

Migrating from OpenLAB CDS EZChrom Edition to OpenLab CDS Version 2.3 – Workstation to Workstation

User Guide



Agilent Technologies

Notices

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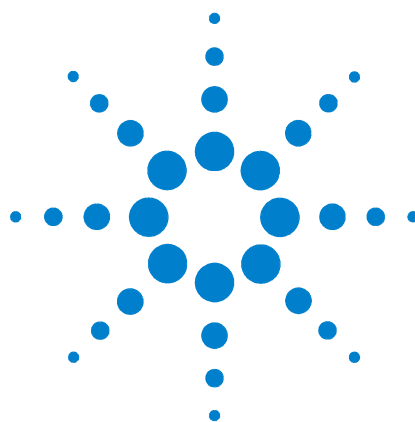
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Introduction

Overview 6

Migration is the process of moving your OpenLAB CDS EZChrom Edition methods and data to the new OpenLAB CDS version 2.3 environment. For OpenLAB CDS version 2.1 and higher, there are two versions of the workstation available: the basic Workstation, where all files are stored in the local file system of the computer, and OpenLAB CDS Workstation Plus, in which all files are stored in a content management database. This document includes information on how to copy files to both versions. Migration of other configurations is described in separate documents.

NOTE

This document describes migration procedures *without* the use of the Agilent Migration Tools for OpenLAB. For OpenLAB CDS EZChrom Edition, Agilent recommends using the Migration Tools for OpenLAB to migrate instrument information and data to OpenLAB CDS Workstation and Workstation Plus. For information on how to use the Migration Tools for OpenLAB, see the *Agilent Migration Tools for OpenLAB User Guide* provided with the OpenLAB CDS version software. Then see [Chapter 4](#) and [Chapter 5](#) of this document for information on how to migrate your methods.

This chapter provides an overview of the process required to migrate your existing OpenLAB CDS EZChrom Edition environment to OpenLAB CDS Workstation and Workstation Plus version 2.3.



Overview

This document describes migration of a standalone workstation running OpenLAB CDS EZChrom Edition to a standalone workstation running OpenLAB CDS Workstation or Workstation Plus version 2.3. Included are procedures for moving your existing environment to the OpenLAB CDS version 2.3; transferring data, methods, and reporting templates. [Figure 1](#) provides a graphical overview.

Before you start migration, the following assumptions apply:

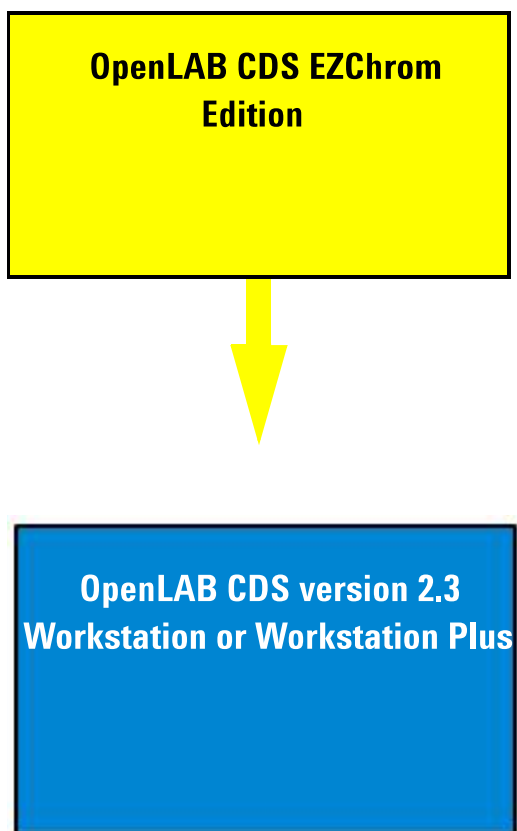
- You are familiar with the use of both data systems.
- You have one PC with OpenLAB CDS EZChrom Edition A.04.07 or higher installed. The files and data are stored locally or on a mapped network share location, without a back end database.
- You have a separate PC with OpenLAB CDS Workstation or Workstation Plus version 2.3 software installed. For information on supported instruments, see the *OpenLAB CDS Requirements Guide* supplied with your OpenLAB CDS version 2.3 software.

NOTE

Standalone workstation configuration assumes the workstations are not on a network. This document may describe optional procedures using a network, where use of a network makes the procedure easier.

NOTE

The procedures contained in this document have been tested when migrating from OpenLAB CDS EZChrom Edition A.04.07. At the time of writing this document, there are no known issues in using this procedure with earlier versions of OpenLAB CDS EZChrom Edition.



NOTE: Use of the Migration Tools for OpenLAB is recommended for exporting data from OpenLAB CDS EZChrom Edition and importing the data to OpenLAB CDS Workstation or Workstation Plus. (Steps 1 - 4)

Step 1: Read and perform the actions described in [“Before You Start”](#) on page 12.

Step 2: Copy all files to be migrated from OpenLAB CDS EZChrom Edition to a USB stick or hard drive.

Step 3: Move USB stick or hard drive to computer where OpenLAB CDS version 2.3 is installed.

Step 4: For OpenLAB CDS Workstation Plus version 2.3: Using FTP, copy result folders for all instruments and report templates from USB drive to OpenLAB CDS version 2.3 project folders. Copy method files to file system on OpenLAB CDS version 2.3 computer, or leave on USB drive. See [“Copying Files from OpenLAB CDS EZChrom Edition to OpenLAB CDS Workstation or Workstation Plus”](#) on page 20.

For **OpenLAB CDS Workstation version 2.3:** copy result folders and files directly to project folders in OpenLAB CDS Workstation version 2.3. See [“Copying Files from OpenLAB CDS EZChrom Edition to OpenLAB CDS Workstation or Workstation Plus”](#) on page 20.

Step 5: Migrate acquisition method. See [“Migrating Methods — Acquisition Parameters”](#) on page 37.

Step 6: Migrate processing method. See [“Migrating Methods — Data Analysis Processing Parameters”](#) on page 41.

Step 7: Migrate raw and results data. See [“Migrating Raw and Results Data”](#) on page 49.

Step 8: Recreate sequence. See [“Working With Sequences”](#) on page 57.

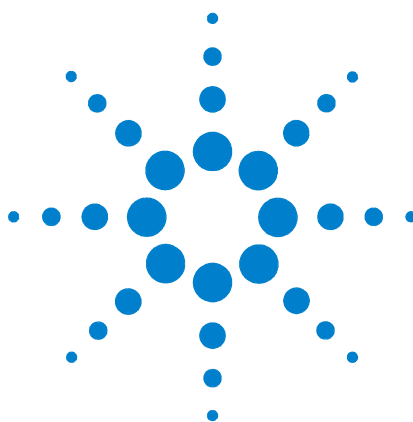
Step 9: Migrate report templates. See [“Migrating Intelligent Reporting Templates”](#) on page 59.

Figure 1 Steps for migrating OpenLAB CDS EZChrom Edition to OpenLAB CDS Workstation or Workstation Plus version 2.3

Table 1 gives a high level overview of the current migration capability from OpenLAB CDS EZChrom Edition to OpenLAB CDS Workstation or Workstation Plus version 2.3. When the migration status is “yes”, this means that capability exists. A notation of “yes” does not mean that the functionality automatically migrates.

Table 1 OpenLAB CDS EZChrom Edition functions and OpenLAB CDS Workstation or Workstation Plus version 2.3 migration status

Function	Migration Status
Raw Data Read & Display	Yes
Result Data Read & Display	Yes — For data stored in Result Package Mode. No — For data stored in File Mode or Advanced File System, raw data must be imported and then reprocessed with an OpenLAB CDS version 2.3 processing method.
Method	Yes Splits into: <ul style="list-style-type: none"> • Acquisition Method — RC.NET only • Processing Method (Compound import) • Sample Prep Method — Migration not yet supported.
Sequence Templates	Create new sequences
Reports	Classic Reports = No Advanced Reports = No Intelligent Reports = Yes
Instrument Configurations	Instrument configurations are taken from the meta data in the results
Custom Parameters	Not migrated. Must be manually added in OpenLAB CDS version 2.3.
Drivers	Yes— RC.NET only Note: See the <i>OpenLAB CDS Requirements Guide</i> supplied with your OpenLAB CDS version 2.3 software to verify that the instrument drivers are supported with OpenLAB CDS version 2.3



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This chapter provides planning information and steps you should perform prior to the migration of methods and data files from an OpenLAB CDS EZChrom Edition standalone workstation to OpenLAB CDS Workstation or Workstation Plus.



Facts to Know About OpenLAB CDS

Compatibility

Files created in OpenLAB CDS are not readable by OpenLAB CDS EZChrom Edition.

UV- libraries (*.lib), Easy Sequence templates (*.est), standard/classic report templates (.srp and .rep), and advanced report templates (.tpl) that operate in the OpenLAB CDS EZChrom Edition environment are not supported in OpenLAB CDS.

Planning your migration

Successfully executing your data system migration requires collaboration and a planned approach.

Agilent is taking steps, in the form of self-help resources, documentation, migration services, and connections with partners to help workstation customers handle this change. Contact your sales team for information on available resources.

The evolution of OpenLAB CDS EZChrom Edition Automation Toolkit in OpenLAB CDS

OpenLAB CDS version 2.3 does not support the OpenLAB CDS Automation Toolkit (ATK). OpenLAB CDS includes a reporting system that can be used to create text files for data interchange with other systems.

As OpenLAB CDS evolves, additional capabilities such as a Software Development Kit (SDK) will be available to aid you in customizing OpenLAB CDS workflows. Contact your Agilent representative about availability of these resources.

Custom calculations

The new Custom Calculation Editor feature in OpenLAB CDS offers a flexible, fully integrated way to create custom calculations. These are defined in the Custom Calculation Editor using the Microsoft Visual Basic .NET syntax that is similar to Excel formulas. Simple custom calculations can also be done as part of custom reports. For information on how to use the Custom Calculation Editor, see the OpenLAB CDS online help.

NOTE

It is important to note that the results of any calculations are stored as part of the data record and are securely stored in the repository. Custom calculations are stored explicitly with the results. Calculations done as expressions within the report template are not stored with the results.

Custom reports

Custom reports are created in data analysis reporting. The reporting is much simpler to use and allows for easy creation and editing of reports. This reporting is already available as Intelligent Reporting in the OpenLAB CDS EZChrom Edition.

Method setup in OpenLAB CDS

OpenLAB CDS has three method types: a sample preparation method, an acquisition method (using RC.NET), and a centralized, instrument-independent processing (data analysis) method, which are saved in individual files. The separation of method files enables you to use the individual parts more efficiently. For example, you can now combine acquisition methods for different instruments with the same data analysis processing method. This new approach replaces the all-in-one method design in OpenLAB CDS EZChrom Edition.

Storage concepts for OpenLAB CDS Workstation and Workstation Plus

OpenLAB CDS Workstation Plus Includes Content Management (formerly called Data Store). Your data, methods and report templates are now stored in a common repository on your workstation. You can browse, access, and manage all your data from the Data Selection view in Data Analysis. Furthermore, you can take advantage of the built-in data management features.

OpenLAB CDS Workstation Provides an open file system for those who prefer an NTFS file-based system. The file-based system can be set up in a secure or non-secure manner. (Note: If file system security has been enabled, you must be logged into the computer as a member of the local Windows group AgtSfsGroup in order to access the project folders.)

Before You Start

Before you start the process of migrating from OpenLAB CDS EZChrom Edition to OpenLAB CDS, review the following information and perform any required tasks.

Supported software versions

OpenLAB CDS EZChrom Edition methods can be migrated from revision A.04.06 and A.04.07, and A.04.07 SR1 and SR2.

Back up your existing OpenLAB CDS EZChrom Edition files

Make sure you have backed up your OpenLAB CDS EZChrom Edition methods, sequences, report templates, results, and data files to a secure location.

Print copies of your OpenLAB CDS EZChrom Edition methods and sequences

From the OpenLAB CDS EZChrom Edition, print copies of your methods and sequences (either hard copies or as PDF files) to use as reference when you migrate your files to OpenLAB CDS.

Create projects in OpenLAB CDS

Create projects in OpenLAB CDS before you copy the files you want to migrate. For information on how to create projects, see the OpenLAB CDS online help and documentation.

Create and configure instruments in OpenLAB CDS

Create and configure the instruments in OpenLAB CDS. These instruments should match the configuration of the instruments used when the methods were created in OpenLAB CDS EZChrom Edition. For information on how to create and configure instruments in OpenLAB CDS, see the online help and documentation. For information on supported instruments and required firmware, see the *OpenLAB CDS Requirements Guide* supplied with your software.

Set the appropriate privileges in OpenLAB CDS

Make sure you have the required user privileges for migrating your system. An administrator with role of “everything” has all of the privileges required. For information on how to set user privileges, see the OpenLAB CDS online help.

Obtain a USB memory stick or hard drive for use in migration

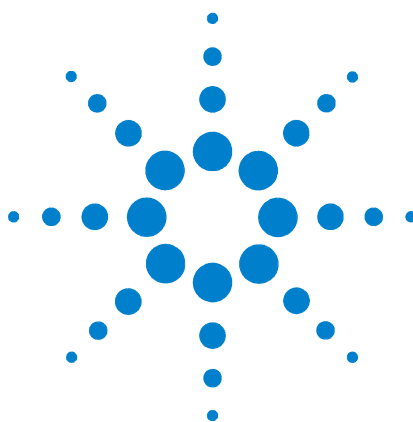
Obtain a USB memory stick or external USB hard drive with sufficient capacity for the files you want to migrate. The method files, data/result files, and (if necessary) intelligent reporter templates (.rdl files) you want to migrate will be copied to the USB drive or memory stick. You can also copy the files to a mapped network drive that is accessible from the OpenLAB CDS computer.

For information on how to copy files into OpenLAB CDS, see [Chapter 3](#), “Copying Files from OpenLAB CDS EZChrom Edition to OpenLAB CDS,” starting on page 15.

For Further Information, Help, and Assistance

If you need help evaluating and planning how you approach your migration project, or are interested in learning about a networked configuration for your laboratory, contact your local Agilent Account Manager or Professional Services Representative. To find your local representative, go to <http://www.agilent.com/en-us/contact-us/page> and select your country.

2 Planning the Migration to OpenLAB CDS Standalone Workstation System



3

Copying Files from OpenLAB CDS EZChrom Edition to OpenLAB CDS

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This chapter describes how to copy result sets and report template files from an OpenLAB CDS EZChrom Edition workstation to OpenLAB CDS Workstation or Workstation Plus using a USB memory stick or hard drive. It also describes the process for moving OpenLAB CDS EZChrom Edition methods into OpenLAB CDS Workstation (file based system) or Workstation Plus with Content Management.



Resources for Copying Files

In order to migrate raw data and results files and report templates to OpenLAB CDS, you must first copy them into the OpenLAB CDS projects. The tool you use to accomplish this depends on your product and the quantity of files you need to transfer.

Table 2 Options for copying files into OpenLAB CDS

Tool	Tool location and instructions	Recommended for
Migration Tools for OpenLAB (Recommended)	Provided on OpenLAB CDS installation media and run as part of the OpenLAB CDS Installer.	Migration to OpenLAB CDS Workstation or Workstation Plus from OpenLAB CDS EZChrom Edition Workstation.
Copy and Paste	No tool required. See "" on page 36.	<ul style="list-style-type: none"> • Migration of data <i>after</i> installation of OpenLAB CDS Workstation, or if Migration Tools for OpenLAB were not executed upon installation. • Copying files and folders to OpenLAB CDS Workstation.
FTP (File Transfer Protocol)	Windows explorer or commercially available FTP tools. See "Procedure for Copying Files from OpenLAB CDS EZChrom Edition to OpenLAB CDS Workstation Plus Using FTP" on page 22.	<ul style="list-style-type: none"> • Copying folders to OpenLAB CDS Workstation Plus. • Migration of data <i>after</i> installation of OpenLAB CDS, or if Migration Tools for OpenLAB were not executed upon installation. • Smaller amounts of data, for example a few Gigabytes. Easy to use but slow for large amounts of data.
Agilent Content Management Bulk Import Utility	Installed as part of OpenLAB CDS Workstation Plus and accessed from Start > Program Files. See "Procedure for Copying Files to OpenLAB CDS Workstation Plus Using Bulk Import Utility" on page 24.	<ul style="list-style-type: none"> • Copying folders to OpenLAB CDS Workstation Plus. • Migration of data <i>after</i> installation of OpenLAB CDS, or if Migration Tools for OpenLAB were not executed upon installation. • Large amounts of data, for example more than a few Gigabytes. More complex to use but takes less time.
OpenLAB CDS Content Management Browser	Installed as part of OpenLAB CDS Workstation Plus and accessed from Start > Program Files. See "Copying files into OpenLAB CDS Workstation Plus using the Content Browser" on page 68.	<ul style="list-style-type: none"> • Migration of data <i>after</i> installation of OpenLAB CDS, or if Migration Tools for OpenLAB were not executed upon installation. • Copying a few files only. Does not copy folders. Use for occasional copying of files not included with your initial file transfer.

File Locations in OpenLAB CDS EZChrom Edition

This section describes the locations of different file types within OpenLAB CDS EZChrom Edition.

OpenLAB CDS EZChrom Edition files are stored in the project folder assigned to the instrument. The project is defined and assigned in the OpenLAB CDS EZChrom Edition Control Panel ([Figure 2](#)).

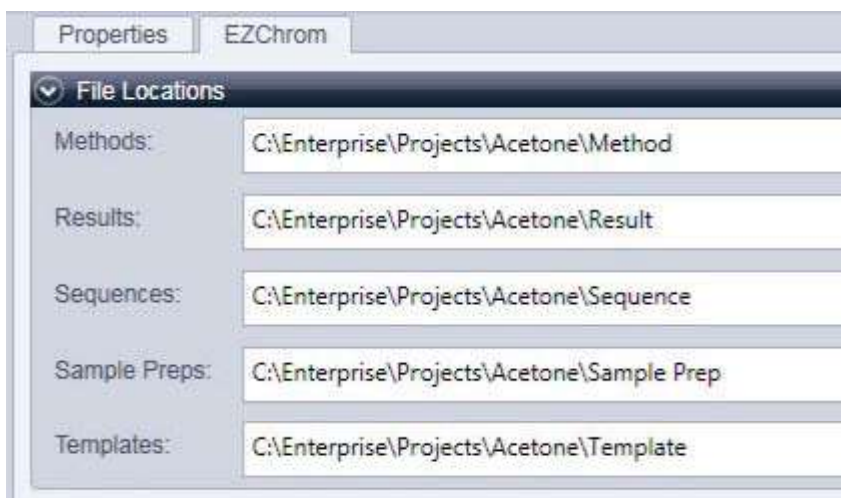


Figure 2 Example of file locations within a project in OpenLAB CDS EZChrom Edition

The OpenLAB CDS EZChrom Edition setting for Result Set Mode defines how the data is stored and which files are copied into the result folders.

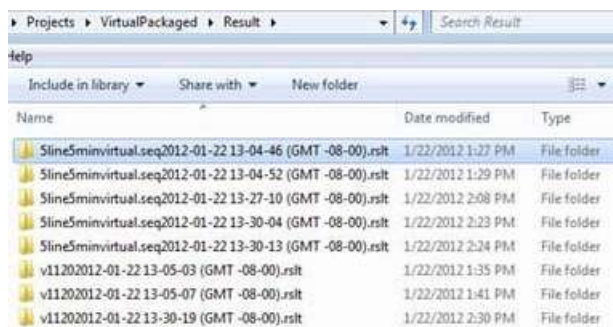
File Mode

If the project Result Set Mode is set to File Mode, the methods, sequences, sample prep, and template files are located in their original project folders. For information on how to copy files when the Result Set Mode is set to File Mode, see [“Copying Files Using the OpenLAB CDS Workstation Plus Content Management Content Browser”](#) on page 67.

Result Package Mode

If the project Result Set Mode is set to Result Package Mode, a sub-folder is created in the project Result .rslt folder for each analysis ([Figure 3](#)). Additional contents of that folder (such as method, sample prep, and template files) ([Figure 4](#)) are set in the Project properties. Copying result set folders is done using FTP, using the procedure described in [“Copying Files from OpenLAB CDS EZChrom Edition to OpenLAB CDS Workstation or Workstation Plus”](#) on page 20.

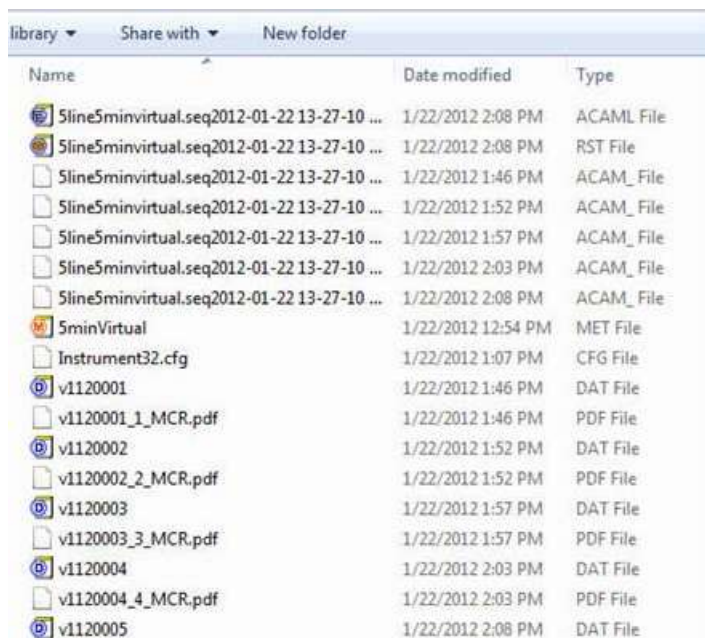
3 Copying Files from OpenLAB CDS EZChrom Edition to OpenLAB CDS



The screenshot shows the 'Result' package mode in OpenLAB CDS EZChrom Edition. The breadcrumb path is 'Projects > VirtualPackaged > Result'. Below the breadcrumb, there are buttons for 'Include in library', 'Share with', and 'New folder'. A table lists the contents of the result set, with columns for Name, Date modified, and Type.

Name	Date modified	Type
Sline5minvirtual.seq2012-01-22 13-04-46 (GMT -08-00).rslt	1/22/2012 1:27 PM	File folder
Sline5minvirtual.seq2012-01-22 13-04-52 (GMT -08-00).rslt	1/22/2012 1:29 PM	File folder
Sline5minvirtual.seq2012-01-22 13-27-10 (GMT -08-00).rslt	1/22/2012 2:08 PM	File folder
Sline5minvirtual.seq2012-01-22 13-30-04 (GMT -08-00).rslt	1/22/2012 2:23 PM	File folder
Sline5minvirtual.seq2012-01-22 13-30-13 (GMT -08-00).rslt	1/22/2012 2:24 PM	File folder
v11202012-01-22 13-05-03 (GMT -08-00).rslt	1/22/2012 1:35 PM	File folder
v11202012-01-22 13-05-07 (GMT -08-00).rslt	1/22/2012 1:41 PM	File folder
v11202012-01-22 13-30-19 (GMT -08-00).rslt	1/22/2012 2:30 PM	File folder

Figure 3 Example result sets for sequence runs in OpenLAB CDS EZChrom Edition Result Package Mode



The screenshot shows the contents of a sequence result set folder in OpenLAB CDS EZChrom Edition Result Package Mode. The breadcrumb path is 'library > Share with > New folder'. A table lists the contents of the folder, with columns for Name, Date modified, and Type.

Name	Date modified	Type
Sline5minvirtual.seq2012-01-22 13-27-10 ...	1/22/2012 2:08 PM	ACAML File
Sline5minvirtual.seq2012-01-22 13-27-10 ...	1/22/2012 2:08 PM	RST File
Sline5minvirtual.seq2012-01-22 13-27-10 ...	1/22/2012 1:46 PM	ACAM_ File
Sline5minvirtual.seq2012-01-22 13-27-10 ...	1/22/2012 1:52 PM	ACAM_ File
Sline5minvirtual.seq2012-01-22 13-27-10 ...	1/22/2012 1:57 PM	ACAM_ File
Sline5minvirtual.seq2012-01-22 13-27-10 ...	1/22/2012 2:03 PM	ACAM_ File
Sline5minvirtual.seq2012-01-22 13-27-10 ...	1/22/2012 2:08 PM	ACAM_ File
5minVirtual	1/22/2012 12:54 PM	MET File
Instrument32.cfg	1/22/2012 1:07 PM	CFG File
v1120001	1/22/2012 1:46 PM	DAT File
v1120001_1_MCR.pdf	1/22/2012 1:46 PM	PDF File
v1120002	1/22/2012 1:52 PM	DAT File
v1120002_2_MCR.pdf	1/22/2012 1:52 PM	PDF File
v1120003	1/22/2012 1:57 PM	DAT File
v1120003_3_MCR.pdf	1/22/2012 1:57 PM	PDF File
v1120004	1/22/2012 2:03 PM	DAT File
v1120004_4_MCR.pdf	1/22/2012 2:03 PM	PDF File
v1120005	1/22/2012 2:08 PM	DAT File

Figure 4 Contents of sequence result set folder in OpenLAB CDS EZChrom Edition Result Package Mode

File Locations in OpenLAB CDS

Storage of files in OpenLAB CDS EZChrom Edition and OpenLAB CDS are project-based. Once you create a project, all method, sequence, data, result, and analysis and reporting template files are stored within the project folder (Figure 5). Note that the project folder names are slightly different than they are in OpenLAB CDS EZChrom Edition.

OpenLAB CDS Workstation Projects are created in the Projects Root Path that was designated during OpenLAB CDS Workstation installation.

OpenLAB CDS Workstation Plus Projects are created in the projects folder in content management. In order to work on migration of files in OpenLAB CDS, make sure the files are copied into the appropriate project locations in OpenLAB CDS, using procedures outlined in [“Copying Files from OpenLAB CDS EZChrom Edition to OpenLAB CDS Workstation or Workstation Plus”](#) on page 20.

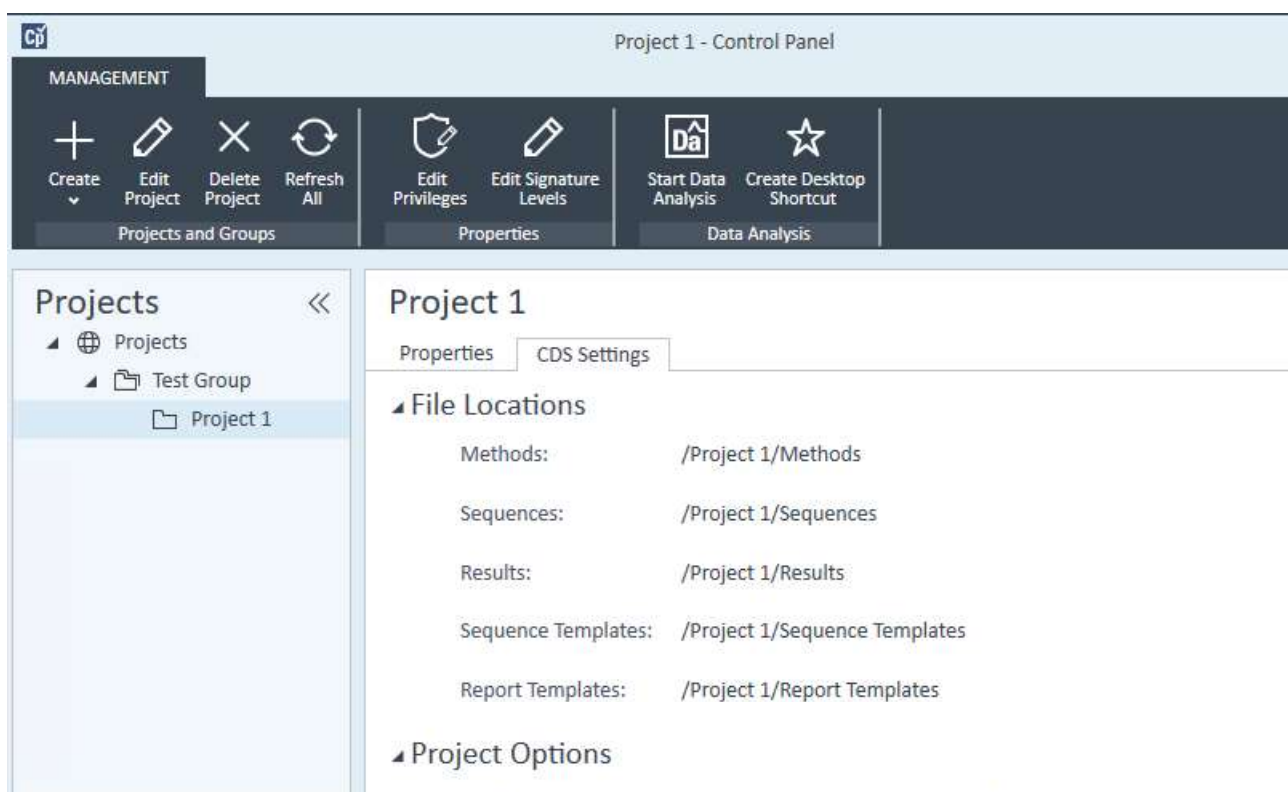


Figure 5 Project file locations in OpenLAB CDS Workstation

Copying Files from OpenLAB CDS EZChrom Edition to OpenLAB CDS Workstation or Workstation Plus

If you are operating in a standalone workstation environment (not networked), transfer of files is done using a USB memory stick or external USB hard drive. Use the appropriate procedure, depending on what version of OpenLAB CDS Workstation you are using: [“Procedure for Copying Files from OpenLAB CDS EZChrom Edition to OpenLAB CDS Workstation Plus Using FTP”](#) on page 22 or [“”](#) on page 36.

Important Notes

- If your workstations are connected to a network, you can use the same procedures to transfer the files to the new location using a mapped network share on the target PC instead of a USB drive.
- If your OpenLAB CDS EZChrom Edition Result Set Mode is set to File Mode and you are copying into OpenLAB CDS Workstation Plus, you must use the Content Management Content Browser to copy individual files to the OpenLAB CDS Workstation Plus storage locations. You can only copy files using this method; you cannot copy folders. (See [“Copying Files Using the OpenLAB CDS Workstation Plus Content Management Content Browser”](#) on page 67.) If you are copying files to OpenLAB CDS Workstation (file based system), you can copy the files directly.
- For OpenLAB CDS Workstation (file based system) it is not necessary to use FTP, as you can directly copy and paste files into the appropriate OpenLAB CDS Workstation project folders.
- If you are copying files into an OpenLAB CDS Workstation with secure project folders enabled, you must be logged into that computer as a member of the local Windows group **AgtSfsGroup**. For example, local Windows user **AgtSfsUser** is the default user created when the **Secure 'Projects Root Path'** option was enabled.

Procedure for Copying Files into OpenLAB CDS Workstation

Because OpenLAB CDS Workstation uses the local file system for all system folders, you can simply copy and paste the OpenLAB CDS EZChrom Edition files you want to migrate into the appropriate project folder for OpenLAB CDS Workstation. (See “[File Locations in OpenLAB CDS](#)” on page 19.)

- a Copy result set folders into the Results folder of the desired OpenLAB CDS project ([Figure 5](#)).
- b Copy the Intelligent Reporting templates (.rdl) into the Report Templates folder of the desired OpenLAB CDS project ([Figure 5](#)).
- c Copy method files (.met) into the \Methods folder of the desired project.

NOTE

Because method files have a different structure in OpenLAB CDS, method files (.met) created in OpenLAB CDS EZChrom Edition cannot be read directly by the OpenLAB CDS software. Create new OpenLAB CDS methods using the **New Method from EZChrom** option, as described later in this document.

NOTE

If you are copying files into an OpenLAB CDS Workstation with secure project folders enabled, you must be logged into that computer as a member of the local Windows group **AgtSfsGroup**. For example, local Windows user **AgtSfsUser** is the default user created when the **Secure 'Projects Root Path'** option was enabled.

Procedure for Copying Files from OpenLAB CDS EZChrom Edition to OpenLAB CDS Workstation Plus Using FTP

Before you start

In order to use FTP, you must be an OpenLAB CDS Workstation Plus user with “Everything” permission. You will need to know your login credentials to proceed.

- 1 Copy the OpenLAB CDS EZChrom Edition project folders or result sets folders containing data, results, methods, sequences, and report templates to a USB memory stick or a USB external hard drive.

NOTE

In order for OpenLAB CDS Workstation Plus to work with raw and results data from OpenLAB CDS EZChrom Edition, the raw (.dat), results (.rst) and ACAML (.acaml) files must be available. Make sure to copy the entire results set folder for a given run or all results set folders for a sequence.

- 2 Move the USB memory stick or USB hard drive to the computer where OpenLAB CDS Workstation Plus is installed.
- 3 In Windows Explorer, type `FTP://<server name>/` and then press **Enter**, where `<server name>` is the name of the OpenLAB CDS server. (By default, this is `localhost` or the name of the PC for workstations.) In the Log On As dialog, type your OpenLAB CDS User name and Password, then click **Log On**. You now have access to the Content Management folder where the OpenLAB CDS Workstation Plus project folders are located.
- 4 Use FTP to copy files and folders into OpenLAB CDS Workstation Plus (Figure 6).
 - Copy data and results files or result sets folders into the OpenLAB CDS Workstation Plus “Results” folder for the appropriate project.
 - Copy Intelligent Reporter files (.rdl) to the Report Templates folder of the appropriate project.
 - Copy method files (.met) into the Methods folder for the appropriate project.

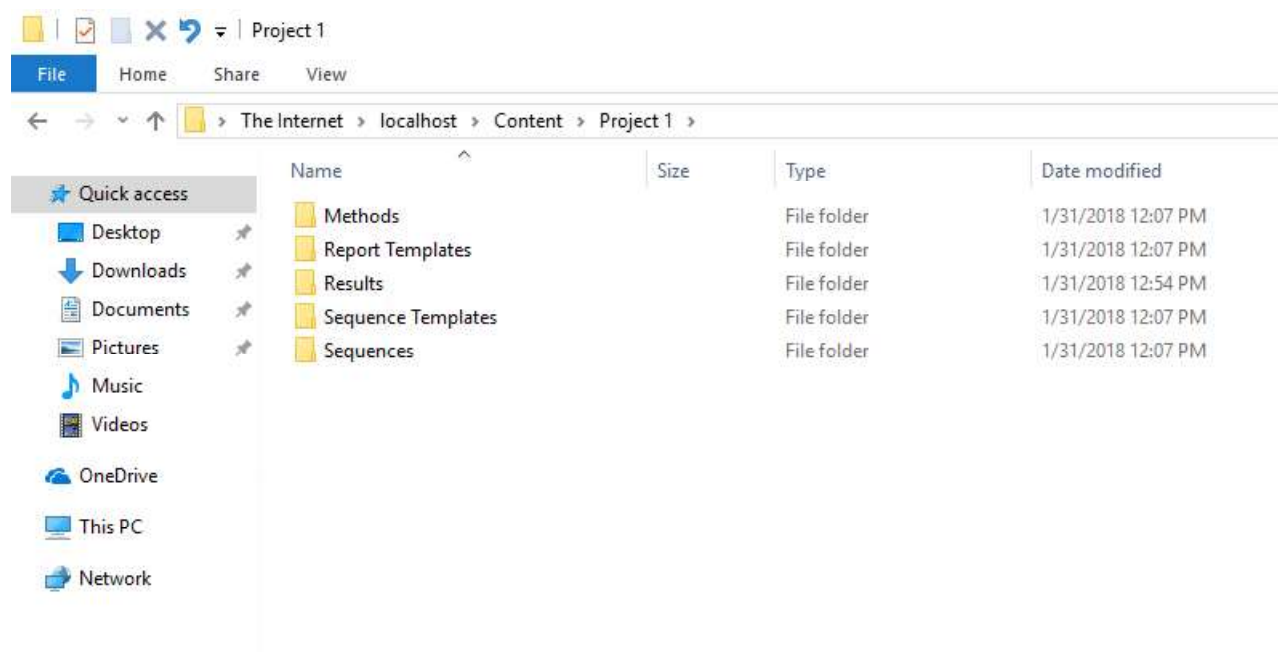


Figure 6 Access to OpenLAB CDS Workstation Plus project folders via FTP

When uploading files using FTP, note the following:

- Do not select the OpenLAB CDS Workstation Plus Archive folder to upload file via FTP.
- Make sure no files are checked out in the upload folder. Uploading a new version of a file will fail.
- Make sure you have the proper access to the repository to upload files and create folders.

NOTE

If you have large amounts of data (for example, 100s of gigabytes), the performance of FTP may be insufficient. In this case, use the Content Management Bulk Import Utility provided with OpenLAB CDS Workstation Plus.

Procedure for Copying Files to OpenLAB CDS Workstation Plus Using Bulk Import Utility

Perform the steps outlined in Before You Start, then use the Import Tool to upload the data into OpenLAB CDS.

Prepare the data for import

- 1 Copy the OpenLAB CDS EZChrom Edition project folders or result sets folders containing data, results, methods, sequences, and report templates to a USB memory stick or a USB external hard drive.

NOTE

In order for OpenLAB CDS Workstation Plus to work with raw and results data from OpenLAB CDS EZChrom Edition, the raw (.dat), results (.rst) and ACAML (.acaml) files must be available. Make sure to copy the entire results set folder for a given run or all results set folders for a sequence.

- 2 Move the USB memory stick or USB hard drive to the computer where OpenLAB CDS Workstation Plus is installed. Copy each project folder or result sets folders into the `contentstore` directory (for example, `C:\DSDData\DSContent\contentstore\`).

NOTE

“C:\DSDData\DSContent\contentstore” may not be your currently configured contentstore. Check with your system administrator for the location of your active contentstore before copying files. The Content Management Import Tool will not work if files reside outside of the active contentstore.

The location of the content store can be found using the Content Management System Configuration report that is created when OpenLAB CDS is installed. From the Start menu go to All Programs > Agilent Technologies > OpenLAB Content Management, right-click on Server Configuration, and select Open file location. Double-click on the `configurator.xml` file to open it, and find the Content Store entry in the table labelled Data Store Content Summary. Use the Content Store value, such as “C:\DSDData\DsContent”. If the `configurator.xml` does not open, right-click on the file and 'Open Using' Notepad. Scroll down to `<ContentStore>` and observe the `<ContentStore>` value, such as “C:\DSDData\DsContent</ContentStore>”

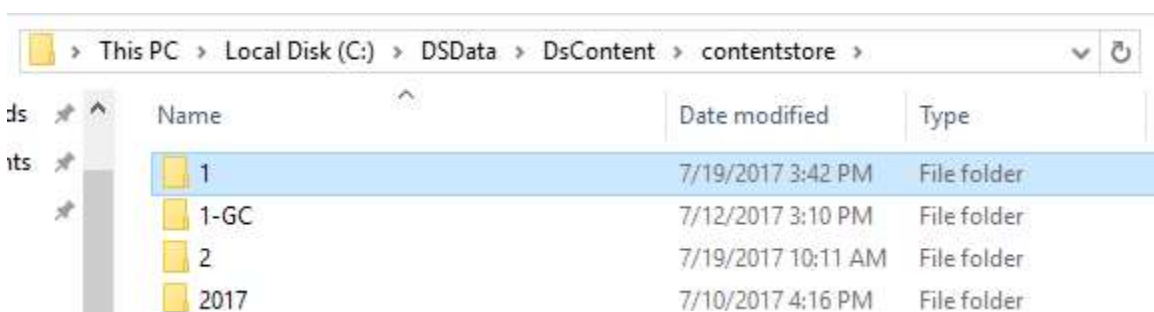


Figure 7 Folder “1” under contentstore directory

Verify projects in OpenLAB CDS

For each project folder (for example, folder “1” and “2” in [Figure 8](#)), verify (or create if necessary) an OpenLAB CDS project to upload the EZChrom data into. Use the following procedure to create each project. In the following procedure, project “1” is used as an example.

- 1 Launch OpenLAB CDS Control Panel, and create a project with the same name as the EZChrom folder named “1”. (Repeat for each project folder with data to be imported.)

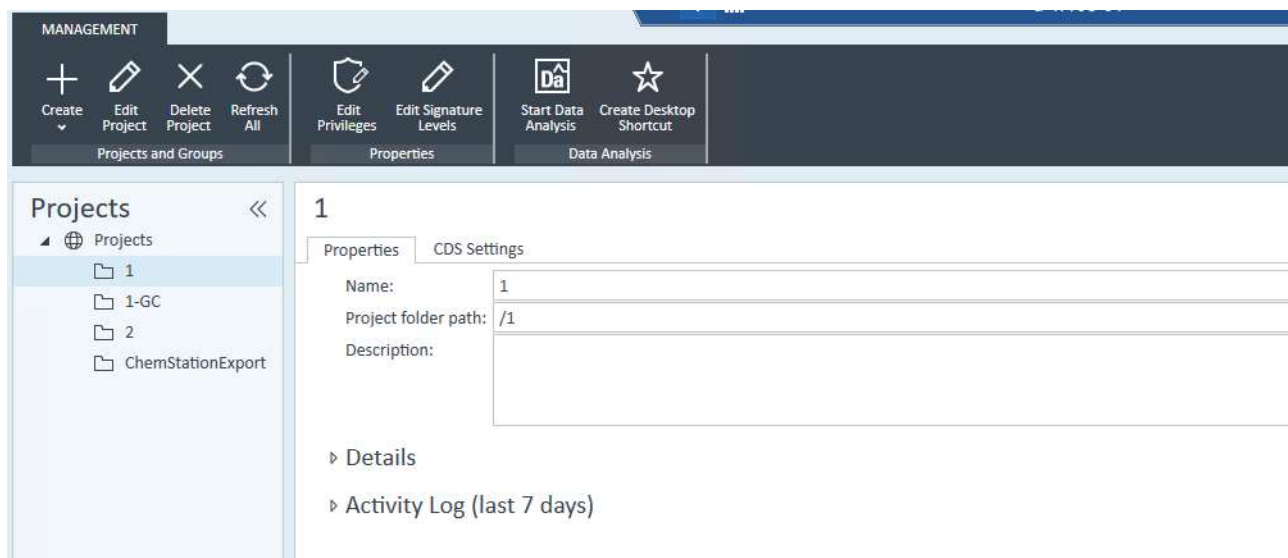


Figure 8 Project “1” created in the Control Panel

- 2 Open Content Management: localhost/datastore, and log in as Administrator. Make sure folder “1” along with the subfolders (Methods,

3 Copying Files from OpenLAB CDS EZChrom Edition to OpenLAB CDS

Report Templates...) are created for project “1.” (Check that folders and subfolders were created for all project folders to be imported.)

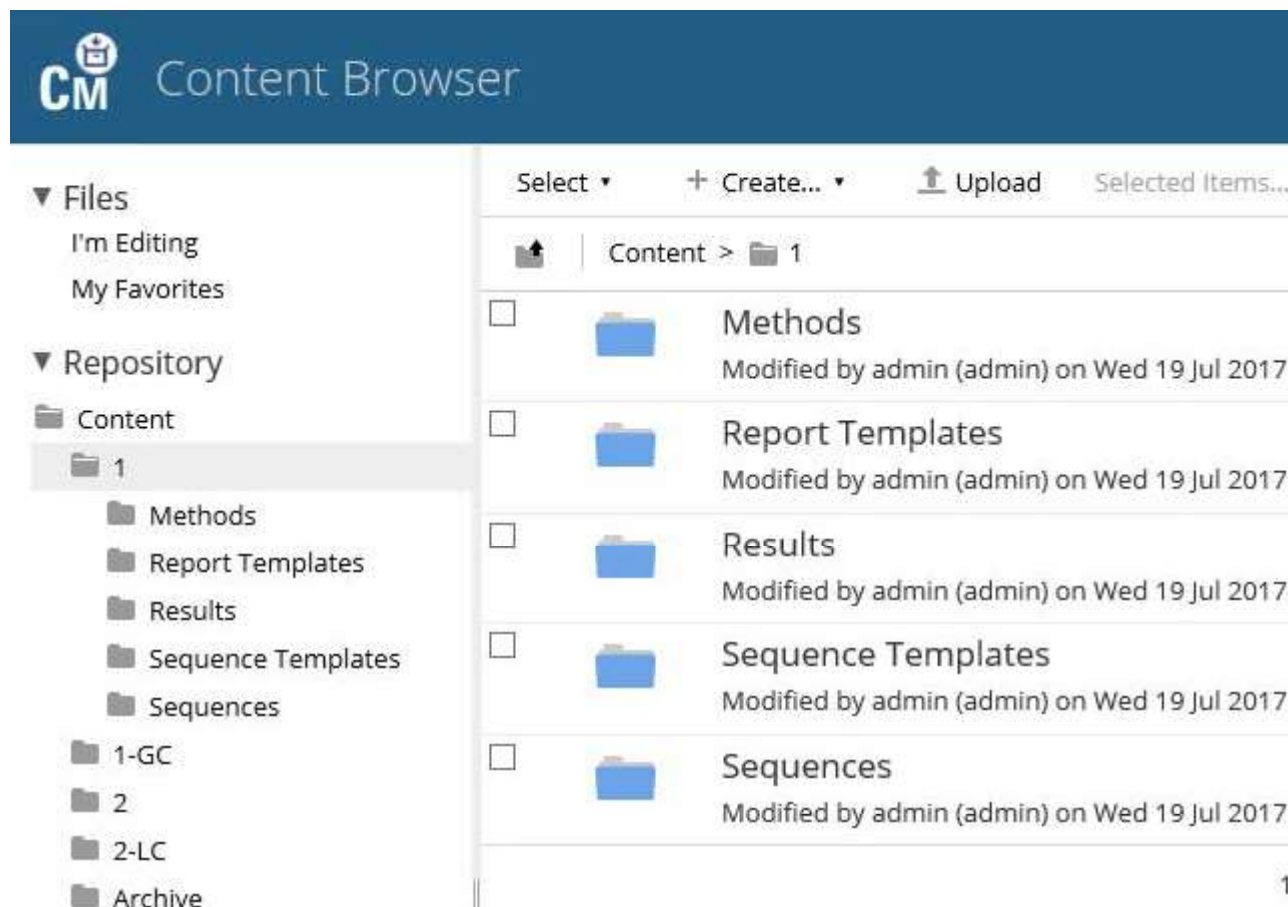


Figure 9 Folder “1” is created for project “1” in Content Management

Import data using the Import Tool

- 1 Open the Content Management Import Tool by one of the following two methods:
 - Type the following address into the browser:
<http://localhost/alfresco/service/agilent/bulk/import/filesystem>

NOTE

The Content Management Import Tool is part of Content Management. It is not an add-on. It is accessible directly using the link shown above.

OR

- Launch from **Start > All Programs > Agilent Technologies > Bulk Import Utility** (Windows 7) or **All apps > Agilent Technologies > Bulk Import Utility** (Windows 10).
- 2 Log in as the administrator used for Content Management.

← → ↻ | localhost/alfresco/service/agilent/bulk/import/filesystem

CM Content Management Import Tool v1.0

This tool provides a mechanism for importing large amounts of data very quickly into Content Management.

Data that needs to be imported must be copied into a folder - Import Directory - under the content store directory for Content folders and files contained in the Import Directory will be imported. Note that this directory must NOT be modified in any manner.

Please provide the full path for the Import Directory below.

The data being imported can be placed into a new or existing folder (Target folder) of your choice. The Target folder path will be stored in the OpenLABDataStore. Please note that the forward slash character(/) must be used as a separator when specifying the target folder.

Please provide the target folder path in Content Management to which files and folders must be imported.

Initiate Bulk Import

Please note that you may need to perform further validation on the imported data as per your needs.

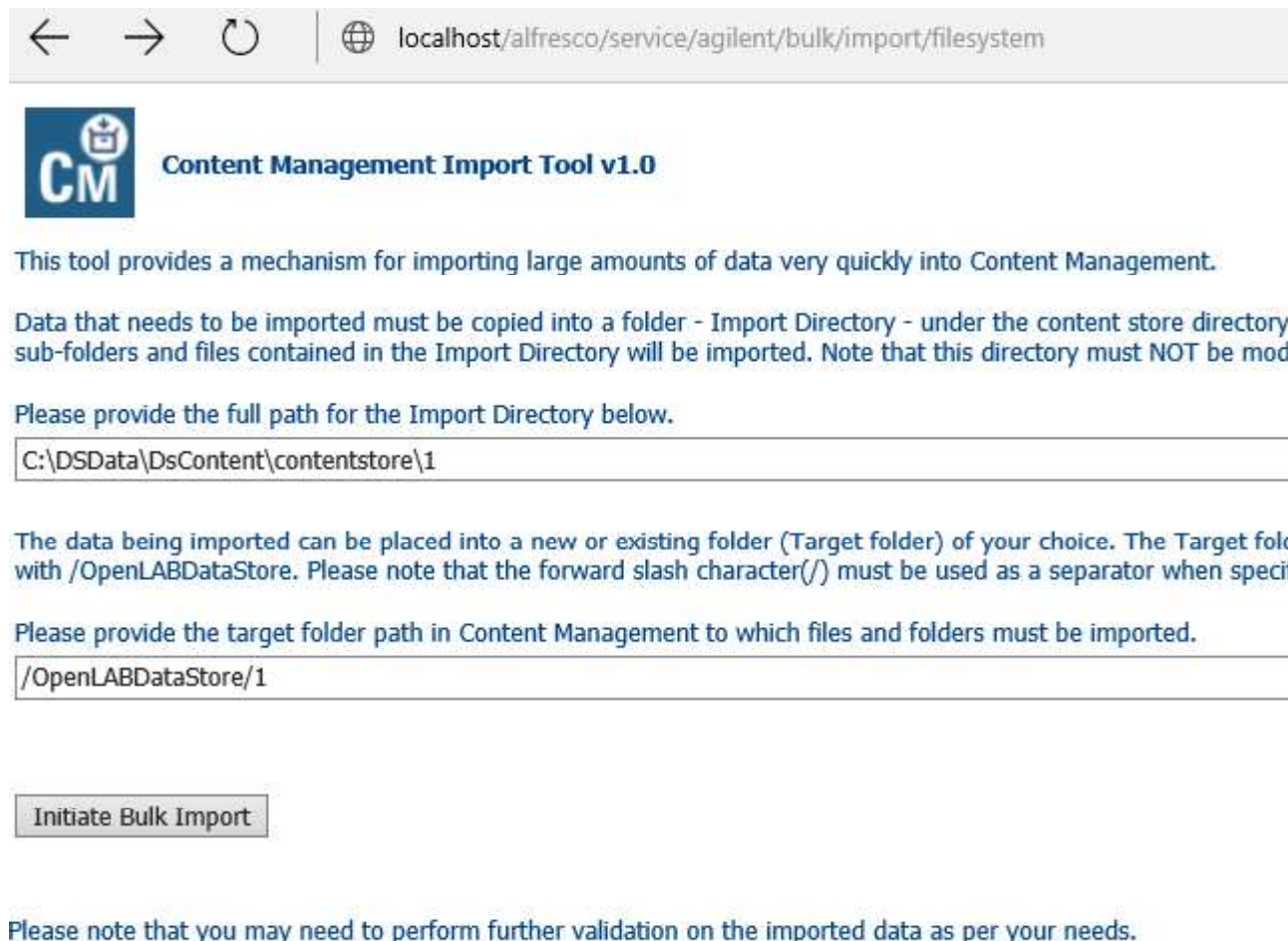
Figure 10 Content Management Import Tool

- 3 In the first field, type the full path for the import folder where your data is located. (In this example, this is the C:\DSDData\DSContent\contentstore\1. See [“Prepare the data for import”](#) on page 24.) All sub-folders and files contained in the import directory will be imported into OpenLAB CDS by the Import Tool.

CAUTION

IMPORTANT: Do not modify this folder in any manner during or after the import is completed.

- 4 In the second field, type the Target Folder path within Content Management where the data will be imported, starting with /OpenLABDataStore (in this example, /OpenLABDataStore/1). Note that the forward slash character (/) must be used as a separator when specifying the target folder location.



← → ↻ | localhost/alfresco/service/agilent/bulk/import/filesystem

Content Management Import Tool v1.0

This tool provides a mechanism for importing large amounts of data very quickly into Content Management.

Data that needs to be imported must be copied into a folder - Import Directory - under the content store directory sub-folders and files contained in the Import Directory will be imported. Note that this directory must NOT be mod

Please provide the full path for the Import Directory below.

The data being imported can be placed into a new or existing folder (Target folder) of your choice. The Target folc with /OpenLABDataStore. Please note that the forward slash character(/) must be used as a separator when specif

Please provide the target folder path in Content Management to which files and folders must be imported.

Initiate Bulk Import

Please note that you may need to perform further validation on the imported data as per your needs.

Figure 11 Content Management Import Tool with import locations filled in

- Click **Initiate Bulk Import** to start the upload. A page with the progress status appears.



Figure 12 Content Management Import Tool progress status

Once the upload is finished, the page will display “Idle” with Status of “Successful.”

3 Copying Files from OpenLAB CDS EZChrom Edition to OpenLAB CDS

- 6 Open Content Management and refresh the page. The OpenLAB EZChrom Edition data under `C:\DSData\DsContent\contentstore\1` should be uploaded into: `/OpenLABDataStore/1`.

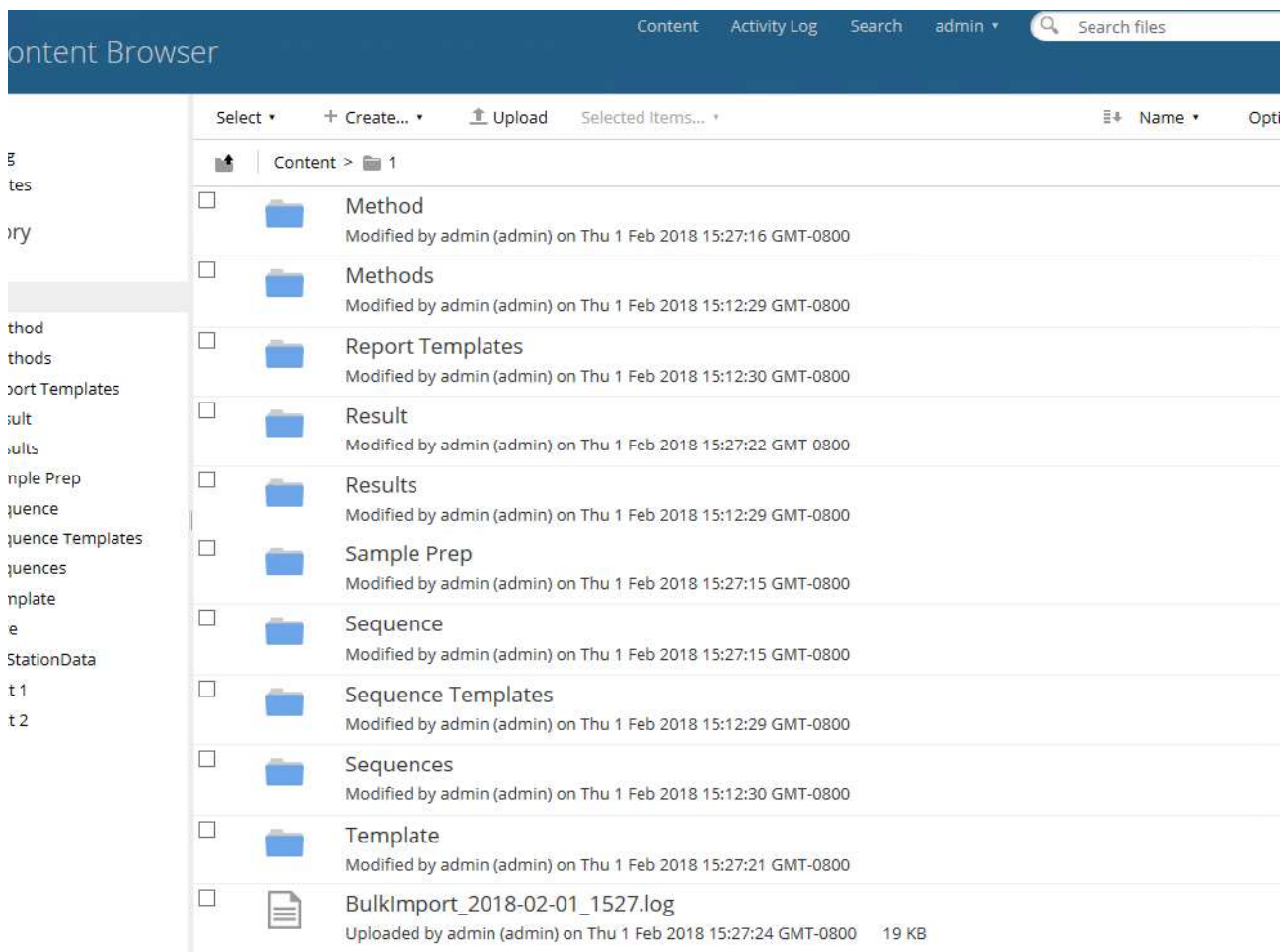


Figure 13 Data from Import Directory successfully uploaded into the target folder

The `BulkImport_(timestamp).log` file contains details of the bulk import process. The content is downloadable and searchable.



BulkImport_2017-07-19_1617.log 1.1

Modified by admin (admin) on Wed 19 Jul 2017 16:18:03 GMT-0700

★ Favorite

Comment



Previous

Next

1

/ 15

-

+

```

16:17:09,768 Bulk import started from "C:\DSData\DsContent\contentstore\1"...
16:17:09,796 Skipping "C:\DSData\DsContent\contentstore\1\Methods" as it already
exists in the repository and replace existing is false.
16:17:11,631 Linked ContentStore file iql.cfg of size 609 bytes into repository
path "/OpenLABDataStore/1/iql.cfg".
16:17:11,631 Linked ContentStore file HP78QK00.ini of size 158 bytes into
repository path "/OpenLABDataStore/1/HP78QK00.ini".
16:17:11,631 Linked ContentStore file RapidControl.InstrumentConfig.xml of size
60,347 bytes into repository path
"/OpenLABDataStore/1/RapidControl.InstrumentConfig.xml".
16:17:11,631 Linked ContentStore file CONFIG.REG of size 660,936 bytes into
repository path "/OpenLABDataStore/1/CONFIG.REG".
16:17:11,631 Linked ContentStore file HP68501.CFG of size 2,093 bytes into
repository path "/OpenLABDataStore/1/HP68501.CFG".
16:17:11,631 Linked ContentStore file ChemStationPerInstrumentSettings.config of
size 852 bytes into repository path
"/OpenLABDataStore/1/ChemStationPerInstrumentSettings.config".
16:17:11,631 Linked ContentStore file instrument.config of size 6,077 bytes into
repository path "/OpenLABDataStore/1/instrument.config".
16:17:11,631 Linked ContentStore file RTL.INI of size 134 bytes into repository
path "/OpenLABDataStore/1/RTL.INI".
16:17:12,871 Linked ContentStore file def_GC.S of size 7,863 bytes into repository
path "/OpenLABDataStore/1/Sequence/def_GC.S".
16:17:12,871 Linked ContentStore file LoadTest.S of size 42,041 bytes into
repository path "/OpenLABDataStore/1/Sequence/LoadTest.S".
16:17:12,871 Linked ContentStore file Seq 26-5-17.S of size 16,969 bytes into
repository path "/OpenLABDataStore/1/Sequence/Seq 26-5-17.S".
16:17:14,328 Linked ContentStore file Seq 26-5-17.LOG of size 5,410 bytes into
repository path "/OpenLABDataStore/1/Data/Seq 26-5-17 2017-05-26 09-35-03/Seq 26-5-
17.LOG".
16:17:14,328 Linked ContentStore file sequence.acaml of size 127,259 bytes into
repository path "/OpenLABDataStore/1/Data/Seq 26-5-17 2017-05-26 09-35-
03/sequence.acaml".
16:17:14,329 Linked ContentStore file Seq 26-5-17.S of size 16,959 bytes into
repository path "/OpenLABDataStore/1/Data/Seq 26-5-17 2017-05-26 09-35-03/Seq 26-5-
17.S".
16:17:14,329 Linked ContentStore file Seq 26-5-17.B of size 3,621 bytes into
repository path "/OpenLABDataStore/1/Data/Seq 26-5-17 2017-05-26 09-35-03/Seq 26-5-
17.B".
16:17:14,329 Linked ContentStore file Methods.Reg of size 590 bytes into repository
path "/OpenLABDataStore/1/Data/Seq 26-5-17 2017-05-26 09-35-03/Methods.Reg".
16:17:14,329 Linked ContentStore file CS1bk.ini of size 145 bytes into repository
path "/OpenLABDataStore/1/Data/Seq 26-5-17 2017-05-26 09-35-03/CS1bk.ini".
16:17:14,805 Linked ContentStore file info.mth of size 761 bytes into repository
path "/OpenLABDataStore/1/Methods/FID_TCD.M/info.mth".
16:17:14,805 Linked ContentStore file i7673.mth of size 1,056 bytes into repository
path "/OpenLABDataStore/1/Methods/FID_TCD.M/i7673.mth".
16:17:14,805 Linked ContentStore file injector.mth of size 66 bytes into repository
path "/OpenLABDataStore/1/Methods/FID_TCD.M/injector.mth".
16:17:14,805 Linked ContentStore file damethod.reg of size 15,574 bytes into
repository path "/OpenLABDataStore/1/Methods/FID_TCD.M/damethod.reg".
16:17:14,805 Linked ContentStore file recalib.mth of size 10 bytes into repository
path "/OpenLABDataStore/1/Methods/FID_TCD.M/recalib.mth".
16:17:14,805 Linked ContentStore file rpthead.txt of size 2,808 bytes into
repository path "/OpenLABDataStore/1/Methods/FID_TCD.M/rpthead.txt".
16:17:14,806 Linked ContentStore file iql.mth of size 3,857 bytes into repository
path "/OpenLABDataStore/1/Methods/FID_TCD.M/iql.mth".
16:17:16,460 Linked ContentStore file IQ1.MTH of size 2,849 bytes into repository
path "/OpenLABDataStore/1/Methods/ISTD_ex.M/IQ1.MTH".

```

Figure 14 Bulk Import log file

3 Copying Files from OpenLAB CDS EZChrom Edition to OpenLAB CDS

The methods imported from OpenLAB CDS EZChrom Edition are imported into the OpenLAB CDS Methods folder in the project. (Both OpenLAB CDS EZChrom Edition and OpenLAB CDS methods are located in the Methods folder.)

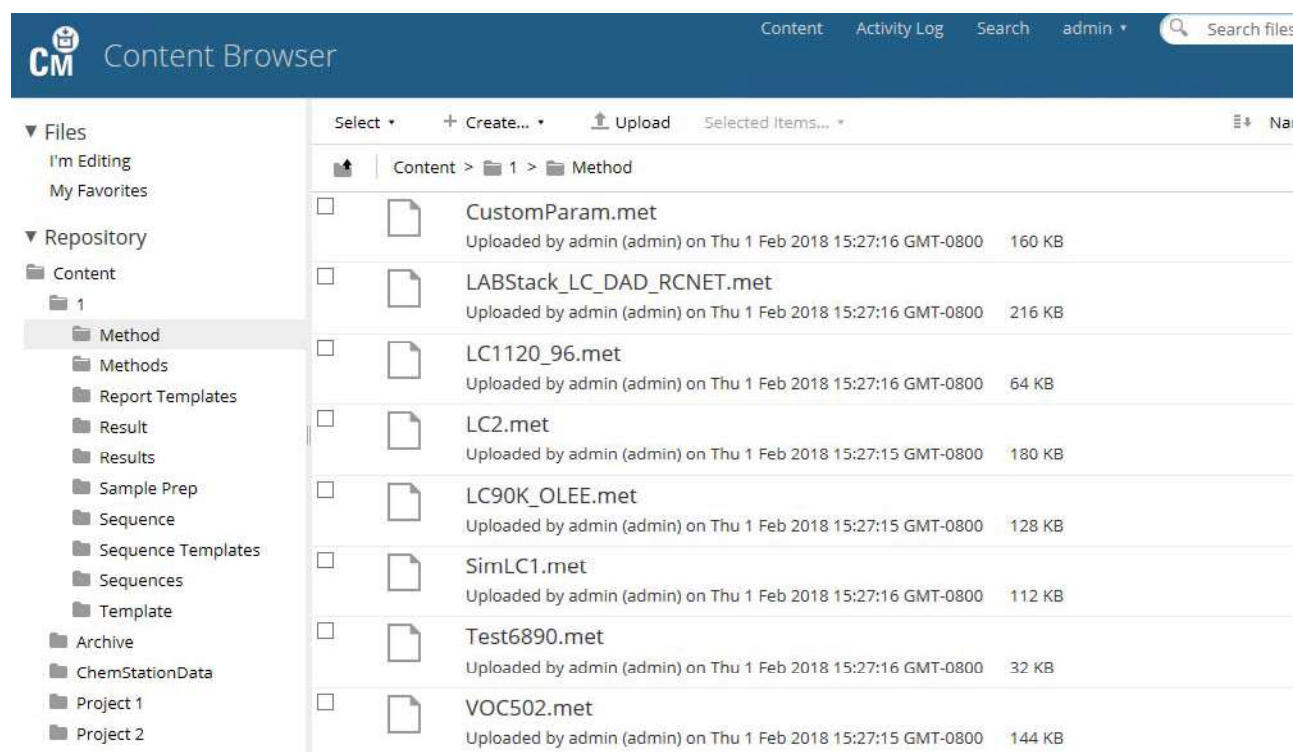


Figure 15 Imported methods under the Method folder

- 7 The folder that contains the imported OpenLAB EZChrom Edition results is called Result. In OpenLAB CDS, results are stored in the Results folder. Therefore, in order to access the imported results from OpenLAB CDS Data Analysis, you must delete the existing Results

folder and rename the Data folder containing the imported results to “Results,” using the following procedure.

- a To delete the existing Results folder, hover the mouse over the Results folder, and on the right side, click **More**.

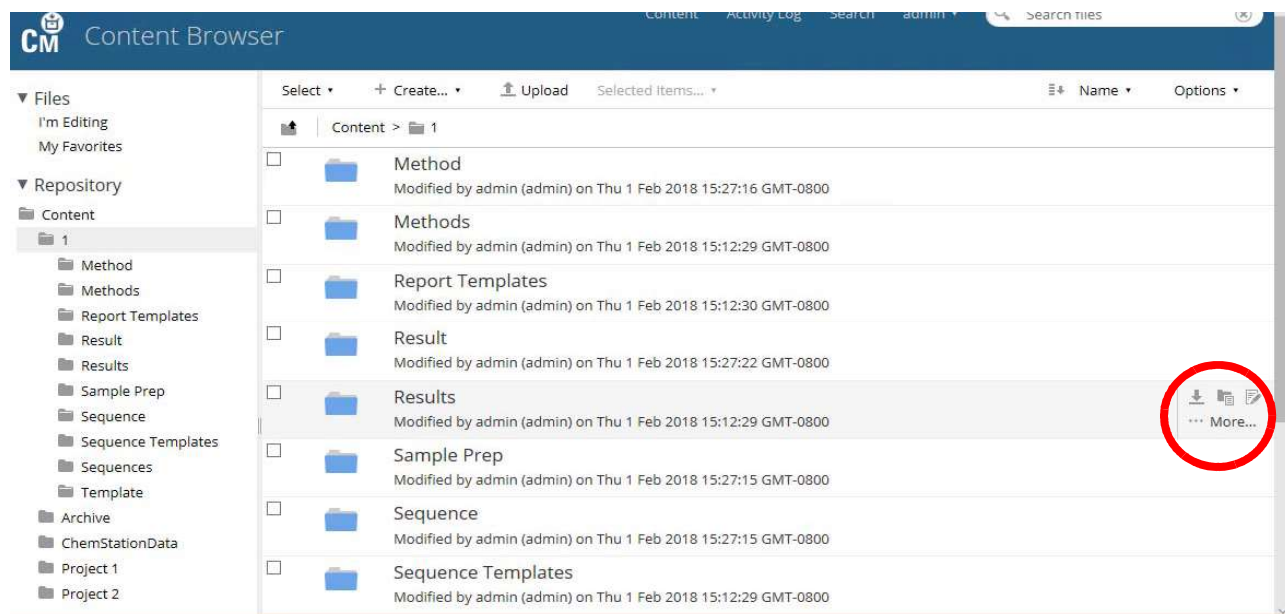


Figure 16 More button for the Results folder

- b In the menu that appears, click **Delete Folder**.

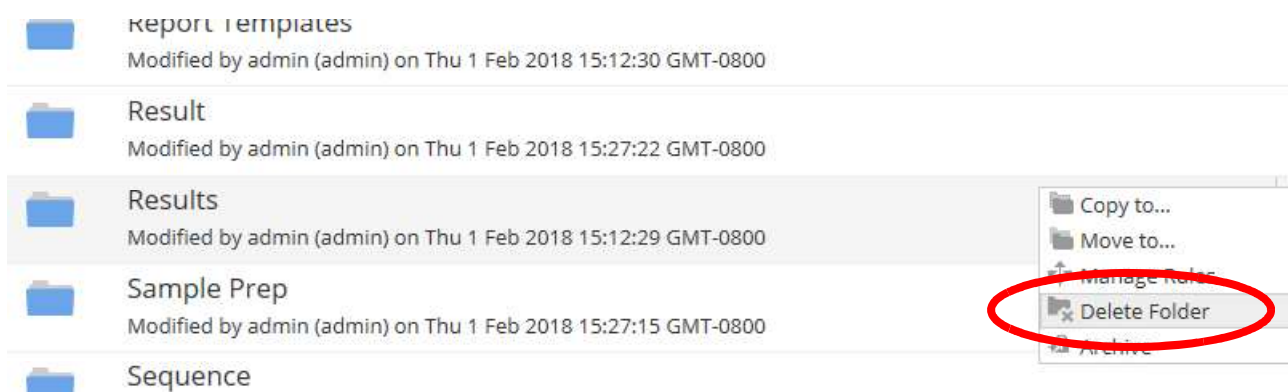


Figure 17 Delete Folder for Results

- c In the confirmation dialog, click **Delete**.

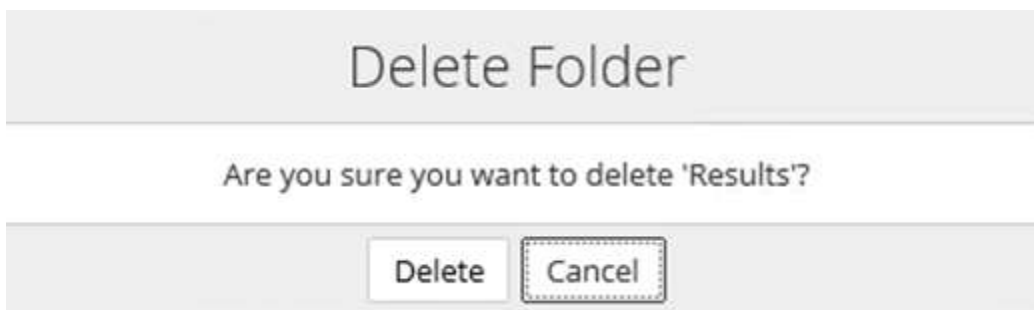


Figure 18 Confirmation dialog for deleting results folder

- d Hover the mouse over the “Data” folder, and click on the **Edit Properties** icon on the right.

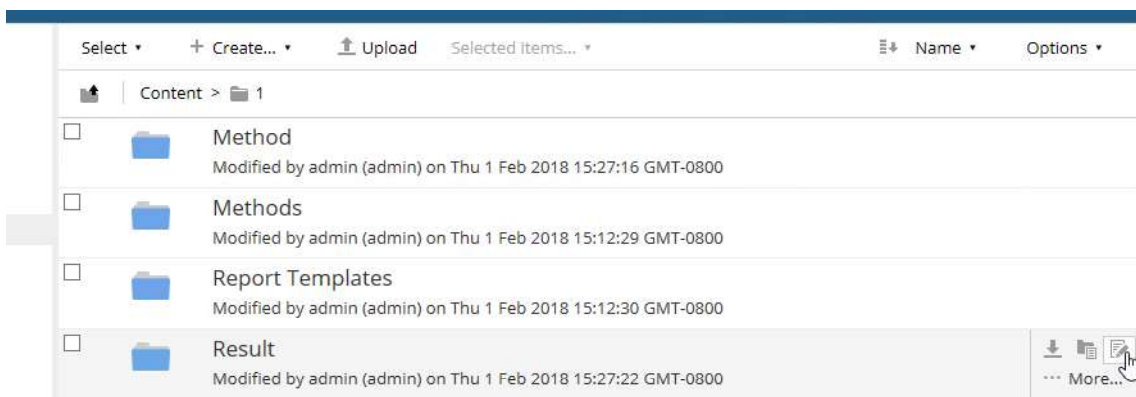


Figure 19 Edit Properties icon when you hover the mouse over the Data folder

- e In the Edit Properties dialog, change the Name from “Result” to “Results” and delete the Title.

Edit Properties: Data

[All Properties...](#)

*** Required Fields**

Name: *
Results

Title:
|

Description:

Save Cancel

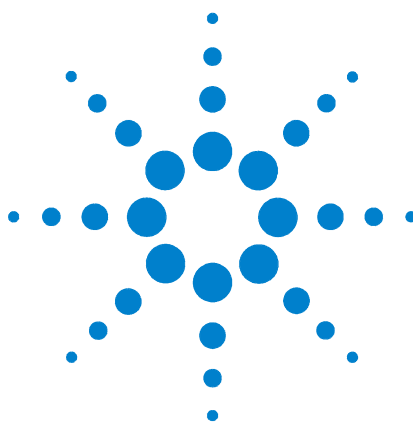
Figure 20 Edit Properties for Results folder

- f** Click **Save**.
- 8** Perform [step a](#) through [step f](#) above for each of the following folders:
 Method to Methods
 Template to Report Templates

NOTE

Although the Sample Prep and Sequence folders are copied to the project by the Bulk Import Utility, the OpenLAB CDS EZChrom Edition Sample Prep and Sequence files are not directly readable by OpenLAB CDS.

3 Copying Files from OpenLAB CDS EZChrom Edition to OpenLAB CDS



4 Migrating Methods — Acquisition Parameters

Migrating an RC.NET Driver Acquisition Method [38](#)

This chapter provides stepwise procedures for migrating RC.NET acquisition parameters from your existing OpenLAB EZChrom Edition method to an OpenLAB CDS acquisition method (.amx file).

NOTE

OpenLAB CDS supports RC.NET (RapidControl .NET) based drivers *only*. It does not support any previous generation of drivers. Classic drivers are non-RC.NET device drivers that existed prior to the introduction of the RC.NET standard in 2007.



Migrating an RC.NET Driver Acquisition Method

OpenLAB CDS only supports drivers based on the RC.NET standard. Migration of Sample Prep is not yet supported.

Prerequisites for migrating RC.NET acquisition methods

Before you start to migrate methods, read [“Before You Start”](#) on page 12.

Instrument connection

Make sure the instrument that will be controlled by the method is connected to the OpenLAB CDS system and powered on.

Steps for migrating RC.NET driver acquisition method

- 1 From the OpenLAB CDS Control Panel, configure the instrument. In order to ensure migration of all acquisition parameters, make sure the configuration matches the configuration of the instrument in OpenLAB CDS EZChrom Edition exactly. Otherwise, OpenLAB CDS adapts the acquisition method to the current instrument configuration. For more information, see the “How Method Resolution Works” topic in the online help.
- 2 Launch the instrument from the Control Panel.
- 3 Navigate to OpenLAB CDS Acquisition.
- 4 Select the **File** tab at the top left side of the window.
- 5 Choose **New Method from EZChrom**.
- 6 When the Select EZChrom Method dialog is displayed, use it to navigate to and open the desired method file.
- 7 The file is imported.

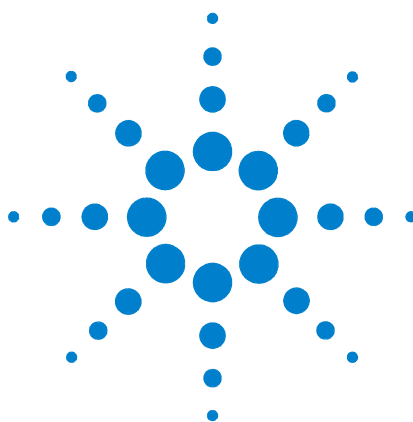
NOTE

If the destination instrument configuration is not the same as the source, then method resolution will be triggered, and the required choices must be selected. See the online help for information on method resolution.

Only the instrument setup parameters are imported. No other parameters of the OpenLAB CDS EZChrom Edition method are imported to the OpenLAB CDS acquisition method.

Sample Prep methods

Migration of sample prep methods is not currently supported. Re-create your sample prep methods in OpenLAB CDS. For information on how to create sample prep methods, see the OpenLAB CDS online help.



5 Migrating Methods — Data Analysis Processing Parameters

Before You Start Data Analysis Migration 42

Steps for Migrating Data Analysis Processing Method 42

Important differences 46

This chapter provides procedures for moving data analysis processing parameters from your existing OpenLAB CDS EZChrom Edition to OpenLAB CDS.



Before You Start Data Analysis Migration

Before you start to migrate processing (data analysis) methods, read “Before You Start” on page 12.

NOTE

OpenLAB CDS Data Analysis imports parameters only from OpenLAB CDS EZChrom Edition methods that include a peak table. Methods without identified compounds are not imported.

Steps for Migrating Data Analysis Processing Method

In OpenLAB CDS, methods are split into three different method types (sample preparation method, acquisition method and processing method). The following procedure describes how to import parameters into a processing method (.pmx file). A processing method contains all the information and parameters needed to process the raw data and generate results.

Steps for migrating processing parameters

An OpenLAB CDS EZChrom Edition method can be used as a base to create a new processing method in OpenLAB CDS Data Analysis. Once the method is created, you must complete sections that are not imported in OpenLAB CDS.

- 1 Start the OpenLAB CDS Data Analysis and switch to the Data Processing view.
- 2 In the ribbon, select the **Processing** tab.
- 3 Click **New Method**, then from the menu select **New Method from EZChrom** (Figure 21).

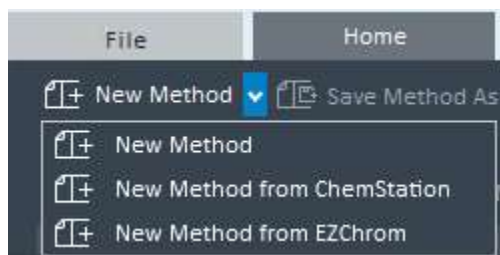


Figure 21 New Method menu

- 4 In the Create New Processing Method dialog box (Figure 22 on page 43), select the required method configuration, then click **Browse** to select the EZChrom method file (*.met).

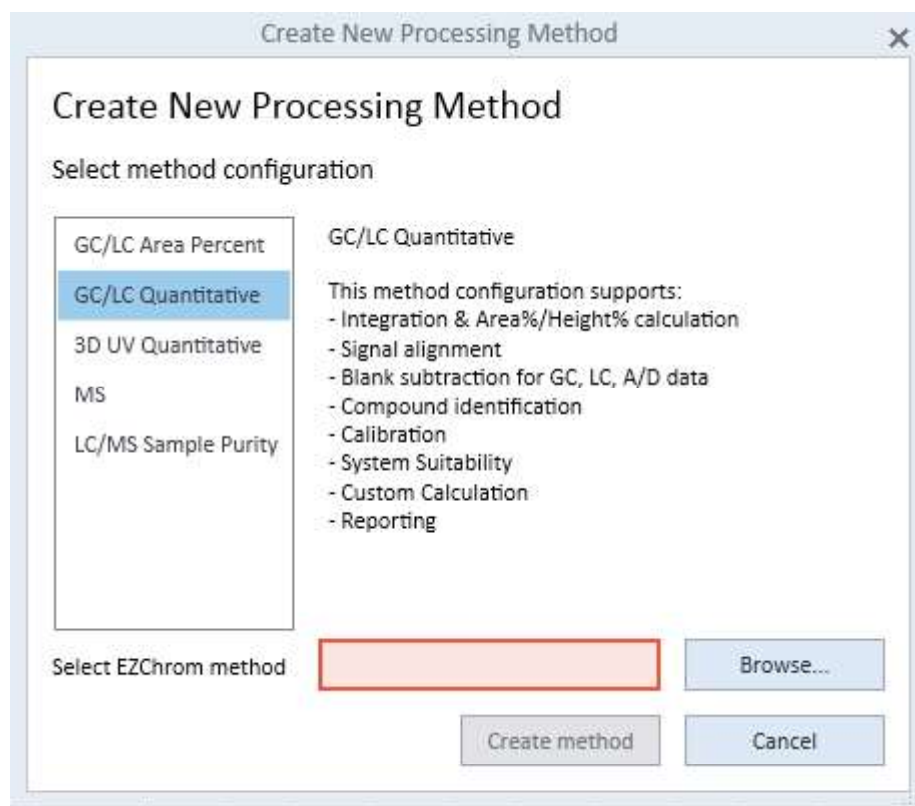


Figure 22 Create New Processing Method dialog box

CAUTION

Choose the method configuration carefully. You cannot change it afterwards. For a description of the possible options, see the OpenLAB CDS online help.

- 5 Click **Create method**.

The following parameters of the EZChrom method are imported into a new processing method:

- Signal name
- Compound name
- Expected retention time
- Retention time window

- Flag if a compound is an internal standard (ISTD)
- Associated ISTD that a compound refers to
 - If there is only one ISTD, it is the associated ISTD of all other compounds.
 - ISTDs with an empty name are ignored.
 - Groups that are used as ISTD are ignored.

NOTE

ISTD amounts are not imported. A warning is displayed if there is an ISTD compound without an ISTD amount. Update the amount for this ISTD in the calibration parameters.

NOTE

ISTD information is not shown by default in a processing method. To view the ISTD columns, go to the **Compounds > Calibration** node, General tab, then select Internal standard.

- 6 Under **Compounds > Identification**, select the signal for each compound, if not defined already.

NOTE

In order to select a signal for a compound, import example raw data (single run or a result set). See [“Procedure for Migrating Raw and Results Data”](#) on page 51.

- 7 In OpenLAB CDS, there are two selections for how concentrations are calculated. To select the calculation that is like OpenLAB CDS EZChrom Edition, go to **Compounds > Calibrations** and select the **General** tab. In the drop-down menu for Concentration calculation, select **Amount * Multipliers / Dil. factor**.

CAUTION

By default, the selection for Concentration calculation is **Amount * Multipliers * Dil. Factor**. To calculate concentrations the way it is done in OpenLAB EZChrom Edition, select **Amount * Multipliers / Dil. factor**. See [“Two results: Amount and Concentration”](#) on page 69 or the online help for more information.

- 8 Using a printed copy of the OpenLAB CDS EZChrom Edition method, manually complete your processing method, including compound calibration information and integration events. For details on how to create OpenLAB CDS methods, see the Data Analysis online help.

- 9 Print the OpenLAB CDS processing method. Use this for comparison to your original OpenLAB CDS EZChrom Edition method printout.
- 10 Test and validate the processing method to prove that the desired results are calculated. To do this, load OpenLAB CDS EZChrom Edition data, process it with the newly created method and compare the results with the results from the OpenLAB CDS EZChrom Edition system. See [Chapter 6](#), “Migrating Raw and Results Data,” starting on page 49.

NOTE

Agilent recommends comparing the integration and quantitation results created in OpenLAB CDS with the ones generated on an OpenLAB CDS EZChrom Edition system before the method is used in production.

- 11 Create (or choose) a suitable Intelligent Report. (See [Chapter 8](#), “Migrating Intelligent Reporting Templates”.)

NOTE

Not all features of an OpenLAB CDS EZChrom Edition method are supported yet in the Data Analysis. OpenLAB CDS EZChrom Edition methods using unsupported features cannot be created in the Data Analysis. (See “[Supported functions](#)” below.)

Supported functions

[Table 3](#) gives an overview of the available functions in OpenLAB CDS. See the online help for details about how all of these parameters are set, how they work, and what formulas are used.

Table 3 Functions supported by Data Analysis in OpenLAB CDS version 2.3

Function	OpenLAB CDS EZChrom Edition	Supported by OpenLAB CDS version 2.3 Data Analysis
Curve Models	Fit Type: <ul style="list-style-type: none"> Point-to-Point Linear Quadratic Cubic Average RF Force through zero enable or disable	Linear, Quadratic, Exponential, Logarithmic, Log/log, with Origin (0,0 point) Ignore, Include, Force, or Connect. Note: OpenLAB CDS version 2.3 does not support "Point-to-Point" calibrations. A single point calibration must "include" the origin.
Weighting method	<ul style="list-style-type: none"> 1/Amount 1/Amount² 1/Response 1/Response² 	<ul style="list-style-type: none"> 1/Amount 1/Amount² 1/Response 1/Response²
Curve modes	N/A	Curve, Manual RF, Reference curve with correction factor

Table 3 Functions supported by Data Analysis in OpenLAB CDS version 2.3 (continued)

Function	OpenLAB CDS EZChrom Edition	Supported by OpenLAB CDS version 2.3 Data Analysis
Quantitation types	ESTD, ISTD, Norm%,	ESTD, ISTD, Norm%,
RF Definition	Response/Amount or Amount/Response	Response/Amount or Amount/Response
Response based on	Quantitate types: Area or Height	Area, Area%, Height, or Height%. For timed groups and named groups, only Area and Height are available.
Bracket calibration	Bracketing: <ul style="list-style-type: none"> • None • Standard • Sequence • Seq. w/Back Calc 	<ul style="list-style-type: none"> • Overall (Sequence) • Non-overlap • Overlapped (Standard)
Compound types	Standard single peak compounds, timed groups with multiple time ranges, and named compound groups	Standard single peak compounds, timed groups with multiple time ranges, and named compound groups

Important differences

There are some differences in the way some features are implemented in the OpenLAB CDS Data Analysis. Take this into account when migrating an OpenLAB CDS EZChrom Edition method into OpenLAB CDS Data Analysis. For details, see [“Important Differences from OpenLAB CDS EZChrom Edition”](#) on page 69 and the OpenLAB CDS online help. These differences include:

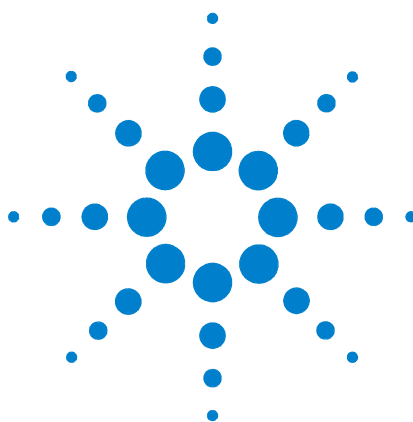
- Calculation of amount and concentration
- Response based on – defined per compound
- Automatic retention time update – defined per compound
- Run types other than clearing calibration are not supported
- New bracketing calibration

Other Data Analysis functionality

The Data Analysis offers a wealth of additional functionality listed below, but some features of the OpenLAB CDS EZChrom Edition method (for example, UV Library search, 3D plot, Iso Plot, fraction collection) are not available yet. Evaluate the available functionality to decide whether or not your specific OpenLAB CDS EZChrom Edition methods can be transferred to OpenLAB CDS Data Analysis.

The following additional functionality is available in OpenLAB CDS Data Analysis, but is implemented with new algorithms so method parameters from OpenLAB CDS EZChrom Edition cannot simply be translated.

- Multi-Detector signal alignment
- UV spectra extraction parameter
- UV Impurity Check
- Compound confirmation by UV spectra
- System Suitability calculations (Column performance, Signal to Noise, Peak Resolution, Peak widths, Tailing, and so on.)
- Custom Calculation Editor
- Reporting



6 Migrating Raw and Results Data

Before You Start Migrating Raw and Results Data 50

Procedure for Migrating Raw and Results Data 51

Differences in Peak Areas and Heights 55

OpenLAB CDS Data Analysis can directly read the raw data and results as they have been created on an OpenLAB CDS EZChrom Edition. This chapter describes the different data types and how to work with the data in Data Analysis.



Before You Start Migrating Raw and Results Data

Before you start to migrate data (raw and results), read [“Before You Start”](#) on page 12.

Data format and Agilent Common Analytical Markup Language (ACAML) file requirements

OpenLAB CDS Data Analysis reads raw/result data generated with OpenLAB CDS EZChrom Edition. It evaluates the raw data and the ACAML (Agilent Common Analytical Markup Language) files. Therefore, in order to work with OpenLAB CDS EZChrom Edition data, both the raw and ACAML files must be present.

NOTE

ACAML files are generated by OpenLAB CDS EZChrom Edition A.04.01 and higher. To generate an ACAML file that you can use with OpenLAB CDS Data Analysis, you must first reprocess the data with OpenLAB CDS EZChrom Edition A.04.01 or higher.

NOTE

OpenLAB CDS can also import raw .DAT files (without the ACAML present). However, you must reprocess it with an OpenLAB CDS processing method in order to see any results information.

Procedure for Migrating Raw and Results Data

After the OpenLAB CDS EZChrom Edition data has been copied into the Results folder of a specific project, OpenLAB CDS Data Analysis works with the data seamlessly without the need to migrate or import it. (See [Chapter 3](#), “Copying Files from OpenLAB CDS EZChrom Edition to OpenLAB CDS,” starting on page 15.)

Data Selection view

The data selection tree shows the folder structure of the data path given in the Data Analysis project in the Control Panel. Navigation is very similar to the Windows explorer. Selecting a folder shows the content of the folder in the injection list on the right of the tree.

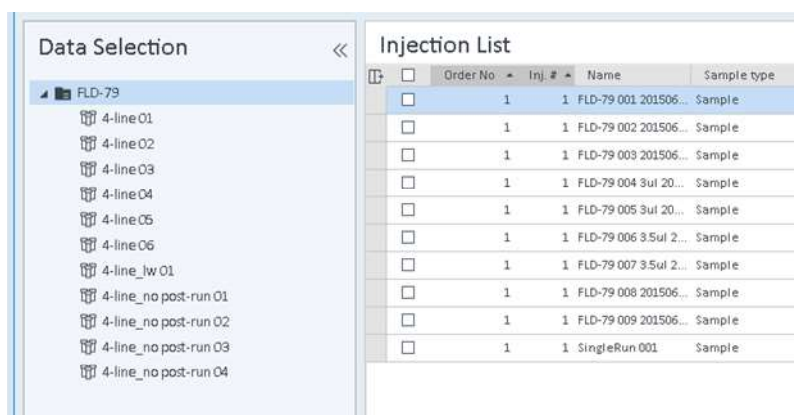


Figure 23 Data Selection tree view in OpenLAB CDS

The tree can contain the following items:

(Folders) A folder contains other folders, result sets, or single runs. If it contains result sets, they are shown as sub-nodes in the tree. If the folder contains single runs, the respective data files are listed in the Injection List window on the right. You can load one or multiple single runs. Single runs as well as sequences created in file mode are shown in these folders ([Figure 24](#)).

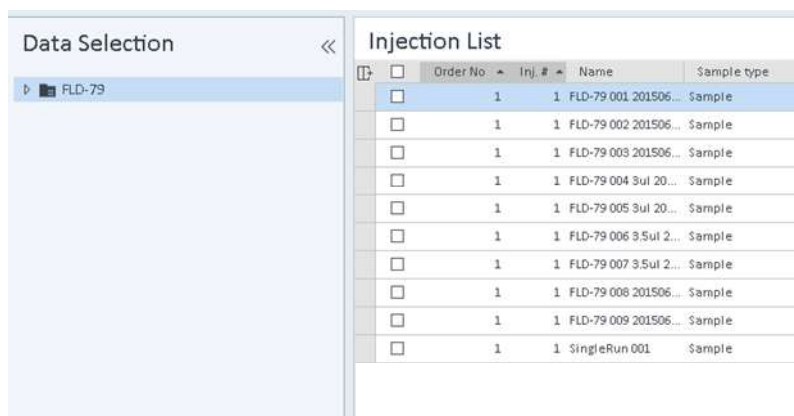


Figure 24 Folders showing single runs from File Mode or Result Package Mode



(Result sets) The contained data files (injections) are listed in the Injection List window. You can only load the entire result set; loading parts of a result set is not supported. Single runs acquired in result package mode are also shown as individual result sets.

NOTE

Results sets that were created in OpenLAB CDS EZChrom Edition without the ".rslt" extension will not load properly in the Data Analysis. Use the Windows explorer to rename the result set folder from <Name of folder> to <Name of folder>.rslt.

Procedure for loading data

- 1 Start the OpenLAB CDS Data Analysis for the project into which the data from OpenLAB CDS EZChrom Edition has been copied.
- 2 In the Data Selection view, click on the result set folder or single run folder and then click **Load Data** to load the data into the "Data Processing" view.
- 3 If the data were not yet processed, you are prompted to select how to process the data. For information on the processing options, see the OpenLAB CDS online help.

Create New Processing Method

Selection contains unprocessed data. What type of method do you wish to use?

Select method configuration

GC/LC Area Percent	GC/LC Quantitative
GC/LC Quantitative	This method configuration supports:
3D UV Quantitative	- Integration & Area%/Height% calculation
MS	- Signal alignment
LC/MS Sample Purity	- Blank subtraction for GC, LC, A/D data
	- Compound identification
	- Calibration
	- System Suitability
	- Custom Calculation
	- Reporting

☒ Auto import processing method

New method name: Same as imported method

Link only Link and process No method

Figure 25 Selections for loading unprocessed raw data

After the data are loaded into the data processing view, the chromatograms, meta data (sample information such as name, sample type, and so on) and calculated results can be displayed. If an ACAML file is available as part of the OpenLAB CDS EZChrom Edition data, the acquisition method parameters can also be displayed.

Users with the appropriate privileges can link a native Data Analysis processing method to the OpenLAB CDS EZChrom Edition data to reprocess the raw data and calculate new results. Linking a method is also required in order to display spectral data.

For more information on linking a method, see the online help.

NOTE

EZChrom data without the ACAML files, for example data from EZChrom Elite 3.x, cannot be opened directly in OpenLAB CDS Data Analysis. (See [“Data format and Agilent Common Analytical Markup Language \(ACAML\) file requirements”](#) on page 50.) Import these files using the import functionality in the Import/Export tab of the Data Selection view.

Opening result sets with bracketing

When opening an OpenLAB CDS EZChrom Edition result set that already uses a bracketing mode, the bracketing mode is selected in the Injection List window, but no brackets are applied yet.

- 1 Change the bracketing mode to None.
- 2 Change the bracketing mode back to the initial mode.

The brackets are correctly displayed.

Differences in Peak Areas and Heights

When the same sample is acquired by OpenLAB CDS EZChrom Edition and OpenLAB CDS, the observed peak areas and peak heights in OpenLAB CDS EZChrom Edition are different from those in OpenLAB CDS. The difference in observed heights and areas is due to the difference in signal treatments by the two different CDS platforms.

OpenLAB CDS records and displays the height and area after applying detector scaling factors, whereas OpenLAB CDS EZChrom Edition displays the unscaled “counts”.

The difference in signal treatments does not affect calibrated quantitation results, Area %, or Height %.

NOTE

When you import OpenLAB CDS EZChrom Edition data into OpenLAB CDS, the EZChrom units for peak area and peak height are maintained.

Adjusting areas and heights for comparison

Using the OpenLAB CDS Intelligent Reporting or Custom Calculation, the scaling factor can be applied in order to adjust the OpenLAB CDS areas and heights for better comparison with areas and heights reported in OpenLAB CDS EZChrom Edition.

Scaled areas/heights with detector-specific units can be obtained by multiplying the unitless EZChrom “counts” by the matching detector specific scaling factor, as shown below.

$$\text{Peak Height [CDS 2.3]} = \text{Peak Height [EZChrom]} * \text{Scaling factor}$$

$$\text{Peak Area [CDS 2.3]} = \text{Peak Area [EZChrom]} * \text{Scaling factor}$$

Likewise, unscaled areas/heights, i.e. detector counts, can be obtained by dividing the OpenLAB CDS data by the scaling factor.

$$\text{Peak Height [EZChrom]} = \text{Peak Height [CDS 2.3]} / \text{Scaling factor}$$

$$\text{Peak Area [EZChrom]} = \text{Peak Area [CDS 2.3]} / \text{Scaling factor}$$

NOTE

Scaling factors described below apply only to Agilent GC and LC detectors listed.

Scaling factors for Agilent GCs

In order to obtain OpenLAB CDS equivalent values for GC signals in the appropriate scale for each detector, the reported value in EZChrom must be divided by 7680 for all detector types. This is based on the GC Least Significant Value (1/7680), i.e. the scaling factor to put into the formulas is 1/7680.

Scaling factors for Agilent LCs

For Agilent LC detector signals the scaling factors used to transform Peak Area and Height from counts to detector units are as follows:

VWD Detector Models - G1314A\G1314B\G1314C\G1314D\G1314E\G1314F\G7114A\G7114B

Scaling Factor = 0.000059604644775390625 mAU (=1000/2²⁴)

DAD\MWD Detector Models - G1315A\G1315B\G1315C\G1315D\G1365A\G1365B\G1365C\G1365D

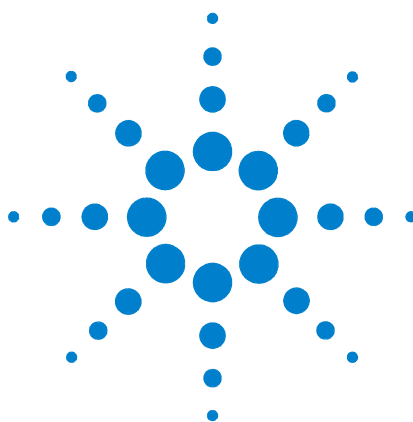
Scaling Factor = 0.000476837158203125 mAU (=1000/2²¹)

DAD Detector Models - G4212A\G4212B

Scaling Factor = 0.000007450580596923828125 mAU (=1000/2²⁷)

FLD Detector Models - G1321A\G1321B\G1321C

Scaling Factor - .0000059604644775390625 mAU (=1000/2²⁴)



7 Working With Sequences

Before You Start Working With Sequences 58

Recreating Sequences in OpenLAB CDS 58

Sequences from OpenLAB CDS EZChrom Edition cannot be used directly in OpenLAB CDS. This chapter provides information for recreating your OpenLAB CDS EZChrom Edition sequences in OpenLAB CDS.



Before You Start Working With Sequences

In OpenLAB CDS, you create sequences from simple data input or using Sequence/Analysis templates to help improve productivity.

The Sequence Template Editor allows you to define an injection pattern, which can simply be applied to create the required sequence.

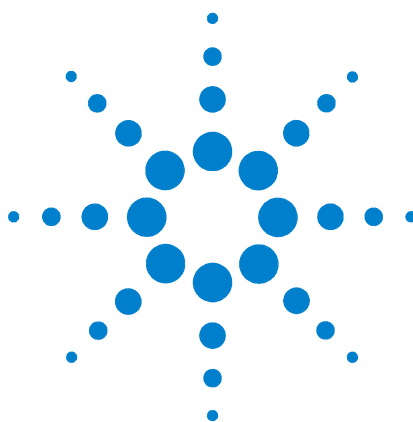
Before you start to work with sequences, read [“Before You Start”](#) on page 12.

Recreating Sequences in OpenLAB CDS

In OpenLAB CDS, there are three ways to recreate a Sequence table. You can:

- Complete the Sequence table manually.
- Use a sequence creation template.
- Import or drag and drop a .csv file into the Sequence table. For an example of a sequence in .csv format, see [“Example of .CSV Sequence Format”](#) on page 71.

See the OpenLAB CDS online help for instructions on how to create a sequence.



8

Migrating Intelligent Reporting Templates

OpenLAB Intelligent Reporting Templates 60

Testing Migrated Report Templates 61



OpenLAB Intelligent Reporting Templates

The reporting functionality provided with OpenLAB CDS is based on Microsoft reporting technology provided with, for example, Microsoft SQL server. This technology was introduced to Agilent CDS systems with OpenLAB CDS A.01.01 in 2011. The layout, report items and their format that make up the reports are defined in report template files with the file extension *.rdl (report definition language by Microsoft).

This chapter covers the technical migration of report templates generated with the built-in Report Template Editor of OpenLAB CDS EZChrom Edition to OpenLAB CDS.

Backward compatibility

With OpenLAB CDS reporting functions are similar to OpenLAB CDS EZChrom Edition. However, OpenLAB CDS offers additional features and enhancements compared to previous versions. These changes affect the report template files (*.rdl) as well as the OpenLAB result files (*.acaml).

OpenLAB CDS provides the following backward compatibility with intelligent reporting:

Intelligent reporting template (*.rdl) files:

- You can load, modify, and use any report template file generated with an earlier version of OpenLAB CDS in the report template editor of OpenLAB CDS.
- Report template files generated with the report template editor of OpenLAB ECM Intelligent Reporter require minor modifications to the RDL file in order to reuse them. If you need assistance to modify these files, contact an Agilent business partner who is knowledgeable in use of Intelligent Reporting.
- You can use report template files generated with Microsoft Business Intelligence studio and similar editors with OpenLAB CDS but you cannot edit them.

Data analysis result (*.acaml) files:

Some data fields are populated with a different label, or the format or meaning of the content has changed from OpenLAB CDS EZChrom Edition. A selection of the most commonly used fields is presented in [“Report items that do not migrate well”](#) on page 62. If none of the modified fields are present in the report template, you can use it without any further modifications. If a modified field is used in the report template, the template may require a minor modification.

Testing Migrated Report Templates

In order to test the successful migration of a report template Agilent recommends the following procedure:

- 1 Review the report template for potential break points.
- 2 Compare reports of representative test data, freshly acquired on OpenLAB CDS EZChrom Edition and OpenLAB CDS.

NOTE

Due to the changes described in “[Report items that do not migrate well](#)” on page 62, you should revalidate your report templates against data acquired with OpenLAB CDS. The revalidation effort depends on the formal requirements and the complexity of your report templates.

Comparison test

Preconditions

- A set of methods used with a specific report template is identified.
- Migration of the acquisition methods is completed according to procedures outlined in [Chapter 4](#), “Migrating Methods – Acquisition Parameters,” starting on page 37.
- Migration of the processing methods is completed according to procedures outlined in [Chapter 5](#), “Migrating Methods – Data Analysis Processing Parameters,” starting on page 41.

Procedure

To ensure complete independence of test results, it is recommended that you perform report comparisons on independently-acquired results sets:

- 1 Identify representative sample mixtures (calibration standards, samples, for example) previously used for migration of the acquisition and data analysis parts of the legacy methods.
- 2 Rerun these samples or load the previously generated result set and the associated methods in OpenLAB CDS EZChrom Edition.
- 3 Generate a reference report using the report template you are migrating.
- 4 Transfer the result set, method, and report template to a system with OpenLAB CDS installed See [Chapter 3](#), “Copying Files from OpenLAB CDS EZChrom Edition to OpenLAB CDS,” starting on page 15 for more details.
- 5 If the report template contains references to custom fields or custom parameters, make sure the test project in OpenLAB CDS contains the

same set of custom parameters (make sure the names and data types match when setting up). Note that custom parameters work differently in OpenLAB CDS. See the online help for additional information.

- 6 Re-analyze the same representative sample mixtures with an instrument controlled by OpenLAB CDS, in the same order as with OpenLAB CDS EZChrom Edition. For migrating the report templates, it is not necessary to re-analyze on the same instrument, but the hardware setup should be comparable. For example, if your report template does not contain signal-specific filters, you could use a 2nd instrument with a DAD detector instead of a VWD.
- 7 Use the newly created result and the migrated report template to generate a report for comparison against the reference report.
 - Watermarks in the report indicate that the template is not yet accepted after import. To accept the template, load the template into the Template Editor in the Reporting view and click **Accept template**. Note that an Accepted template file can no longer be used in OpenLAB CDS EZChrom Edition.
 - Verify the correctness of result calculations by an independent calculation method used during the initial template validation process.
 - Verify that all expected fields are filled with expected values.
 - If the previous verification steps are passed, perform additional verifications with other methods using the same template.

In case one of these verification steps fails, inspect the report template for data items that are listed in the following list of potential break points.

Report items that do not migrate well

Table 4 on page 63 shows the most important report items that do not necessarily return identical values when migrating existing report templates to OpenLAB CDS.

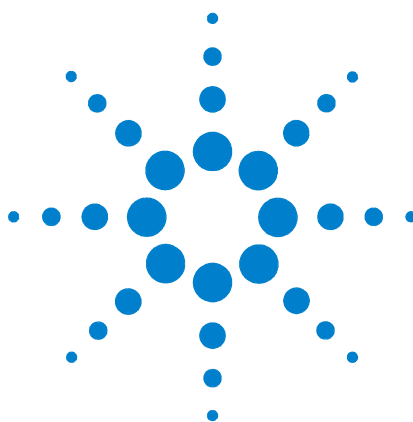
Normally, only a few parameters need to be adjusted in a template. If one of these parameters is used for data filtering or report item grouping, the impact could be highly visible.

Table 4 OpenLAB CDS Intelligent Reporting Templates developed with OpenLAB CDS EZChrom Edition

Data context	Data field	OpenLAB CDS EZChrom Edition	OpenLAB CDS version 2.3
Sample			
	Dilution factors	Up to 5 dilution factors and 5 multipliers.	Up to 5 dilution factors. The DA method defines whether it is used as a multiplier or divisor. Note: Changing from “divisor” to “multiplier” may invalidate the report template.
Signal	Description and name		The syntax of the signal description has changed slightly for specific detectors. Signal names or description are often used in filter conditions. Adjust these filter conditions if needed.
Compound	Amount	<p>OpenLAB CDS EZChrom Edition A.04.05 and earlier:</p> <ul style="list-style-type: none"> Multiplier and dilution factor are applied to calculate the amount <p>OpenLAB CDS EZChrom Edition A.04.05 Software Update 3 and later:</p> <ul style="list-style-type: none"> Multiplier and dilution factor are not applied to calculate the amount. These factors are applied to the field compound_concentration. 	<p>Amount is calculated using the calibration curve of the compound as defined in the method. Multiplier and dilution factor are not applied to calculate the amount. To use value with multiplier and dilution factor applied, use field compound_concentration instead.</p> <p>If no multiplier or dilution factor is used, the amount and concentration field values are identical.</p>
	Response factor	Default method setting: amount /response	Default: Response /amount.
	Custom field 01-10	Limited to 10 compound specific custom fields	No longer limited to 10 custom fields. Compound specific custom parameters are now written to field Compound_CustomFields.
	Type	No distinction between known (identified) peaks and calibrated peaks	Distinction between unknown, known (identified) and calibrated peaks. Compound type numbers are often used in filter conditions. Adjust these filter conditions if needed.
Peak	Peak inflection	Start - down tick End - up tick	Start - up tick End - down tick

Table 4 OpenLAB CDS Intelligent Reporting Templates developed with OpenLAB CDS EZChrom Edition

Data context	Data field	OpenLAB CDS EZChrom Edition	OpenLAB CDS version 2.3
Live system values	User name	=UserName	Replaced by =ECMOperator
	Result set path		Replaced by Injection > Data file directory
	Method comment	=MethodComment	Use “single data analysis method parameter” to display the DA method comment on the reports. Syntax: Method_Information.ID_method_description

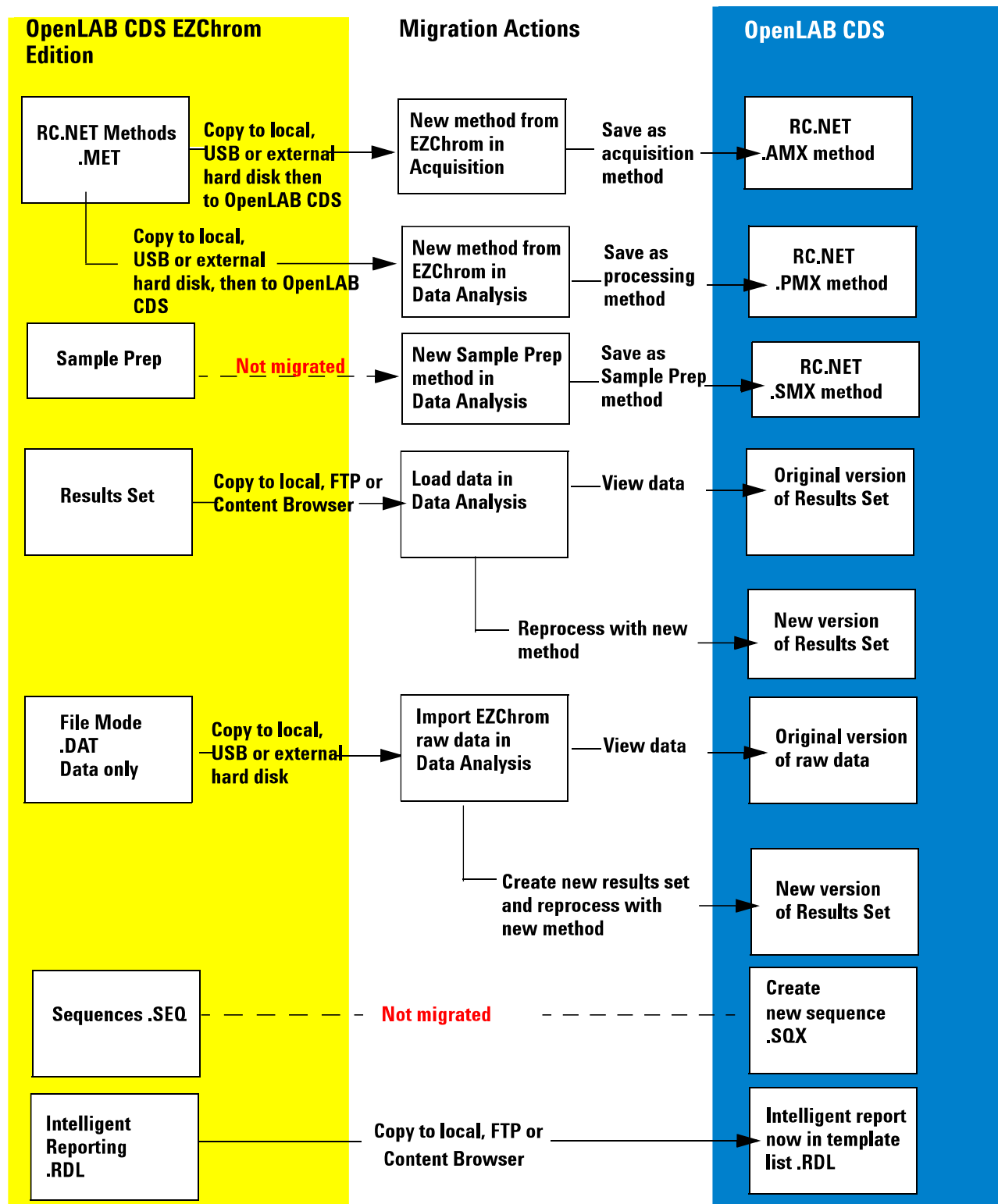


9 Appendix

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Workflow for Migration (Without Migration Tools)

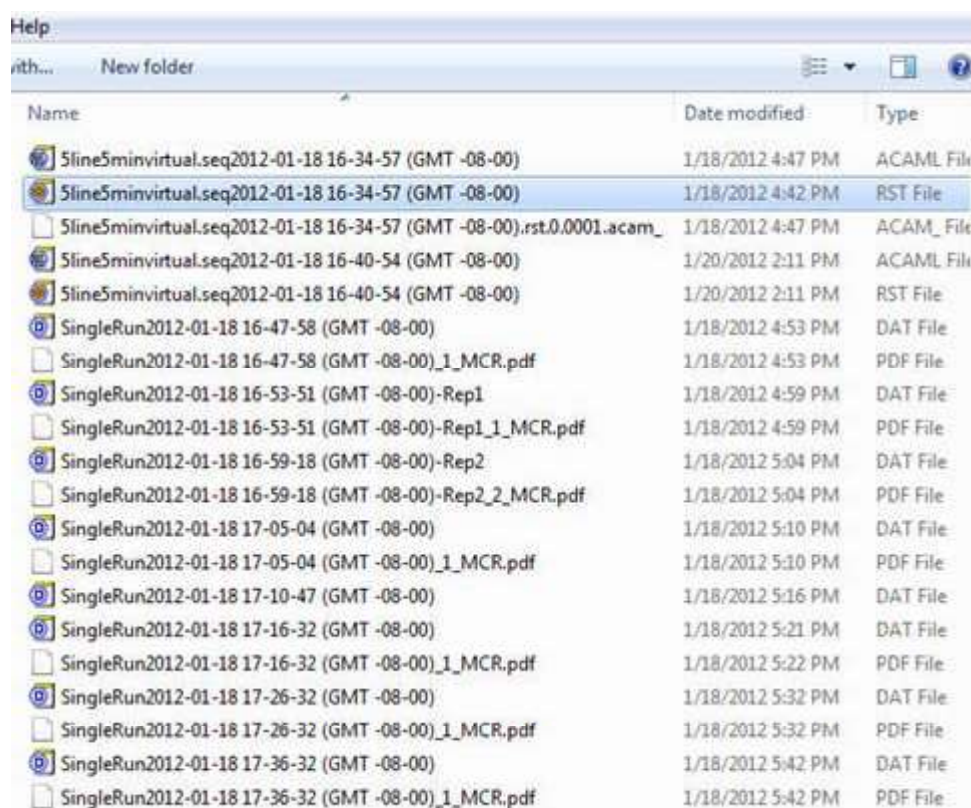


Copying Files Using the OpenLAB CDS Workstation Plus Content Management Content Browser

The recommended approach to copying files into OpenLAB CDS Workstation Plus is using FTP, as described in [Chapter 3](#), “Copying Files from OpenLAB CDS EZChrom Edition to OpenLAB CDS,” starting on page 15. You can also copy individual files (not folders) into OpenLAB CDS Workstation Plus using the following procedure, which is recommended when the OpenLAB CDS EZChrom Edition project Result Set Mode is set to File Mode.

File Mode

If the OpenLAB CDS EZChrom Edition project Result Set Mode is set to File Mode, the methods, sequences, sample prep, and template files are located in their original project folders. Results from all analyses by default are placed in the Results folder for the project, or in the result path set for the sequence ([Figure 26](#)).



Name	Date modified	Type
5line5minvirtual.seq2012-01-18 16-34-57 (GMT -08-00)	1/18/2012 4:47 PM	ACAML File
5line5minvirtual.seq2012-01-18 16-34-57 (GMT -08-00)	1/18/2012 4:42 PM	RST File
5line5minvirtual.seq2012-01-18 16-34-57 (GMT -08-00).rst.0.0001.acam_	1/18/2012 4:47 PM	ACAM File
5line5minvirtual.seq2012-01-18 16-40-54 (GMT -08-00)	1/20/2012 2:11 PM	ACAML File
5line5minvirtual.seq2012-01-18 16-40-54 (GMT -08-00)	1/20/2012 2:11 PM	RST File
SingleRun2012-01-18 16-47-58 (GMT -08-00)	1/18/2012 4:53 PM	DAT File
SingleRun2012-01-18 16-47-58 (GMT -08-00)_1_MCR.pdf	1/18/2012 4:53 PM	PDF File
SingleRun2012-01-18 16-53-51 (GMT -08-00)-Rep1	1/18/2012 4:59 PM	DAT File
SingleRun2012-01-18 16-53-51 (GMT -08-00)-Rep1_1_MCR.pdf	1/18/2012 4:59 PM	PDF File
SingleRun2012-01-18 16-59-18 (GMT -08-00)-Rep2	1/18/2012 5:04 PM	DAT File
SingleRun2012-01-18 16-59-18 (GMT -08-00)-Rep2_2_MCR.pdf	1/18/2012 5:04 PM	PDF File
SingleRun2012-01-18 17-05-04 (GMT -08-00)	1/18/2012 5:10 PM	DAT File
SingleRun2012-01-18 17-05-04 (GMT -08-00)_1_MCR.pdf	1/18/2012 5:10 PM	PDF File
SingleRun2012-01-18 17-10-47 (GMT -08-00)	1/18/2012 5:16 PM	DAT File
SingleRun2012-01-18 17-16-32 (GMT -08-00)	1/18/2012 5:21 PM	DAT File
SingleRun2012-01-18 17-16-32 (GMT -08-00)_1_MCR.pdf	1/18/2012 5:22 PM	PDF File
SingleRun2012-01-18 17-26-32 (GMT -08-00)	1/18/2012 5:32 PM	DAT File
SingleRun2012-01-18 17-26-32 (GMT -08-00)_1_MCR.pdf	1/18/2012 5:32 PM	PDF File
SingleRun2012-01-18 17-36-32 (GMT -08-00)	1/18/2012 5:42 PM	DAT File
SingleRun2012-01-18 17-36-32 (GMT -08-00)_1_MCR.pdf	1/18/2012 5:42 PM	PDF File

Figure 26 Example results folder using File Mode in OpenLAB CDS EZChrom Edition

Copying files into OpenLAB CDS Workstation Plus using the Content Browser

NOTE

You can only upload files using the OpenLAB Content Browser. You cannot upload folders.

- 1 Open Content Management (**Start > All Programs > Agilent Technologies > Content Browser**) and log in as an administrator.
- 2 On the Content Management ribbon, click **Content**. (Be sure that you have selected Show Folders from the Options menu in order to have your folders displayed.)

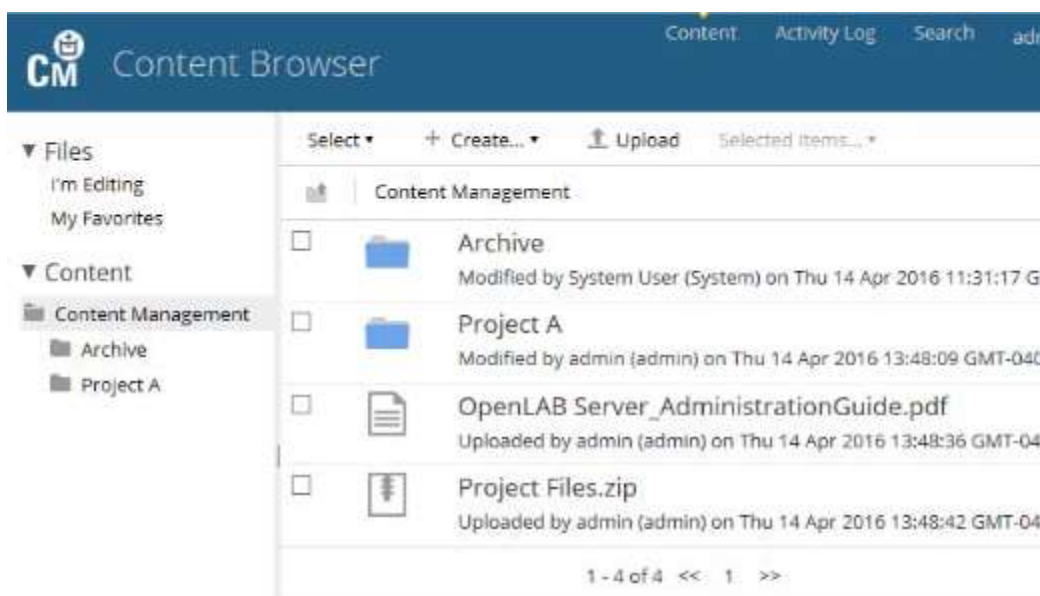


Figure 27

- 3 Click the Content Management folder where you want to copy the files, then click **Upload**.
- 4 In the Upload Files window, click **Browse** (for Internet Explorer) or **Select Files to Upload** (for Google Chrome).
- 5 Browse to and select the files you want to upload, then click **Open**. The selected files are imported into the OpenLAB CDS Content Management folder you selected.

Important Differences from OpenLAB CDS EZChrom Edition

Method differences

In OpenLAB CDS, methods are separated into the following individual files. These files are saved in the Methods folder. For more information, see the OpenLAB CDS online help.

- Acquisition Methods (*.amx)
- Sample Prep methods (*.smx)
- Processing methods (*.pmx)
- Custom Calculation files (*.ccf)

Calculations

Two results: Amount and Concentration

OpenLAB CDS Data Analysis calculates two quantitative results: Amount and Concentration.

Amount Calculated using the calibration curve of the compound as defined in the method. This value is not corrected by any factors and can have its own unit defined in the method (for example, “mg”).

Concentration The “corrected amount” which can have a separate unit defined (for example, “mg/ml”).

Depending on the choice for concentration calculation in the processing method, the concentration is calculated in OpenLAB CDS as follows:

$$\text{Concentration} = \text{Amount} * \text{Multipliers} * \text{Dilution}$$

(This is default and the way concentration was calculated in OpenLAB CDS ChemStation Edition.)

or

$$\text{Concentration} = \text{Amount} \times \left(\frac{\text{Multipliers}}{\text{DilutionFactors}} \right)$$

(This is the way amount was calculated in OpenLAB CDS EZChrom Edition.)

The Norm% result is also stored and reported as the “Concentration” value.

Clearing the calibration curve and run types

In OpenLAB CDS, automatic clearing of the calibration curve is defined in the sequence table (or Injection List in the Data Analysis). The “Run Type” column in the table allows you to define whether all calibration points (of all levels) or only all points of the respective level of the calibration standard are removed before processing a specific calibration standard injection. (See [Figure 28](#).) If the Run Type is not set, the calibration points will be averaged with already existing calibration points. This is similar to the setup in the sequence table of an OpenLAB CDS EZChrom Edition system, but it is important to know that all other “Run Types” are not yet supported.

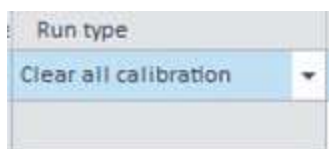


Figure 28 Run type selection in OpenLAB CDS sequence table

New bracketing calibration

The bracketing definition in OpenLAB CDS is included in the sequence/injection list table. With a single selection box you define the type of bracketing (None, Overall, non-Overlap and Overlap) to use when processing a result set. Refer to the online help for more information.



Figure 29 Bracketing mode selections in OpenLAB CDS

Example of .CSV Sequence Format

An example of a comma separated variable (.csv) file for an OpenLAB CDS sequence is shown in the following figure.

```
Vial, Sample type, Acq. method, Proc. method, Inj/Vial, Volume, Injection source , Sample amount,
Sample name, Data file, Sample prep method
Vial 1, Sample, LC-01.amx, LC-01.pmx, 1, 1.0, Als, 1.0, Sample-1, Sample-1, LC-01.smx
Vial 2, Blank, LC-02.amx, LC-02.pmx, 2, 2.0, Als, 2.0, Sample-2, Sample-2, LC-01.smx
Vial 3, Double blank, LC-03.amx, LC-03.pmx, 3, 3.0, Als, 3.0, Sample-3, Sample-3, LC-01.smx
Vial 4, Cal. Std., LC-04.amx, LC-04.pmx, 4, 4.0, Als, 4.0, Sample-4, Sample-4, LC-04.smx
Vial 5, QC check, LC-05.amx, LC-05.pmx, 5, 5.0, Als, 5.0, Sample-5, Sample-5, LC-05.smx
Vial 6, Spike, LC-06.amx, LC-06.pmx, 6, 6.0, Als, 6.0, Sample-6, Sample-6, LC-06.smx
Vial 7, Sys. Suit., LC-07.amx, LC-07.pmx, 7, 7.0, Als, 7.0, Sample-7, Sample-7, LC-01.smx
```

Figure 30 Example .csv file for an OpenLAB CDS sequence

Supported sequence column headers in OpenLAB CDS

The following is a list of supported sequence column headers for import to OpenLAB CDS. For more information on importing sequences in .csv format, see the OpenLAB CDS online help.

Table 5 Sequence columns supported by OpenLAB CDS

Supported columns	Unsupported columns
Acq. method	Action
Data file	Bracket
Dil. factor 1	Expected barcode
Dil. factor 2	Injection source
Dil. factor 3	Sample prep method (different file extension from OpenLAB CDS EZChrom Edition)
Dil. factor 4	State
Dil. factor 5	Use Method
Inj/Vial	
ISTD amt 1	
ISTD amt 2	
ISTD amt 3	
ISTD amt 4	
ISTD amt 5	

Table 5 Sequence columns supported by OpenLAB CDS (continued)

Supported columns	Unsupported columns
Level	
Multiplier 1	
Multiplier 2	
Multiplier 3	
Multiplier 4	
Multiplier 5	
Proc. method	
Run type	
Sample amount	
Description	
Sample name	
Sample type	
Target 1	
Target 2	
Target 3	
Target 4	
Target 5	
Type	
Vial	
Volume	



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