Agilent OpenLAB Chromatography Data System (CDS)

ChemStation Edition

Reusing Data from ChemStation B.04.03 SP1 and SP2 in OpenLAB CDS ChemStation Edition C.01.06

Agilent Technologies

Notices

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Contents

1 Reusing Your Data in OpenLAB CDS ChemStation Edition with OpenLAB Data Store or OpenLAB ECM

This chapter describes a manual procedure for transferring ChemStation Sequences that were stored in containers (now called result sets), from a ChemStation file system into OpenLAB CDS ChemStation Edition with Data Store or ECM.

These instructions support the transfer of data from ChemStation B.04.03 SP1 to OpenLAB CDS ChemStation C.01.04 or higher.

Sequence Data Stored in Result Sets

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). If you use a central data storage system (*OpenLAB ECM* or *OpenLAB Data Store*), the complete result set (sequence/methods/data files/report templates) is transferred to the central repository as one entity.

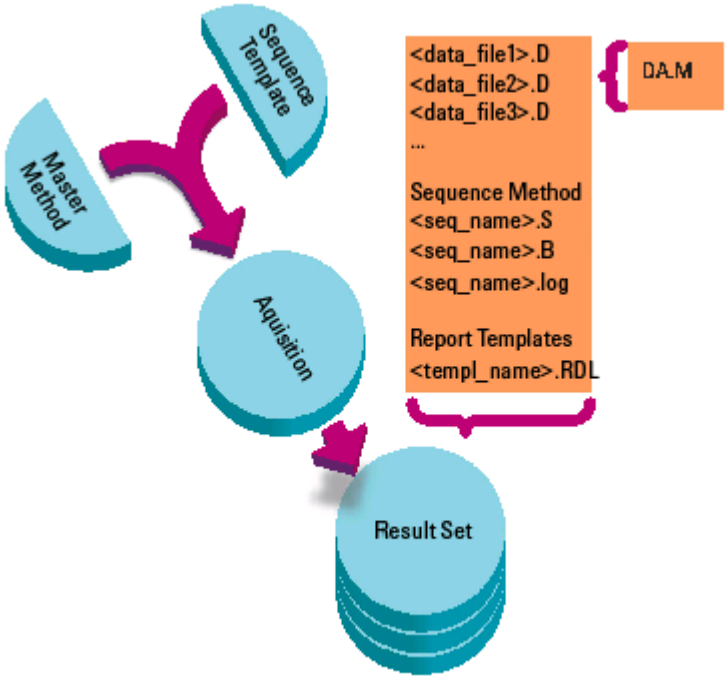


Figure 1 Sequence Acquisition with Unique Folder Creation ON

The methods in the folder Chem32\1\methods serve as master methods. They remain unchanged during acquisition and data analysis.

Similarly, the sequences in the folder Chem32\1\sequence serve as sequence templates that can be used to rerun (but not reprocess) a sequence several times.

Report Templates in the folder Chem32\repstyle serve as a starting point for developing your own report templates.

NOTE

If your data is not in this format, Agilent recommends changing your configuration now, to be ready to migrate easily in the future.

See "Step 1 – Verify Containers are in Use." on page 7, for more details on this.

Transferring ChemStation Data to OpenLAB Data Store or OpenLAB ECM

Requirements

The user who will carry out this transfer must be part of the Local Administrator group.

The user should have administrative privileges in ChemStation and in OpenLAB Shared Services (the **Everything** privilege in OpenLAB Control Panel) so he can edit the method and sequence data path, select the ECM or Data Store path in the transfer settings, and create and configure instruments in OpenLAB Shared Services.

The data to be transferred must be stored in containers (result sets).

Step 1 – Verify Containers are in Use.

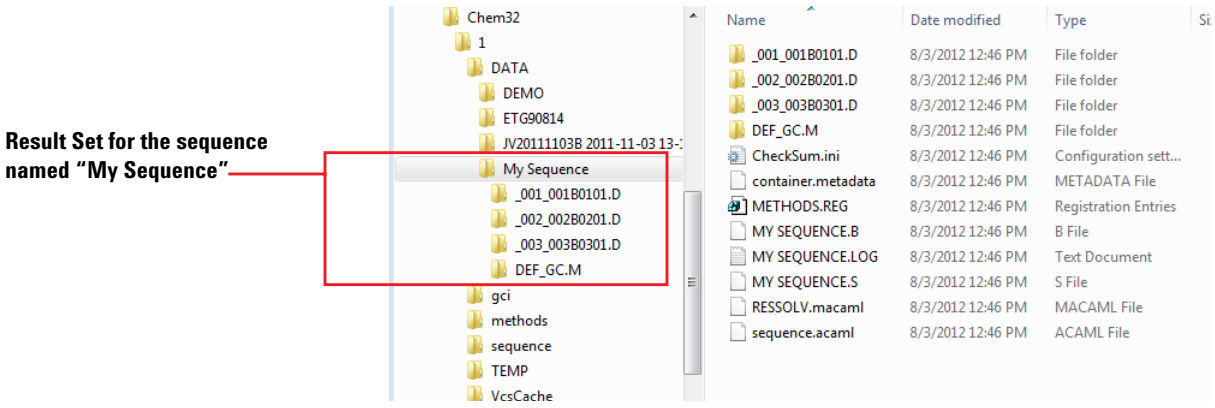
Only data stored in a container (result set) will transfer to Data Store or ECM.

Before continuing, verify that the data being transferred is in a container. Data in containers will look similar to the screen capture below. Notice that all the data files, the sequence file, and the methods used in the sequence are grouped in a single folder. This folder, known as the *container* in ChemStation B.04.03, is now called the *result set*.

NOTE

If you see the data is not in this format, Agilent recommends changing your configuration now, to be ready to migrate easily in the future.

For old data that is not in a container, create one as described in step 2.



For more details on ChemStation data Structure please refer to the *OpenLAB CDS ChemStation Edition Concepts and*

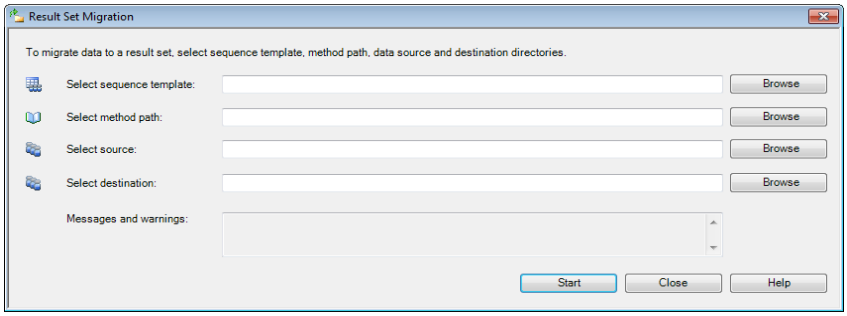
Workflows guide (M8301-90015).

Step 2 – Create a Result Set for Results that are not in a Container.

Use the **Result Set Migration** screen in ChemStation to make containers (result sets) for the data to be uploaded to Data Store or ECM.

NOTE Only use this procedure if you are certain about the sequence and method that was used to produce the data.

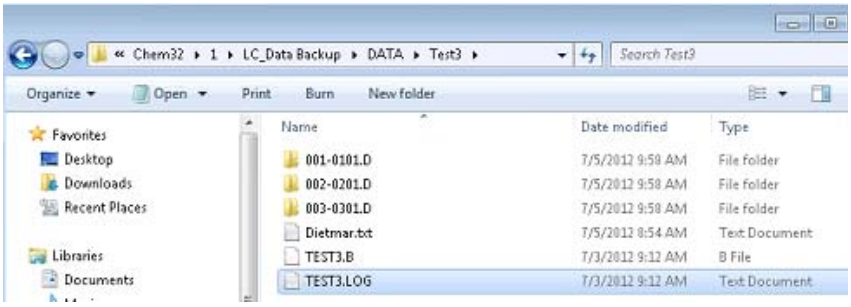
1 From the Data Analysis view of the OpenLAB ChemStation, select **Sequence > Result Set Migration...** to open the Result Set Migration dialog.



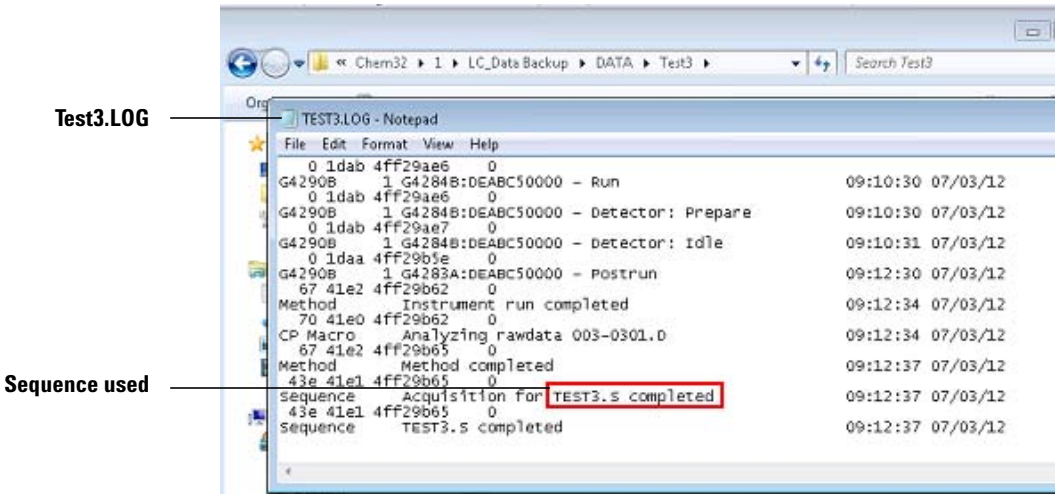
2 Navigate to, and select the sequence template from the ChemStation B.04.03 backup data acquired for that instrument folder.

If you do not know which sequence was used, please refer to *.log in data folder.

This figure highlights the log file (Test3.log) in the Test3 data folder:

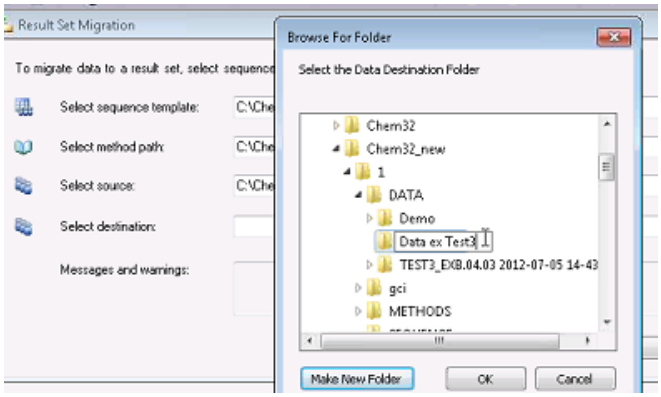


This figure shows the Test3.log file opened in Notepad, with the name of the sequence file highlighted:



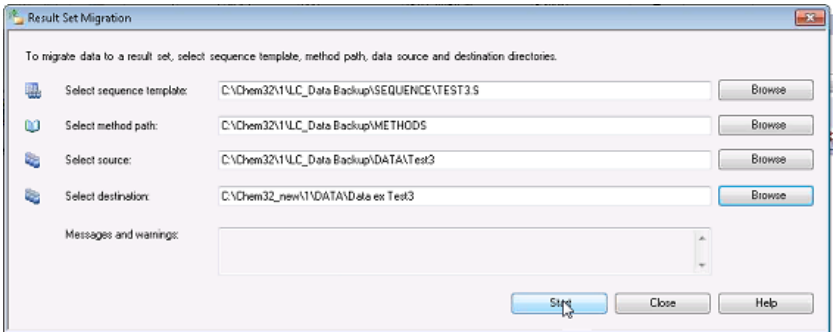
3 Select the Method folder from the ChemStation B.04.03 backup location.

4 Select the source folder from the ChemStation B.04.03 backup location.

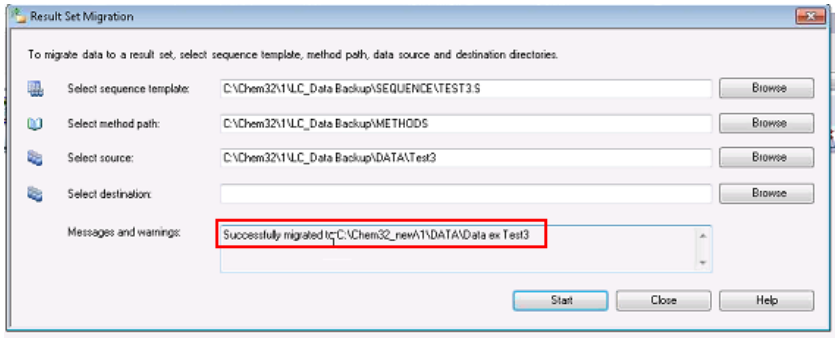


5 Select the destination folder. Create a new subfolder within the data folder structure of the upgraded C.01.04 location and select it as the destination.

6 Click **Start**.



7 If the result set migration was successful, an appropriate message will be displayed as highlighted in the figure below.



For more information on result sets refer to ChemStation documentation.

Step 3 – Manually Transfer Data Into OpenLAB Data Store or OpenLAB ECM.

1 Setup a client PC with a Data Store or ECM connection.

For ECM, please refer to the ECM Installation Guide.
For Data Store, please refer to the Data Store Installation Guide.

2 Create folders for your data, methods, and sequences in Data Store or ECM.

3 In the ChemStation **Method and Run Control** view, browse to **Data Store** or **ECM > Preferences**. In the **Preferences** dialog:

   a Click the **Paths** tab and enter the paths for Sequence, Data, and Methods that were used with the ChemStation file system.

   b Click the **Transfer Settings** tab and select the **Import After Reprocessing** check box. Verify that the data transfer path is set to the correct path.

NOTE

If the **Import After Reprocessing** check box is cleared and grayed out in the Preferences, this option needs to be enabled for the entire workstation in the ChemStation Administration Tool. This tool is accessible to administrators (under **Start Menu > Programs > Agilent Technologies> OpenLAB CDS ChemStation Edition**).

Add Methods from a ChemStation File System to Data Store or ECM

1 From ChemStation Explorer, in the **Method and Run Control** view, click the **Methods** tab and then double-click a method to load it.

2 Click **Data Store** or **ECM > Save Method**.

3 Browse to a folder created in Data Store or ECM and save the method.

4 The method icon in the ChemStation Navigation Pane will change from  to  indicating that the method has been saved to Data Store or ECM.

5 If the instrument configuration of the method being saved does not match the current instrument configuration, the configuration may need to be resolved prior to saving.

Add Sequence Templates from a ChemStation File System to Data Store or ECM

1 From ChemStation Explorer, in the **Method and Run Control** view, click the **Sequence Templates** tab and then double-click a sequence template to load it.

2 Click **Data Store** or **ECM > Save Sequence Template**.

3 Browse to a folder created in Data Store or ECM and save the sequence template.

4 The icon for the sequence template will change from  to  indicating the sequence template has been saved to Data Store or ECM.

Add Data from a ChemStation File System to a Data Store or ECM System

NOTE

For this way of importing data, the **Import After Reprocessing** check box must be selected in the **Preferences > Transfer Settings** dialog or in the ChemStation Administration Tool.

1 From ChemStation Explorer, in the **Data Analysis** view, click the **Data** tab.

2 Double-click data that you want to add to Data Store or ECM. Please note that only data stored in a container or result set will be transferred.

3 Reprocess the data by choosing the Reprocessing Mode and clicking  (**Start Sequence Reprocessing**) in the sequence reprocessing toolset.

4 Data from the file system will appear in Data Store or ECM. The sequence icon in the ChemStation Navigation Pane will change from  to  indicating that the sequence has been saved to Data Store or ECM.

Add Other Files from a ChemStation File System to a Data Store or ECM System

1 In the **Method and Run Control** view or in the **Data Analysis** view, Click **Data Store** or **ECM > Upload Files**.

2 In the **Upload file** dialog, select the file to upload and the target folder in Data Store or ECM.

You can add UV-libraries (*.uvl), column databases (*.mdb), Easy Sequence templates (*.est) or classic report templates (*.frp).

2 Reusing Your Data in a Standalone Open LAB CDS ChemStation Edition C.01.06 System

This chapter describes how to move methods, sequence and data files from a standalone ChemStation Workstation, version B.04.03 SP1 and SP2, to an OpenLAB CDS ChemStation Edition Workstation, version C.01.06 when the data is stored in the container mode.

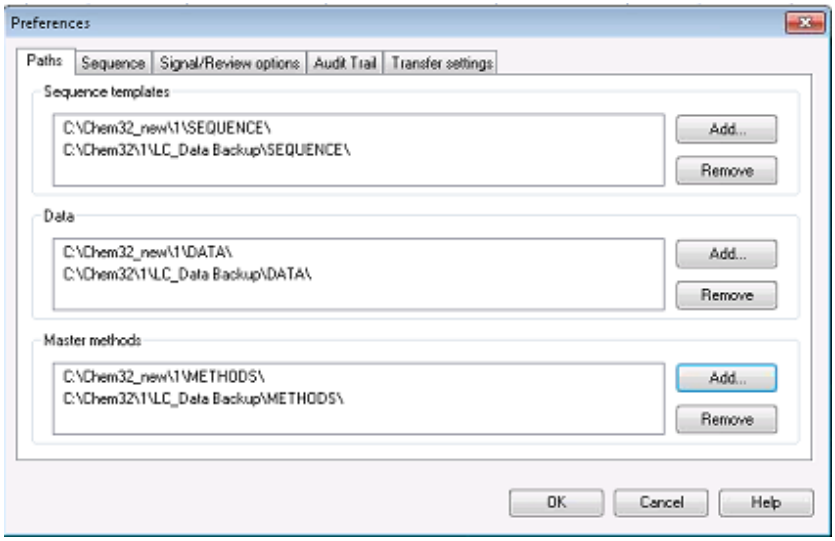
Also included in this chapter is a list of documents that contain more details on reusing data.

Steps to Migrate

1. Manually backup data acquired for all ChemStation B.04.03 SP1 instruments.
2. Run the Configuration Editor and record the following details of each configured instrument. You need these details to reconfigure your instruments in OpenLAB CDS ChemStation Edition C.01.06.
   a. Instrument number
   b. Instrument name
   c. Instrument type
   d. Connection settings (for example, IP address or GPIB address)
3. Uninstall all Add-On Solutions. Refer to the Add-On Solution manual for specific uninstallation instructions.
4. Install OpenLAB CDS ChemStation Edition C.01.06. During the installation, the Master Installer either uninstalls the previous ChemStation or moves it to a different folder before installing OpenLAB CDS ChemStation Edition C.01.06.
   - **If you choose to keep the existing ChemStation folder**, the installed ChemStation files are removed, and all user-created files are moved to a backup folder, for example, Chem32_001.
   - **If you choose to create a new folder**, the existing folder is retained with its original name.
5. To move data which was previously saved in a container mode, add the path from the ChemStation B.04.03 version to the new directory/machine by using the **Preferences > Path > Add** function.
   a. In the Data Analysis view, select **View > Preferences** to open the **Preferences** dialog box.
   b. Click the **Paths** tab.
   c. Press **Add** and navigate to the location of the sequence templates, data, and master methods, that were created by the ChemStation B.04.03 system. (This could be from the backup folder of the ChemStation B.04.03 system, which was prepared before upgrading to C.01.06, or the backup folder Chem32_001 generated by C.01.06 Master Installer.)

d Click **OK**.

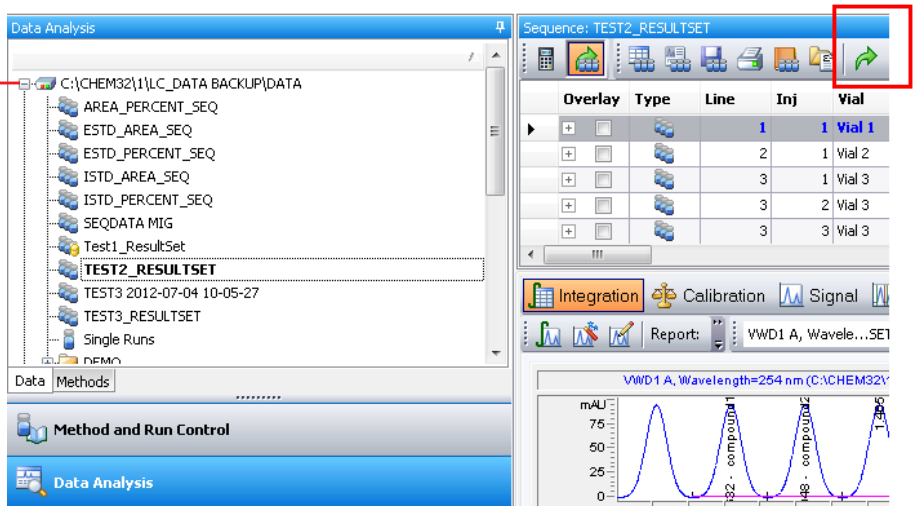
The selected paths and all the sequence templates, data, and master methods stored in them are now displayed in the ChemStation Explorer.



6 Double-click each sequence, one at a time, to load the associated data files into ChemStation memory, then click the **Start Reprocessing** icon to reprocess the data and generate a C.01.06 ChemStation result set. Please see the Checksum.ini and Sequence.acaml file for the time stamp to confirm that the data was reprocessed.

Start Reprocessing icon

Path identified in step 5



Facts to Know for Data Migration

Compatibility of ChemStation Entities

In general, forward compatibility is guaranteed. This means that it is possible to load methods, sequence templates and data from previous versions in newer versions. This is especially true for loading files from any ChemStation rev. B.xx.xx version into OpenLAB CDS ChemStation Edition rev. C.xx.xx. But there is no backward compatibility. Once a method or sequence template has been stored in OpenLAB CDS ChemStation Edition rev. C.xx.xx, it can no longer be used in a ChemStation rev. B.xx.xx. The same is true for data. Loading data files from OpenLAB CDS ChemStation Edition rev. C.xx.xx in ChemStation rev. B.xx.xx is not supported and could lead to serious issues with the data files creating wrong or incomplete results. Therefore Agilent recommends clearly separating ChemStation rev. B.xx.xx files from OpenLAB CDS ChemStation Edition rev. C.xx.xx files within ECM to make sure that files are not loaded in an older version by accident.

Migration of Reporting Templates

Currently there is no migration for old FRP report templates to the new RDL report template format. Old FRP templates will continue to work in OpenLAB CDS ChemStation Edition rev. C.xx.xx, but new RDL templates have to be created from scratch.

Migration of Classic Methods to RC.net Methods

RC.net methods were introduced in ChemStation rev. B.04.02. The method migration (migrating classic methods to RC.net methods) will still work the same way in OpenLAB CDS ChemStation Edition rev. C.xx.xx. An RC.net method cannot be converted back to a classic method.

Estimated Time to Upgrade

The estimated time to upgrade from ChemStation B.04.03 SP1 to OpenLAB CDS ChemStation Edition rev. C.xx.xx is approximately 30 minutes for software upgrade.

List of Detailed Documents to Reference

1. Overview of Upgrade procedures:

   Please refer to the chapter *Overview of the Upgrade Procedure* in the *OpenLAB CDS ChemStation Edition Upgrade Preparation Guide*, (M8301-90032, **CDS_CS-Upgrade.pdf** on disc 2)

2. Result Set Migration and more details on ChemStation data structure:

   Please refer to the chapters *Result Set Migration* and *ChemStation Data Structure* in the *OpenLAB CDS ChemStation Edition Concepts and Workflows Guide* (M8301-90015, **CDS_CS_Concepts.pdf** on disc 2)

3. Upload and reprocess workflows:

   Please refer to the chapter *Working with ChemStation and Central Data Storage* in the *OpenLAB CDS ChemStation Edition with Central Data Storage Concepts Guide* (M8301-90083, **CDS_CS-with-DataStorage.pdf** on disc 2)

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