the new user interface now under **Options > Change User Interface Setting > new laboratory**.

Now your new user interface layout can always be selected from the icon. 

NOTE Each time you change a new user interface or you close the ChemStore Review Client, you will be asked if you want to save the UI settings. Once you have a good layout, you can always say "No" to this questions.

5 Reporting results

Reporting workflow 36
Create report 38

In this chapter you learn how to obtain and filter your data and how to report your results in the ChemStore Review Client.

Reporting workflow

Before you start

Log-on to ChemStore as chemist, refer to Chapter 1, “Introduction”.

Run a query

1 Select the query **Sequence container** that you have created in Chapter 4. You can only see this query when you are logged in as user „chemist“.

2 Click on button **File > Run Query > Sequence container.**

3 To run the query **Sequence container**, click on buttons **Execute** and **Retrieve.**

Filter data for report (optional)

4 Click on button **Table layout** in the main menu and select the Sample tab (or use menu **View > Sample > Table**).

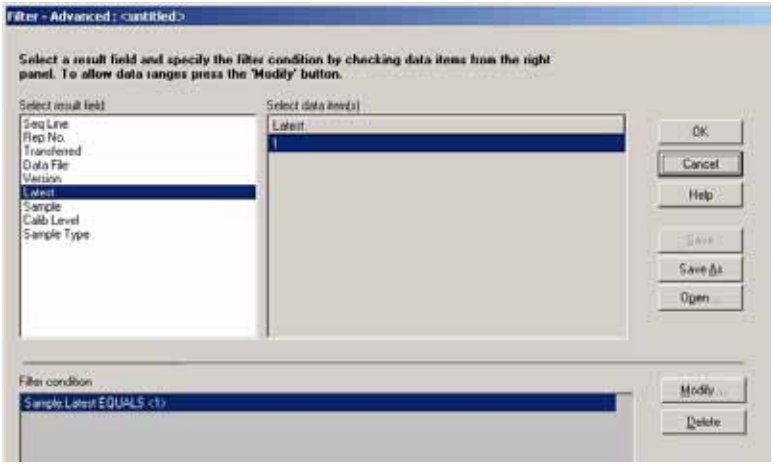

Figure 17 Filter definition

5 Click on button **View > Create Filter** in the main menu to create a filter.

6 Select the result field **Latest** and choose a data item **1** in the table. This will

generate a filter for latest result versions only, in case your query was based on **all result versions.**

Note: Only data items displayed in the table view are available for defining a filter.

7 Click on button **Save as** to save the current filter with the name **Latest versions**.

8 You can turn the current filter on or off in the menu **View > Filter** or by clicking on the button  in the tool bar.

9 Previous result versions will be hidden from the result table, without the need for re-executing the query.

With **View > Filter > Complement Filter** you can inverse the filter condition for e.g. quick toggling between sample and calibration runs. The filter condition would need to be based on the Sample Type, then.

Select report

Click on button **report** in the main menu.

Main menu The following functions for reporting are available in the main menu:

- select report to choose a report from the menu
- preview a report on the screen
- print report to print the report in a file or printer

Create report

Select report

10 Click on button **Report menu,** select a report from the menu or create, edit or manage an report.

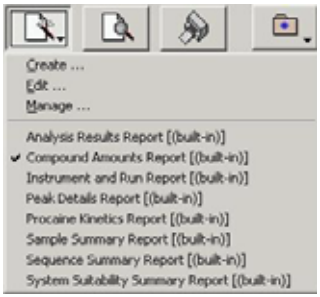

Figure 18 Report template selection

Print report

11 Click on button **Report preview**, the selected report is generated.

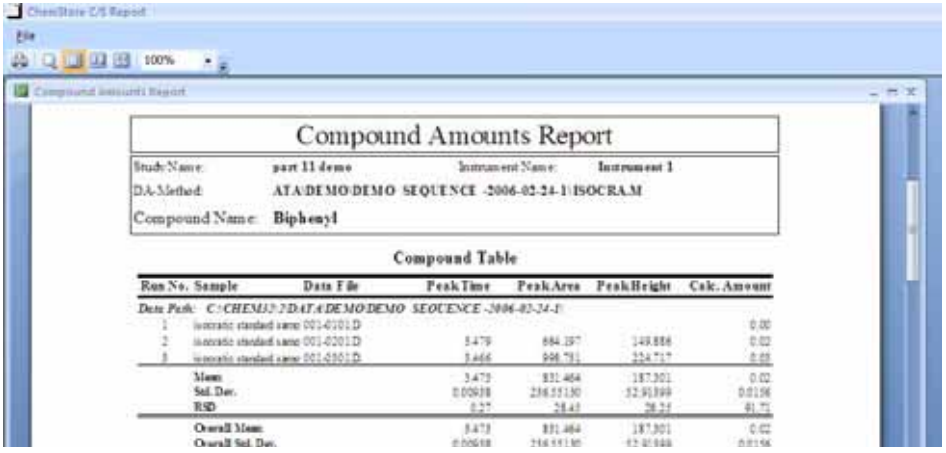

Figure 19 Report preview

6 Batch Reprocessing

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Manual integration 44

In this chapter you learn how to select a transfer process for batch review, how to transfer the batch to ChemStation, and how to edit the results.

If you work in an environment that is regulated according to CFR 21 part 11, Agilent recommends using batch review for data reprocessing. Batch review ensures automatic and full traceability of all results.

Creating and loading batches

Run a query

1 Select the menu **File > Run Query > Part 11 demo latest versions only.**

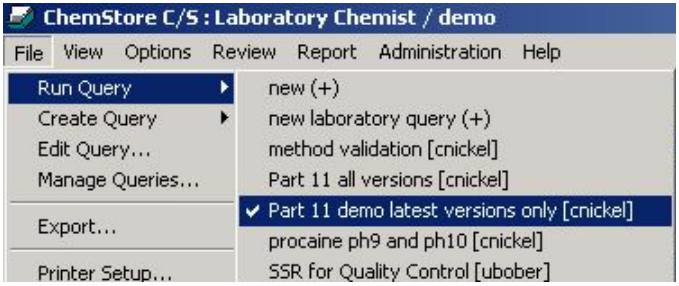

Figure 20 Run query

2 To run the query, click on buttons **Execute** and **Retrieve.**

3 The query is executed.

Create batch

1 Select a sample for batch review with a right-click in the context menu. You can select one or all samples.

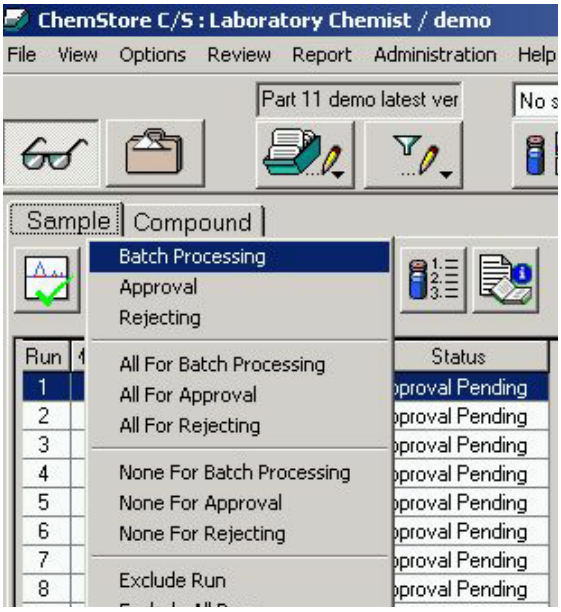

Figure 21 Select sample for Batch Processing

2 Select menu item **Review > Create Batch** or click on button **Create Batch**  .

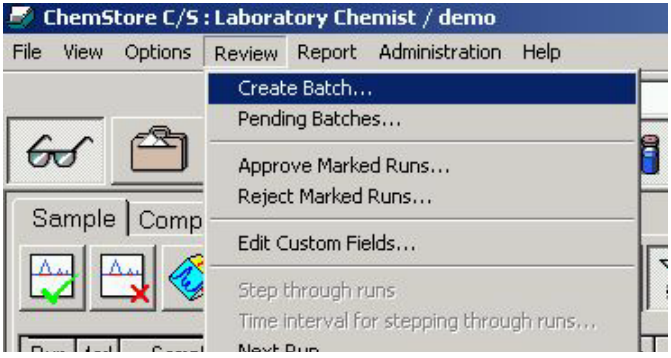

Figure 22 Menu Review > Create Batch

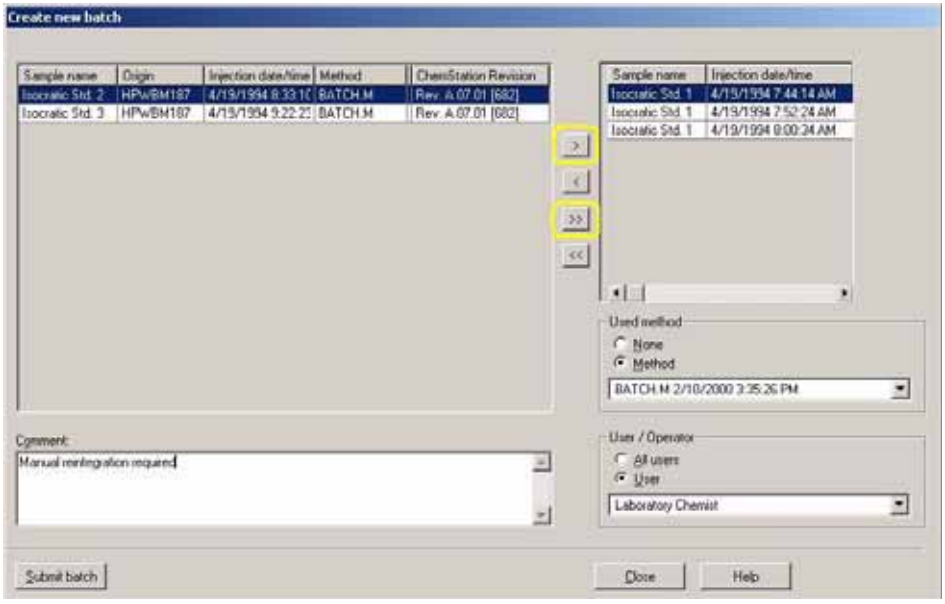

Figure 23 Submit Batch

3 Select and move the samples with the arrows to the right table.

4 Select in the field **Used Method** one of the options **Method** or **None.** Select in the drop-down-list the method you want to use to reprocess the batch (optional).

5 If you want the batch to be reprocessed by a certain user, select the user from the drop-down list.

6 Enter a comment (mandatory).

7 Click on the button **Submit Batch.**

8 Please switch to the ChemStation **Data Analysis** view.

9 Select menu **Batch > Load Batch > ChemStore.**

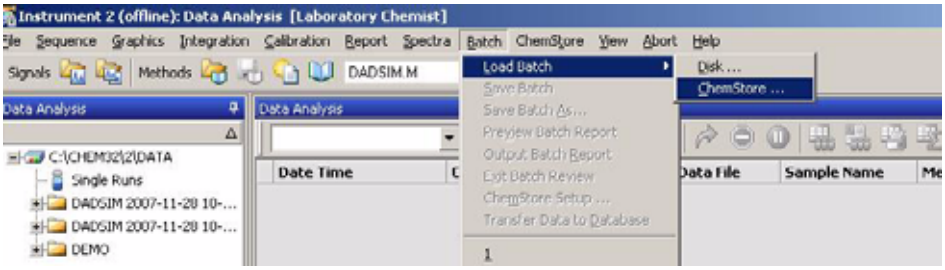

Figure 24 Load batch

10 The batches that are assigned to the current logged in user (or to all users) are displayed.

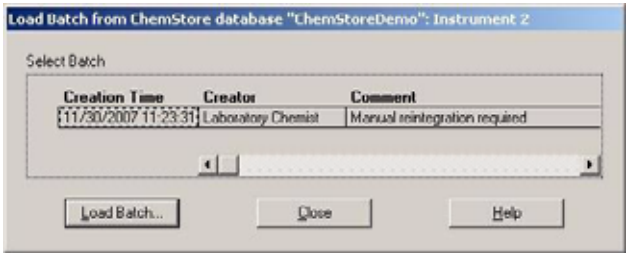

Figure 25 Selected Batch in database

11 Select a batch.

12 Click on button **Load Batch**.

13 The batch is ready for reprocessing and editing.

NOTE Please refer to the manual Security Pack User Guide and the Understanding Your ChemStation manual for more information on batch reprocessing.

Manual integration

Peak integration

In batch review all functions of the data analysis view work the same as without batch review. In batch review, all data files selected for this batch are listed in the lower half of the screen and can easily be selected. Manual integration events can easily be made and stored with each individual chromatogram, as will be shown in this section.

Note: The ChemStation explorer panel and the sample navigation table are hidden while batch mode is activated. Chromatograms can only be loaded through the batch table.

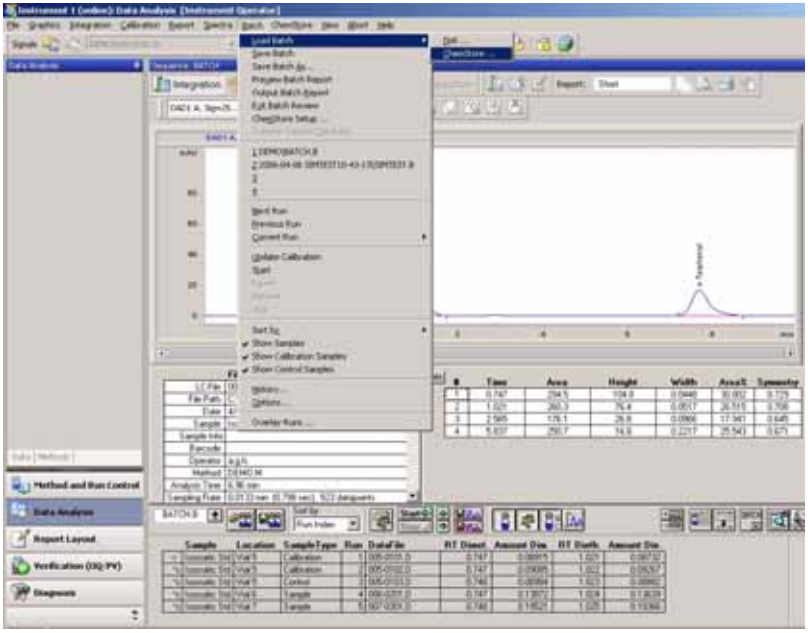

Figure 26 Chromatogram and batch table for sample selection

1 Zoom the y-axis to magnify the baseline position where you want to manually draw a baseline.

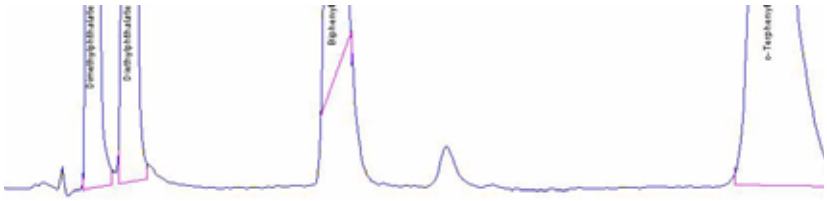

Figure 27 Magnified baseline area

2 Click the manual Draw baseline button or select menu **Integration > Draw Baseline**.

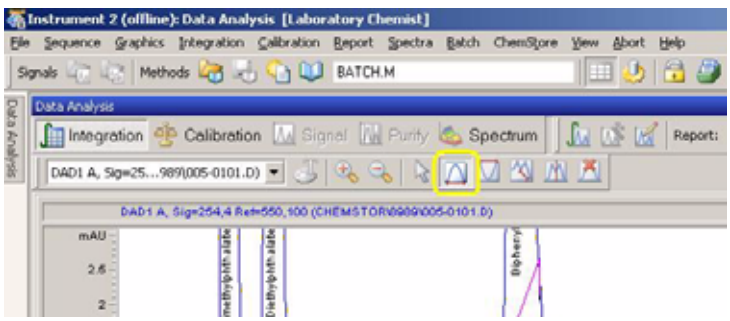

Figure 28 Draw Baseline

3 Draw manually a baseline for the peak you want to integrate.

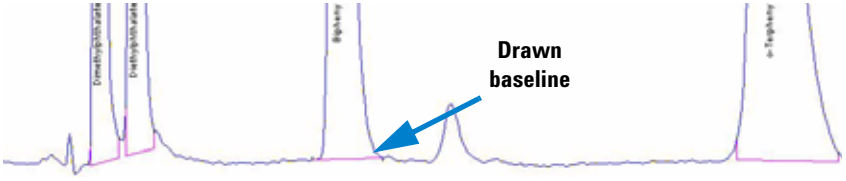

Figure 29 Manually drawn baseline

4 To store the manual baseline, just select the next sample.

Figure 30 Message „modified results“

5 Click on **OK** to save the modified results.

The window **Comment for Batch Processing** opens. It is mandatory to enter a comment stating the reason for the modification.

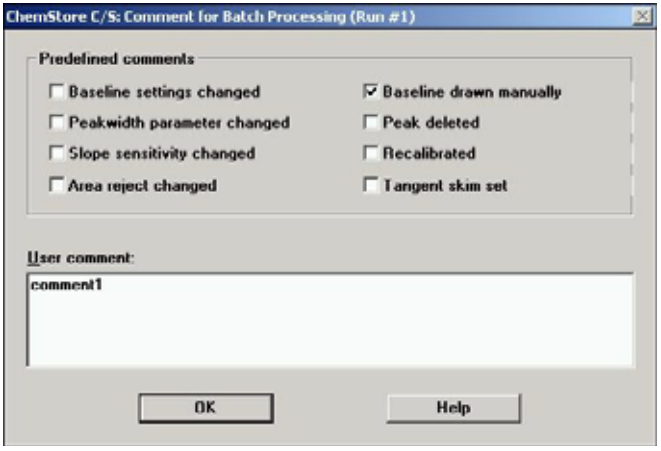

Figure 31 Comment Draw Baseline

6 Enter a comment or select a pre-defined comment.

7 Click on button **OK**.

NOTE

If Security Pack is installed, the changes in the marked run are saved automatically in the ChemStore database. The button **Save Changes** next to the **Start** button is inactive. Is Security Pack not installed, the button **Save Changes** is active and the user has to manually save the made changes.

Update calibration

In batch review, the calibration curve is created using all standards from the batch. Further details on calibration in batch review can be found in the „Understanding Your ChemStation“ manual.

1 Select menu **Batch > Update Calibration**.

2 The program re-calculates the calibration curve by equally weighting all calibration runs.

Before reprocessing the batch

1 Check all runs for valid data.

2 The default of the waiting time between runs is 10 seconds. Select menu **Batch > Options** to change the waiting time between the runs.

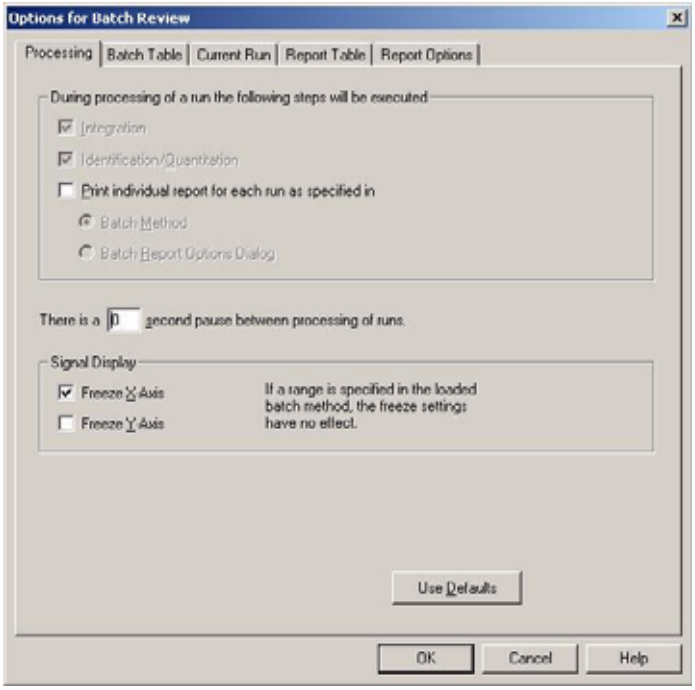

Figure 32 Menu Options for Batch Review

3 Change the pause from 10 to 0 seconds and click on button **OK.**

Reprocess the batch

4 Click on button **Start**  , to reprocess the batch with the new calibration.

The program starts to reprocess the runs automatically. The results are transferred and stored to ChemStore with the new calibration.

5 Select the menu **Batch > Exit Batch Review** to exit the batch.

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In This Book

This guide provides detailed exercises and instructions for the workflow with your Agilent ChemStation Plus.

This guide particularly describes the new functions made available through the integration of Agilent ChemStore into Agilent ChemStation.

Printed in Germany
02/08

G2181-90017

Agilent Technologies