Agilent

ASM Export for OpenLab CDS

User and Installation Guide

Notices

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Software Revision

This guide is valid for revision 1.0 or higher of Agilent ASM Export for OpenLab CDS, until superseded.

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1 Introduction

This solution enables the automatic conversion of OpenLab CDS data stored in ECM to ASM (Allotrope Simplified Model) files (JSON format). Liquid chromatography (LC), supercritical fluid chromatography (SFC), gas chromatography (GC), liquid chromatography/Mass Spectrometry (LC/MS), and gas chromatography/mass spectrometry (GC/MS) data including chromatograms and spectra can be exported to ASM files.

Features

- Export of OpenLab CDS data archived in OpenLab ECM 3.6 and OpenLab ECM XT 2.8 and conversion to ASM (Allotrope Simplified Model) files (JSON format).
- The conversion to ASM files takes place automatically after completion of the analytical data (re)-processing.
- Data is converted according to the Allotrope Liquid Chromatography (LC), Gas Chromatograph (GC), Liquid Chromatography/Mass Spectrometry (LC/MS) and Gas Chromatography/Mass Spectrometry (GC/MS) specification version 09/2026. SFC data is represented using the LC specification.
- The generated ASM files are stored in a customer defined data storage location: an Amazon S3 bucket or a local file system.
- The solution can be managed and monitored through a web-based user interface.

Components

This solution includes the following components:

- ASM Export for OpenLab CDS
  - Main application that includes all back-end functionality and the web-based user interface but excluding the ASM conversion logic (which is a separate component).
  - File name: **Agilent.ASMExport.OpenLabCDS.Setup.msi**
  - Latest version: 1.0.0
- ASM Export for OpenLab CDS Configuration Tool
  - The Configuration Tool is part of ASM Export for OpenLab CDS and becomes available after successful installation of ASM Export for OpenLab CDS. The Configuration Tool properly configures the required connections between the ASM Export for OpenLab CDS application and the OpenLab Shared Services (OLSS) components.
  - File name: **Agilent.ASMExport.OpenLabCDS.ConfigurationTool.exe**
- Allotrope Converter for OpenLab CDS
  - Separate logic to convert an OpenLab CDS result dataset to one or more ASM file(s). This conversion logic component is used by the main ASM Export for OpenLab CDS application.
  - File name: **Agilent.AllotropeConverter.OpenLabCDS.Setup.msi**
  - Latest version: 1.0.0

Additional Services

In addition to the software product, optional professional services are available, including installation support and assisted batch conversion of historical data. Contact your local sales representative for information on available services and associated options.

2 Requirements

OpenLab Topology Requirements

ASM Export for OpenLab CDS operates in an integrated environment where OpenLab CDS is connected to OpenLab ECM 3.6 or OpenLab ECM XT 2.8) through OpenLab Shared Services (OLSS). OLSS enables and provides authentication, data repository (database), activity log, and communication services, while ECM provides centralized storage for CDS data accessed by ASM Export for OpenLab CDS.

ASM Export for OpenLab CDS is only supported for Client/Server topologies (both regular and Enterprise setups) and must be installed on the OpenLab Server machine due to the tight integration with OpenLab Shared Services (OLSS) components (in specific, the Reverse Proxy).

NOTE

ASM Export for OpenLab CDS shares hardware and software resources with the OpenLab Server/Shared Services application (CPU, RAMM, database, …). Ensure the machine is properly dimensioned per OpenLab Server/Shared Services instructions to have a performant ASM Export for OpenLab CDS installation.

Installed Software Requirements

Table 1 shows the software requirements for the OpenLab Server machine on which ASM Export for OpenLab CDS and Allotrope Converter for OpenLab CDS are installed.

Table 2 shows the software requirements for the client machine from where a user accesses the web-based user interface.

Table 1 Software requirements for ASM Export for OpenLab CDS installation

Requirement	Description
Operating System	Any supported OpenLab Server operating system (for details, refer to the OpenLab CDS documentation); ASM Export for OpenLab must be installed in the same machine where OpenLab Server is installed.
Agilent OpenLab ECM 3.6 (if no Agilent OpenLab ECM XT 2.8)	ECM: ECM v3.6 Update 7 or later Web Interface: v3.6 or later
Agilent OpenLab ECM XT 2.8 (if no Agilent OpenLab ECM 3.6)	v2.8 Update 4 or later
Agilent OpenLab Server	v2.8 Update 4 or later
Agilent OpenLab Server database backend	Microsoft SQL Server or PostgreSQL
Agilent OpenLab Shared Services	Any version compatible with installed OpenLab Server and ECM
Amazon S3 bucket (optional)	Bucket can be set up after installation of ASM Export for OpenLab
Microsoft .NET Runtime	v8.0.x (x64) (required for Allotrope Converter for OpenLab CDS)
Microsoft ASP.NET Core Runtime	v10.0.x (x64) (required for ASM Export for OpenLab CDS)
Microsoft .NET Desktop Runtime	v10.0.x (x64) (required for ASM Export for OpenLab CDS)

Table 2 Requirements for web-based user interface clients

Requirement	Description
Operating System	Windows 10 Windows 11
Browser	Google Chrome v107 or later Microsoft Edge v107 or later Mozilla Firefox v104 or later Opera v93 or later

NOTE

The database user account password must comply with the password policy of the database. Failure to meet the password policy requirements may prevent successful configuration of ASM Export for OpenLab CDS. Changes to the password policy after successful configuration might result in a non-functional ASM Export for OpenLab CDS.

Ingestion Source and Transfer Destination Prerequisites

OpenLab ECM 3.6

When using **ECM 3.6** as Ingestion Source, the configured user that interacts with ECM must be granted the following privileges at a minimum:

- **System: Advanced Search** (**Run**) privilege

During configuration of the Ingestion Source, the configuration can only be saved if all required privileges are properly granted (for details, refer to the "Configuring Using the ASM Export for OpenLab CDS Configuration Tool" section on page 20), which is verified by executing a specific API call to explicitly validate the presence of the required privilege for the configured ECM user.

OpenLab ECM XT 2.8

ECM XT 2.8 uses a combination of API features that need to be exposed via specific licensing tiers and user privileges that need to be granted to the users that consume the API.

None of the API features required by ASM Export for OpenLab CDS are gated by licensing; they are available to any authenticated user.

The configured user that interacts with ECM must be granted the following privileges at a minimum:

- **download** (**Download files/folders** in OpenLab Control Panel)
- **viewcontent** (**View content** in OpenLab Control Panel)

During configuration of the Ingestion Source, the configuration can only be saved if all required privileges are properly granted (for details, refer to the "Configuring Using the ASM Export for OpenLab CDS Configuration Tool" section on page 20), which is verified by executing specific API calls (against the root folder as a best effort basis) to validate the presence of the required privileges for the configured ECM user.

Amazon S3

When using an **Amazon S3** bucket as **Transfer Destination**, ASM Export for OpenLab CDS supports two authentication mechanisms. The **Explicit Credentials** toggle in the web-based user interface allows you to choose between the following two:

- **Explicit Credentials:** An AWS Access Key ID and Secret Access Key are explicitly provided (together with the region and bucket name) through the web-based user interface (**Configuration** menu). The underlying S3 client interface is using these long-term credentials directly.
- **No Explicit Credentials:** No explicit credentials are provided through the web-based user interface (only region and bucket name). The underlying S3 client uses the default AWS credential chain, which resolves to the AWS variables defined in the environment variables in the machine running the ASM Export for OpenLab CDS application, the AWS variables defined in the credentials configuration file defined in the machine running the ASM Export for OpenLab CDS application, or to the IAM role attached to the EC2 instance (for cloud-based deployments). Configure your environment using one of the following options when selecting the No Explicit Credentials option:
  - Environment variables: When using environment variables, define the credentials (e.g., **AWS_ACCESS_KEY_ID**, **AWS_SECRET_ACCESS_KEY**, and **AWS_DEFAULT_REGION** when using short-term credentials) in the system-level environment variables. For details, refer to the Amazon documentation.
  - Credentials configuration file: When using a credentials configuration file, create a configuration file (e.g., containing **aws_access_key**, **aws_secret_access_key**, and **aws_session_token** when using short-term credentials) on the file system and refer the system-level environment variable **AWS_SHARED_CREDENTIALS_FILE** to the configuration file. For details, refer to the Amazon documentation.
  - Direct IAM role usage (only applicable for cloud-based OpenLab environments): The S3 client uses the default AWS credential chain and automatically assumes the IAM role assigned to the hosting EC2 instance, ECS task, or runtime environment. When the OLSS server is deployed on-premises, the IAM Anywhere service can be implemented. Use the 8.3 short path for the directory containing aws_signing_helper.exe to avoid issues caused by whitespace characters in the folder path.

Requirements

The IAM user or role must be granted the following privileges on the target bucket at a minimum:

- **s3: ListBucket**
- **s3: PutObject**
- **s3: DeleteObject**

This translates into the following IAM policy as an example:

```
{
  "Version": "2012-10-17",
  "Statement": [
    {
      "Effect": "Allow",
      "Action": [
             "s3:PutObject",
             "s3:ListBucket",
             "s3:DeleteObject",
      ],
      "Resource": [
        "arn:aws:s3:::bucket-name",
        "arn:aws:s3:::bucket-name/*"
      ]
    }
  ]
}
```

During configuration of the **Transfer Destination**, the configuration can only be saved if all required privileges are properly granted (for details, refer to the "Configuring Using the ASM Export for OpenLab CDS Configuration Tool" section on page 20), which is verified by executing the following connectivity test:

1. Authenticate to the configured Amazon S3 bucket and list objects to verify credentials and bucket access.
2. Create a test folder (dts-connectivity-test) inside the Transfer Destination Location.
3. Upload a test file (test-file.txt) inside the test folder.
4. Clean up both the test file and test folder.

NOTE

When using the system-level environment variables or a credentials configuration file approach (No Explicit Credentials), ASM Export for OpenLab CDS does not manage the credentials directly. In those cases, an external mechanism must be used to define and maintain the credentials. After the credentials are updated, the Agilent ASM Export for OpenLab CDS service must be restarted to ensure ASM Export for OpenLab CDS uses the updates credentials.

NOTE

Consider performance, cost, and compliance requirements when choosing an Amazon region. For best performance and lower latency, select a region geographically close to where your data originates or where most users access it. This can also help reduce data transfer costs. Additionally, some organizations must store data in specific regions to meet legal, regulatory, or internal compliance requirements, so verify any data residency rules before creating your bucket.

Local File System

When using **Local File System** as transfer destination, ASM Export for OpenLab CDS does not perform user impersonation. ASM Export for OpenLab CDS writes files using the identity of the ASP.NET Core process itself — whatever account runs the dotnet process (e.g., an IIS Application Pool identity, a Windows service account, or the logged-in user during local dev). For mounted UNC paths (e.g., \\server\share\...), network access relies on the process identity's Kerberos/NTLM credentials.

The process identity must be granted the following privileges on the configured Transfer Destination Location (e.g., C:\my_output_folder\) at a minimum:

- **Read**
- **Write**
- **Create directories**
- **Modify**

During configuration of the Transfer Destination, the configuration can only be saved if all required privileges are properly granted (for details, refer to the "Configuring Using the ASM Export for OpenLab CDS Configuration Tool" section on page 20), which is verified by executing the following connectivity test:

1. Check whether the configured base path directory (Transfer Destination Location) exists.
2. Create a test folder (dts-connectivity-test) inside the Transfer Destination Location.
3. Write a test file (test-file.txt) inside the test folder.
4. Clean up both the test file and test folder.

OpenLab CDS Data Prerequisites

Any analytical data from the supported devices and detectors (for details, refer to the "Supported Systems and Modules" section on page 67) that can be opened in OpenLab CDS 2.8 or OpenLab CDS 3.0 is supported for conversion to ASM files. This includes data originally generated or processed using older versions of OpenLab CDS as well as non-CDS data (e.g., ChemStation data) that has been imported into OpenLab CDS.

3 Installing, Updating, Uninstalling, and Configuring ASM Export for OpenLab CDS

The Allotrope Converter for OpenLab CDS and ASM Export for OpenLab CDS application must be installed in no specific order. Subsequently, the ASM Export for OpenLab CDS Configuration Tool will verify the installation of both components and properly configure the integration with OpenLab Shared Services (OLSS).

Installing and Updating Allotrope Converter for OpenLab CDS

Download the Software

1. Go to FlexNet Operations (FNO) at: https://agilentlicensing.flexnetoperations.com/.
2. Log in with your FNO user ID and password.
3. In the **Downloads** section, search for **ASM Export for OpenLab CDS Installer** in the **OpenLab Add-Ons** folder and download the software to a local drive.
4. Unzip the software package to your local hard drive.
5. Copy the **Allotrope Converter for OpenLab CDS** MSI file to a directory on the OpenLab Server machine (e.g., C:\tmp).

Update the Software

If an older version of **Allotrope Converter for OpenLab CDS** software was installed before, first uninstall the older version of the **Allotrope Converter for OpenLab CDS** software:

1. Open **Settings** (select **Start** and search for “settings”).
2. Select **Apps** > **Installed Apps**.
3. Select **Agilent Allotrope Converter for OpenLab CDS** and click **Uninstall**.
5. Follow the wizard until the uninstallation is completed.

Once the software is uninstalled, run the new installation file (for details, refer to the "Install the Software" section on page 18).

NOTE

To prevent queued tasks from failing during an update of the Allotrope Converter software, complete the following steps before uninstalling the previous version:

- Stop the **Automatic Mode Discovery process**.
- Allow all queued tasks to finish processing.
- Stop the **Processing process** (for details, refer to the "ASM Export for OpenLab CDS Workflow" section on page 27).

After the Allotrope Converter update is complete, restart both the **Automatic Mode Discovery process** and the **Processing process**.

Install the Software

Install the downloaded version of the **Allotrope Converter for OpenLab CDS** software:

1. Double-click the MSI file to launch the installation wizard.
2. When the "Do you want to allow this app to make changes to your device?" prompt appears, select **Yes**.
3. Follow the installation wizard until the installation is complete.

NOTE

The **Allotrope Converter for OpenLab CDS** installation wizard just closes after successful installation; no specific message is displayed. Successful installation can be verified in Windows in **Apps** > **Installed Apps**.

Installing and Updating ASM Export for OpenLab CDS

Download the software

1. Go to FlexNet Operations (FNO) at: https://agilentlicensing.flexnetoperations.com/.
2. Log in with your FNO user ID and password.
3. In the **Downloads** section, search for **ASM Export for OpenLab CDS Installer** in the **OpenLab Add-Ons** folder and download the software to a local drive.
4. Unzip the software package to your local hard drive.
5. Copy the **ASM Export for OpenLab CDS** MSI file to a directory on the OpenLab Server machine (e.g., C:\tmp).

Update the Software

If an older version of the **ASM Export for OpenLab CDS** software was installed before, first uninstall the older version of the **ASM Export for OpenLab CDS** software:

1. Open **Settings** (select **Start** and search for “settings”).
2. Select **Apps** > **Installed Apps**.
3. Select **Agilent ASM Export for OpenLab** CDS and click **Uninstall**.
4. Follow the wizard until the uninstallation is completed.

Once the uninstallation is complete, install the latest version of the software (for details, refer to the "Install the Software" section on page 18).

Install the Software

Install the downloaded version of the **ASM Export for OpenLab CDS** software:

1. Double-click the MSI file to launch the installation wizard.
2. When the “Do you want to allow this app to make changes to your device?” prompt appears, select **Yes**.
3. Follow the installation wizard until the installation is complete.

NOTE

The **ASM Export for OpenLab CDS** installation wizard just closes after successful installation; no specific message is displayed. Successful installation can be verified in Windows in **Apps** > **Installed Apps**. If installation was not successful, the following "debug" installation command can be used to retrieve detailed information: C:\Users\Administrator> msiexec.exe /i <path to MSI file> /l*v install.log.

Configuring Using the ASM Export for OpenLab CDS Configuration Tool

The **ASM Export for OpenLab CDS Configuration Tool** is used for registering the ASM Export for OpenLab CDS application in the OpenLab ecosystem. The Configuration Tool must be executed after successful completion of the ASM Export for OpenLab CDS installation.

The ASM Export for OpenLab CDS Configuration Tool executes the following configuration steps:

- OLSS registration
- Data Repository registration
- Local reverse proxy configuration
- Saving settings to local configuration file
- Restart Windows service

1. Launch the **ASM Export for OpenLab CDS Configuration Tool**:
   a. Select **Start** and search for **ASM Export for OpenLab CDS Configuration Tool**.
   b. Launch **ASM Export for OpenLab CDS Configuration Tool**.
2. To configure the interaction with OLSS, define the following configuration settings:
   - **URL**: The URL of the OLSS REST API (must be the external hostname of the OLSS server).
   - **Username**: The username to be used for interaction with the OLSS REST API. Preferably a local OpenLab administrator with all privileges.
   - **Password**: The password to be used for interaction with the OLSS REST API.
   - **Domain**: The domain to be used for interaction with the OLSS REST API (drop-down populated with values returned by the OLSS REST API). Leave the field blank when using local authentication (no domain).
   - **Language**: The language to be used in the OpenLab Control Panel (drop-down populated with the languages supported by ASM Export; (defaults to the language of the local OLSS installation).

3 Click **Test Connection** to verify the accessibility of the OLSS REST API.
   - The button colors green when connection could successfully be established.
   - The button colors red (and an error message is shown) when the connection could not be established. In certain cases, you are offered to go to log files for troubleshooting.

4 To configure Data Repository, define the following settings:
   - **Base Service URL**: The URL of the Data Repository REST API.
   - **New Database User Password**: The password for the Data Repository database user.
   - **Confirm Database User Password**: Confirm the password for the Data Repository database user. Field colors green if both passwords match and red if both passwords don't match.

   By default, the password fields are pre-filled with the de-obfuscated OpenLab Data Repository user password set during installation.

5 Save the configuration:
   a. When both the **Test Connection** button and **Confirm Database User Password** field color green, click **Save** at the bottom.
   b. Wait for the popup **Configuration successfully applied!** to confirm the configuration is applied (this can take up to 30 seconds). If configuration is not successful, the Configuration Tool log file can be consulted at %ProgramData%\Agilent\LogFiles\ASM Export for OpenLab CDS\ConfigurationTool-<timestamp>

6 Close the popup by clicking **OK**.

7 Close the ASM Export for OpenLab CDS Configuration Tool.

NOTE The ASM Export for OpenLab CDS Configuration Tool must be executed each time a new version of ASM Export for OpenLab CDS is installed.

NOTE The Data Repository password complexity requirements are unknown by the Configuration Tool. When clicking **Save**, the configuration can fail if the provided password does not satisfy the complexity requirements. Ensure the provided Data Repository password satisfies the complexity requirements.

Software Verification Tool (SVT)

The Agilent Software Verification Tool (SVT) qualifies your installation and informs you about successful installation on an existing system.

To run the SVT after installing and configuring both Allotrope Converter for OpenLab CDS and ASM Export for OpenLab CDS, execute the following steps:

1 Obtain the SVT through one of the following means:

- The SVT is included with the Agilent OpenLab CDS software.
- The SVT is included with the ECM Client software.
- Download the SVT from Agilent's SubscribeNet account and install per provided instructions.

2 Start the SVT:

c. Select **Start**.

d. Select **Agilent Technologies**.

e. Click **Software Verification Tool** to open the SVT.

3 Qualify the **Allotrope Converter for OpenLab CDS** installation:

a. Select the **Allotrope Converter for OpenLab CDS** check box.

b. Click **Qualify** to create the Software Verification Report.

4 Qualify the **ASM Export for OpenLab CDS** installation:

a. Select the **ASM Export for OpenLab CDS** check box.

b. Click **Qualify** to create the Software Verification Report.

Network and Firewall Configuration Requirements

The application uses http.sys for HTTP communication. This allows the application to leverage the Windows HTTP Server API for request handling and routing, providing reliable and centralized port binding. The application listens on a configured port (default: 52080), while http.sys manages incoming requests and routes them to the appropriate service endpoint.

The application is exposed via the OpenLab reverse proxy. Ensure that the reverse proxy is reachable, as it is required for normal operation and external access to the application.

Security, Configuration, and Service Account

Configuration Files

The application stores configuration files in the following locations:

- C:\ProgramData\Agilent\ASM Export for OpenLab CDS\config.json
- C:\ProgramData\Agilent\ASM Export for OpenLab CDS\DataProtection-Keys\

Both are secured using Windows Access Control Lists (ACLs) and are accessible only to:

- SYSTEM
- Administrators
- The application's virtual service account

This ensures that configuration settings and sensitive data protection keys are restricted to authorized system-level access only.

Service Account and Access Requirements

The Windows service is installed and runs under the virtual service account:
NT SERVICE\Agilent.OpenLab.DataTransformationService.Server

During installation, a URL ACL reservation is created for:
http://+:52080/openlab/asm-export/

If the service identity is changed, the administrator must ensure that the new account has the appropriate permissions:

- Read access to the config.json file
- Read access to the key directory (DataProtection-Keys)
- Permission to register and use the configured URL namespace (URL ACL)

Failure to grant these permissions may prevent the service from starting or functioning correctly.

Log Files and Temporary Files Folders

The application stores log files and temporary files in the following locations:

- %ProgramData%\Agilent\ASM Export for OpenLab CDS\
- %ProgramData%\Agilent\ASM Export for OpenLab CDS\temp\
- %ProgramData%\Agilent\LogFiles\ASM Export for OpenLab CDS\
- %ProgramData%\Agilent\AllotropeExport\LogFiles\

NOTE

These folders may grow over time, depending on application usage. Ensure that sufficient disk space is available and periodically review and clean up these locations if required, in accordance with your site's IT policies.

Anti-Virus Software Configuration Requirements

The folders listed below must be excluded from all real-time and scheduled antivirus scanning. Scanning these folders can interfere with normal operation and can cause performance issues, unexpected behavior, or data integrity problems. Customers must configure their antivirus software to exclude these folders from all scanning and quarantine actions. Refer to your antivirus vendor's documentation for instructions on configuring exclusions.

Folders to exclude from anti-virus scanning

- %Program Files%\Agilent Technologies\ASM Export for OpenLab CDS\
- %Program Files%\Agilent Technologies\Allotrope Converter for OpenLab CDS\
- %ProgramData%\Agilent\ASM Export for OpenLab CDS\
- %ProgramData%\Agilent\ASM Export for OpenLab CDS\temp\
- %ProgramData%\Agilent\ASM Export for OpenLab CDS\DataProtection-Keys\
- %ProgramData%\Agilent\LogFiles\ASM Export for OpenLab CDS\
- %ProgramData%\Agilent\AllotropeExport\
- *Any user-defined Local File System output folder (i.e., Transfer Destination Location configuration setting)*

Windows Long File Name Support

The application can generate output files in which the full file or directory path exceeds the traditional 260-character path length limit enforced by Microsoft Windows. The application is long-path aware; however, operating-system-level support must be enabled to allow extended path lengths.

Enable Win32 Long Paths

On Windows 10 version 1607 and later (including Windows 11), Win32 long paths must be enabled using the **Enable Win32 long paths** policy or the equivalent **LongPathsEnabled** registry setting. If this setting is not enabled, Windows will continue to enforce the legacy path length limitation, even for compatible applications. In such cases, file access operations and downstream analyses may fail.

For configuration details, refer to the official Microsoft documentation on enabling long file paths on Microsoft Learn.

Verification

Administrators can verify that Win32 long paths are enabled by running the following command from an elevated command prompt on the system where ASM Export for OpenLab CDS is installed:

```
reg query HKLM\SYSTEM\CurrentControlSet\Control\FileSystem
/v LongPathsEnabled
```

A value of 0x1 confirms that long file path support is enabled.

Uninstalling Allotrope Converter for OpenLab CDS and ASM Export for OpenLab CDS

To uninstall **Allotrope Converter for OpenLab CDS**, execute the following steps:

1. Open **Settings** (select **Start** and search for "settings").
2. Select **Apps** > **Installed Apps**.
3. Select **Agilent Allotrope Converter for OpenLab CDS** and click **Uninstall**.
4. Follow the wizard until the uninstallation is completed.

To uninstall **ASM Export for OpenLab CDS**, execute the following steps:

1. Open **Settings** (select **Start** and search for "settings").
2. Select **Apps** > **Installed Apps**.
3. Select **Agilent ASM Export for OpenLab CDS** and click **Uninstall**.
4. Follow the wizard until the uninstallation is completed.

NOTE

The uninstallation wizard does not remove data. This allows you to reinstall the application and continue using the data after re-installation.

4 ASM Export for OpenLab CDS Workflow

Automatic Mode and Manual Data

The application has two distinct **Discovery** and **Processing** workflows: **Automatic Mode** and **Manual Mode**.

The **Automatic Mode** workflow considers data that is generated or updated after installation of ASM Export for OpenLab CDS and discovery is based on continuously monitoring the ingestion source (i.e., ECM storage linked to your OpenLab CDS environment). A periodic polling (user-defined polling frequency; typically, minutes) mechanism is used to data that was generated or updated since the previous polling round.

The **Manual Mode** considers data already available in ECM that you wish to process independently of the **Automatic Mode** process. The **Manual Mode** workflow is an on-demand process. For details, refer to the "Discovery and Processing Processes" section on page 27.

Discovery and Processing Processes

The export of data from ECM to the user-defined transfer destination goes through two distinct and decoupled processes: the **Discovery** process and the **Processing** process (which consists of an **Ingestion**, **Conversion** and **Transfer** step).

The **Automatic Mode Discovery** process uses the periodic polling approach as explained in the "Automatic Mode and Manual Data" section on page 27. The **Manual Mode Discovery** process uses an on-demand approach where a user needs to specify parameters the data needs to satisfy (e.g., timestamp of file in ECM needs to be within a defined date range). Both the **Automatic Mode Discovery** process and **Manual Mode Discovery** processes can be active in parallel and are independent of each other.

Eventually, these **Discovery** processes discover datasets that need to be exported from ECM and converted into ASM files and put the identifiers of these datasets into a single queue. It is important to note that no download from ECM or conversion has happened yet at this point in the overall process. A separate

process – the **Processing** process – periodically queries the queue and processes the listed datasets one by one (or a few in parallel depending on the parallelization setting). This approach effectively throttles the load of incoming data and manages back-pressure properly.

NOTE

The **Discovery** and **Processing** processes can be managed (e.g., started/stopped) independently from each other through the web-based user interface. For details, refer to the "Web-Based User Interface" section on page 33.

NOTE

The **Automatic Mode Discovery** and **Manual Mode Discovery** processes are independent of each other, but they can run in parallel at the same time. For example, the **Automatic Mode Discovery** process can be running and discovering datasets to be processed while a user is configuring and running the **Manual Mode Discovery** process.

NOTE

Processing of data identified by the **Automatic Mode Discovery** process always has priority over processing of data identified by the **Manual Mode Discovery** process.

NOTE

Only the latest version of a dataset is discovered in both Automatic Mode and Manual Mode. In Automatic Mode, only the most recent version within a polling window is discovered (newer versions in subsequent polling windows can be discovered later). In Manual Mode, the most recent version within the specified date range is discovered.

The **Discovery** and **Processing** processes for both **Automatic Mode** and **Manual Mode** are schematically shown in Figure 1.

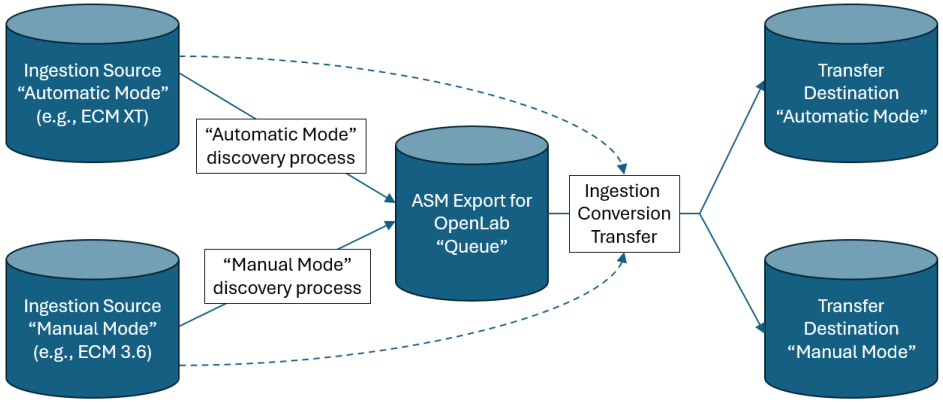


Figure 1 Overview of the Discovery and Processing processes in ASM Export for OpenLab CDS

Ingestion, Conversion, and Transfer

The **Processing** process consists of three distinct sequentially executed steps: **Ingestion**, **Conversion**, and **Transfer**.

Ingestion

The process starts with an **Ingestion** step that effectively downloads the OpenLab CDS data as a single data archive from the configured Ingestion Source (i.e., ECM location) to the machine where the ASM Export for OpenLab CDS application is installed.

The configuration of the Ingestion Source is managed through the web-based user interface (for details, refer to the "Web-Based User Interface" section on page 33).

After successfully downloading the data archive, the data archive is automatically passed on to the **Conversion** step.

NOTE

Data discovery and ingestion rely on predefined folder structures and file-naming conventions in ECM. Manually modifying folder structures or file names may cause data to be excluded from Discovery or Ingestion.

Conversion

After successfully downloading the data in the **Ingestion** step, the downloaded data archive is converted, per the specified conversion configuration, into one or more ASM files using the dedicated Allotrope Converter for OpenLab CDS component.

The configuration of the **Conversion** is managed through the web-based user interface (for details, refer to the "Web-Based User Interface" section on page 33).

As a result of the **Conversion** step, one ASM file is created per injection (for details, refer to the "ASM File Name" section on page 31). Each ASM file is automatically passed on to the **Transfer** step.

Transfer

After successfully generating the ASM files during the **Conversion** step, the ASM files are transferred to the configured transfer destination (e.g., Amazon S3 bucket).

The configuration of the **Transfer** is managed through the web-based user interface (for details, refer to the "Web-Based User Interface" section on page 33).

After successfully transferring the ASM files, the **Processing** process is completed and the next Processing cycle (**Ingestion**, **Conversion**, and **Transfer**) starts.

Parallelization

Parallelization enables the **Processing** process to run concurrently across multiple processes, reducing overall execution time. Configure between one and five processes where using one process runs all the steps sequentially with minimal resource usage and maximum stability, while increasing to two-to-five processes enables parallel execution that can significantly reduce overall execution time.

The parallelization configuration is managed through the web-based user interface (for details, refer to the "Web-Based User Interface" section on page 33).

NOTE

Using a higher number of processes increases CPU, memory, and I/O consumption. While 5 processes can reduce execution time, it also raises the risk of resource contention or failures if the system does not have sufficient capacity. Select the number of processes carefully to balance performance gains against available resources.

ASM File Name

One ASM file is created per injection meaning a single sequence of, for example, five injections will result in five ASM files being created. The file name of the ASM files is composed of the following components:

- **Sequence name:** The name of the sequence as shown in OpenLab CDS (not present for single injection datasets).
- **Injection file name**: The file name of the .dx file corresponding to the injection.
- **Version**: The version of the data as shown in OpenLab CDS.

An example is: **SequenceName-InjectionFile.dx-2025-1002-0959-09391.json**

NOTE

Characters that would result in an invalid Windows or non-recommended Amazon S3 file name are removed or replaced when constructing the file name of the exported ASM files. Leading dots (1 or more) are removed. Leading, internal, and trailing spaces are replaced by an underscore (_). Furthermore, any character not part of A–Z a–z 0–9 ! & - _ . ' ( ) is replaced by an underscore (_).

NOTE

File names are uniquely identified only by the combination of the sequence name (if available), injection file name and the version. If the same data version is processed again, for example, when reprocessing previously processed data via the **Manual Mode** workflow, the existing data will be overwritten in the Transfer Destination.

Error Handling

Retrying Failures

During the **Ingestion, Conversion, and Transfer** steps, retries are performed automatically where appropriate. Since Ingestion Sources and the Transfer Destinations are tested during configuration in the web-based user interface, no retries occur if credentials are invalid (**Fail once**).

For other types of failures, multiple retries are attempted, with exponentially increasing waiting times between attempts (**Retry with exponential back-off**). Each individual Ingestion or Transfer step has a maximum duration of 1 hour, after which the process is forcefully terminated. For details regarding which conversion errors result in **Fail once** or **Retry**, refer to Table 12 on page 70.

Conversion Errors

ASM files are generated and transferred to the configured Transfer Destination only if an input dataset is entirely converted successfully. If an error occurs during the conversion of a sequence (a dataset containing more than one injection), the entire sequence is considered failed — even if some individual injections were processed successfully. In this case, no ASM files are transferred to the Transfer Destination, including those generated from successfully converted injections.

Error Logging

Basic error messaging is available through the web-based user interface. The **Message** column in the **Conversion Log contains applicable error messages.** More detailed error messaging is available in the log files on the server where ASM Export for OpenLab CDS is installed (for details, refer to the "Log Files and Temporary Files Folders" section on page 24).

5 Web-Based User Interface

The application contains a web-based user interface where configuration can be managed, and conversion statistics can be consulted. The web-based user interface is hosted on the OpenLab Server and can be consulted from any client computer having network access to the OpenLab Server.

Configuring HTTPS

ASM Export for OpenLab CDS is accessed through the OpenLab reverse proxy using the **openlab/** path. The reverse proxy also provides secure HTTPS connections.

OpenLab uses self-signed certificates instead of certificates from a public certificate authority. To validate the HTTPS connection, the required certificate must be installed and trusted on each client computer that accesses the web-based user interface.

The self-signed certificates are generated by the Agilent OpenLab Certificate Service Tool. After the OpenLab root certificate has been installed and trusted, certificate management is handled automatically, including certificate issuance and renewal. This ensures secure HTTPS communication between users and the application.

Execute the following steps *on each client computer* that wants to access the web-based user interface.

Agilent OpenLab Certificate Service Tool

Ensure the **Agilent OpenLab Certificate Service Tool** software is installed on the client computer.

If the **Agilent OpenLab Certificate Service Tool** software is already installed, go directly to the "Installing the Certificate" section on page 34.

If the **Agilent OpenLab Certificate Service Tool** software is not yet installed, obtain and install the software:

1. Contact your Agilent sales contact directly to obtain the **Agilent OpenLab Certificate Service Tool**.
2. Copy the MSI to a directory on the client computer that wants to access the web-based user interface (e.g., C:\tmp).
3. Launch the MSI file in administrator mode:
   a. Select **Start** and search for "command prompt".
   b. Right-click **Command Prompt** and select **Administrator mode**.
   c. Execute **msiexec /i** *<path to the MSI>*.
4. Follow the installation wizard until the installation is completed.

Installing the Certificate

1. Open a Windows PowerShell window in administrator mode.
   a. Select **Start** and search for "PowerShell".
   b. Right-click **Windows PowerShell** and select **Run as administrator**.
2. In the PowerShell window, go to the Agilent OpenLab Certificate Tool directory.
   c. Execute **cd "C:\Program Files\Agilent Technologies\OpenLab Platform\"**.
   d. Execute **cd ".\Certificate Service Tool\Bin"**.
3. In the PowerShell window, execute **.\Agilent.OpenLab.CertService.CertTool.exe RegisterRootCert -h** *<OpenLab Server URL>*.

   In the command, replace *<OpenLab Server URL>* with the external facing domain name of the OpenLab Server on which the application is installed.

   Wait for the installation to complete with **Processing finished without errors** (can take up to 10 seconds).
4. Close the Windows PowerShell to complete the HTTPS configuration process.

Accessing the Web-Based User Interface

The user interface can be accessed via:
https://<OpenLab Server URL>/openlab/asm-export/.

The web-based user interface authentication is governed by the authentication provider configured in OpenLab (OLSS). When **Windows Domain** is selected as the authentication provider, the login screen includes a domain dropdown, and users must provide their username, password, and domain. When the **built-in** (internal) authentication provider is used, the domain selection is not shown and only username and password are required.

Authentication is only granted to users having specific privileges assigned through the OpenLab Control Panel. For details, refer to the "Privileges and Roles" section on page 36.

NOTE

To protect the system, login attempts are limited. If too many login requests are made in a short time (>10 connections per minute per IP address), the system will temporarily reject additional attempts with a **429 (Too Many Requests)** response. If multiple users access the system through the same network (e.g., behind a shared company internet connection or load balancer), this limit may be reached more quickly.

NOTE

ASM Export for OpenLab CDS relies directly on the OpenLab authentication configuration. Changing the authentication provider via the OpenLab Control Panel after the application has been installed and configured is strongly discouraged. Such a change will invalidate the existing setup and can render the system non-functional.

Privileges and Roles

Privileges

During configuration of ASM Export for OpenLab CDS via the Configuration Tool, specific privileges are automatically added to the OpenLab Shared Services. These privileges are available in the OpenLab Control Panel where they can be manually assigned to roles.

The privileges listed in Table 3 determine how the application can be used.

Table 3 ASM Export for OpenLab CDS privileges

Privilege	Allows the user to…
Use ASM Export	view the **Home** page, the Help pages, and the **Open-Source Notification**. Without this privilege, access to ASM Export for OpenLab CDS is denied, even when the provided credentials (user, password, and domain where applicable) are correct.
Manage Configuration	view and make changes to the **Configuration** settings, and to start and stop the **Discovery** and **Processing** processes.
View Configuration	view the **Configuration** settings, but not to make changes to them.
View Conversion Log	view, filter/search, sort, and export the **Conversion Log**.
Manage Administration	view and make changes in the **Administration** menu.
View Administration	view the **Administration** menu but not to make changes. Note: The **Activity Log** is managed by a separate privilege (see **View Activity Log**).
View Activity Log	view, filter/search, sort, and export the **Activity Log**. Note: The existing Shared Services privilege is used; no separate **View Activity Log** privilege is added for ASM Export for OpenLab CDS.

Roles

During configuration via the Configuration Tool, specific roles are automatically added to OpenLab Shared Services and privileges are automatically assigned to these roles. These roles are available in the OpenLab Control Panel. They can be manually assigned to users that need access to ASM Export for OpenLab CDS.

The roles that are automatically created are listed in Table 4.

Table 4 ASM Export for OpenLab CDS roles

Role	Description
ASM Export Admin	This role has all privileges and is intended for administrators who need full access to all features and settings in the ASM Export for OpenLab CDS application. Users with this role can make configuration changes and start/stop processes.
ASM Export Analyst	This role has limited privileges and is intended for users who need access to specific features and data within the ASM Export for OpenLab CDS application. Users with this role cannot make configuration changes or start/stop processes.

Table 5 gives an overview of the privileges that are granted to each role. "Yes" means that the privilege is granted to the role by default. "No" means that the privilege is not granted to the role by default. Privileges can still be assigned manually in OpenLab Control Panel if a different access model is required.

Table 5 Overview of privileges assigned to each role

Privilege	ASM Export Admin	ASM Export Analyst
Use ASM Export	Yes	Yes
Manage Configuration	Yes	No
View Configuration	No	Yes
View Conversion Log	Yes	Yes
Manage Administration	Yes	No
View Administration	No	Yes
View Activity Log	Yes	No

Privileges Impact on the User Interface

Depending on the privileges that are granted to the user, certain buttons and fields are disabled or unavailable. Where applicable, appropriate warnings indicate why certain fields and buttons are disabled or unavailable due to lacking privileges.

Main Functionalities

Home Page

The Home Page of the ASM Export for OpenLab CDS web-based user interface is displayed after successful authentication. It consists of the following elements:

- **Main Navigation**

  Provides access to the primary sections of the application: **Conversion Log**, **Configuration**, and **Administration**.

- **Help Icon**

  Provides access to the About section, In-Application Help, and the Open-Source Notification.

- **User Icon**

  Displays the user's login name and full name (if available) and provides the option to log out.

- **Dashboard**

  Provides a quick overview of the system health and job statistics (e.g., the number of completed and pending jobs).

- **Pipeline Configuration**

  Provides a quick overview of the current configuration settings, as defined in the **Configuration** section.

- **System Configuration**

  Provides a read-only overview of system-level configuration settings (not user-definable).

- **Slide-In Status Menu**

  The *Status Slide-In Menu*, always available at the bottom of the **Home** page, provides real-time status information about the **Discovery** process (**Automatic Mode**) and the **Processing** process.

Conversion Log

The **Conversion Log** provides users with detailed information about the conversion jobs that have taken place within the application. It includes records of all conversion activities, including timestamps, status, and any relevant messages or errors.

Configuration

The **Configuration** menu allows users to set up and manage the **Ingestion**, **Conversion,** and **Transfer** settings for the **Automatic Mode** and the **Manual Mode**. Additionally, users can configure, start, and stop the **Discovery** process for the **Automatic Mode** and the **Manual Mode**, as well as configure, start, and stop the **Processing** process.

Administration

The **Administration** menu provides access to features and settings that are typically reserved for administrators or service users. It includes the **Activity Log**, which documents user and system activities within the application, and the **Service Mode**, which is reserved for service users (Agilent employees) to perform specific tasks.

In-Application Help

The web-based user interface includes a built-in **In-Application Help** section designed to guide you through the system. It offers a clear overview of key functionalities, step-by-step explanations of each feature, and a glossary of terms to make navigation easier.

You can access the **In-Application Help** section at any time by clicking the Help Icon in the main navigation bar and selecting **Help** from the menu.

6 ASM Content Description

High-Level ASM File Structure

High-level structure of an LC (including SFC), GC, LC/MS, and GC/MS ASM file specified by the Allotrope Foundation version 09/2026:

- $asm.manifest
- technique aggregate document
  - device system document
    - device document
      - custom information document
  - data system document
  - electronic project record
  - analysis sequence document
    - custom information aggregate document
      - custom information document
  - technique document
    - log
      - log entry
    - fraction aggregate document
      - fraction document
        - location aggregate document
          - location document
        - custom information aggregate document
          - custom information document
    - measurement aggregate document
      - measurement document
        - custom information aggregate document
          - custom information document
        - chromatography column document
        - sample introduction document
        - device control aggregate document
          - device control document
            - custom information document
        - sample document
          - custom information aggregate document
            - custom information document
        - injection document
        - <type> data cube
          - cube-structure
            - dimensions

- measures
- data
  - dimensions
  - measures
  - points
- processed data aggregate document
  - processed data document
    - data processing document
    - peak list
      - peak
        - custom information aggregate document
          - custom information document
      - custom information aggregate document
        - custom information document
- custom information aggregate document
  - custom information document

Measurement Document

The **measurement document** contains a list of entries, one entry per signal. The elements listed below **measurement document** are repeated for every signal in case multiple signals are present in a single ASM file (e.g., multiple detectors were used). The content of the **sample introduction document**, **sample document** and **injection document** are the same for each signal included as they are injection specific in OpenLab CDS; the other documents (e.g., **data cube**) are specific for each signal.

Column Information

Chromatography Column Document

The **chromatography column document** contains information about the column used for a specific measurement. Column information is obtained from two sources: the ACAML file and the acquisition method (amx file). Each source provides different metadata, and complete column information is available only when data from both sources is present. The acquisition method provides the column position; therefore, if the acquisition method is unavailable, the column position (e.g., **front position**) cannot be displayed in the ASM file. Similarly, if neither ACAML file nor the acquisition method provides a column name, the ASM file contains the message "No name provided" for the column name.

When the acquisition method is missing, the application has limited ability to associate columns with detectors. If only a single column is present, the column can still be assigned to the detector. However, when multiple columns are detected, the application cannot determine which column belongs to which detector because the positional information is unavailable.

Device System Document

The **device system document** lists all columns detected in the instrument that generated the data for the injection under consideration. This includes columns that are not directly used by the current injection but are used by other injections within the same sequence. As a result, the **device system document** may contain columns that are not associated with the specific measurement being viewed.

Data Cubes

Raw data signals that represent chromatograms or spectra are exported to the ASM files in **data cubes**.

NOTE

The raw data signals in the data cubes are extracted directly from the original .dx files included in the ECM data package. These signals do not include any additional processing that may occur when the data is opened in OpenLab CDS (e.g. smoothing). As a result, the data stored in the ASM files may differ (slightly) from what is displayed in the OpenLab CDS user interface.

Data Cube Types

The type of **data cube** with respective measures and dimensions depends on the available data type:

- chromatogram data cube: two-dimensional chromatograms for LC, GC, LC/MS, and GC/MS
- three-dimensional ultraviolet spectrum data cube: three-dimensional UV spectra for LC and LC/MS
- mass chromatogram data cube: two-dimensional mass chromatograms for LC/MS and GC/MS
- three-dimensional mass spectrum data cube: sparse three-dimensional mass spectra for LC/MS and GC/MS

Chromatogram Data Cube and Mass Chromatogram Data Cube

The chromatogram data cube and mass chromatogram data cube **cube-structure** property contain the following dimensions and measures:

- Dimensions:
  - retention time (unit: seconds (s))
- Measures:
  - see Table 6

The chromatogram data cube and mass chromatogram data cube **data** property contain the raw measurement data, with the retention time points defined in the **dimensions** property and the corresponding measurement values provided in the **measures** property.

Table 6 Mapping between Allotrope Simplified Model (ASM) data units and OpenLab CDS data units

Technique/Detector	OpenLab CDS unit	ASM concept	ASM unit
LC/UV (DAD, VWD, MVD)	mAU	absorbance	mAU
LC/FLD	LU	fluorescence	RFU
LC/RID	nano RIU	refractive index	nRIU
LC/ELSD (mV)	mV	voltage	mV
LC/ELSD (LSU)	LSU	intensity	RLU
LC/UIB	mV	voltage	mV
LC/MS	Counts	count	Counts
GC/FID	pA	electric current	pA
GC/TCD	(25) µV	voltage	mV
GC/ECD	Hz	frequency	Hz
GC/FPD (incl. DFPD)	(150) pA	electric current	pA
GC/SCD	pA	electric current	pA
GC/NCD	pA	electric current	pA
GC/NPD	pA	electric current	pA
GC/MS	Counts	count	Counts

NOTE

For data acquired with Flame Photometric Detectors (FPD), the OpenLab CDS unit is in some cases "150 pA". In such cases, the unit in the exported ASM files is "pA" and the values are multiplied by 150.

For data acquired with Thermal Conductivity Detectors (TCD), the OpenLab CDS unit is in some cases "25 µV". In such cases, the unit in the exported ASM files is "mV" and the values are divided by 40.

For data acquired with the Universal Integration Bus (UIB), the OpenLab CDS unit is in some cases "V" or "µV". In such cases, the unit in the exported ASM files is "mV" and the values are rescaled accordingly.

For data acquired with Evaporative Light Scattering Detectors (ELSD), the OpenLab CDS unit is in some cases Light Scattering Units (LSU). As LSU is not supported by the ASM schema, the most closely related supported unit Relative Light Unit (RLU) is used. The values are not rescaled.

Three-Dimensional Ultraviolet Spectrum Data Cube

The three-dimensional ultraviolet spectrum data cube **cube-structure** property contains the following dimensions and measures:

- Dimensions:
  - retention time (unit: seconds (s))
  - wavelength (unit: nanometer (nm))
- Measures:
  - absorbance (unit: milli Absorbance Unit (mAU))

The three-dimensional ultraviolet spectrum data cube **data** property contains the raw measurement data. Retention time points and wavelength points defined as separate arrays in the **dimensions** property, while the corresponding measurement values provided in the **measures** property as single flattened array. The values are ordered such that, for each retention time point, the measurements for all wavelength points are stored consecutively.

Three-Dimensional Mass Spectrum Data Cube

The three-dimensional mass spectrum data cube **cube-structure** contains the following dimensions and measures:

- Dimensions:
  - retention time (unit: seconds (s))
  - m/z (unit: mass-to-charge ratio (m/z))
- Measures:
  - count (unit: Counts)

The three-dimensional mass spectrum data cube **data** property contains the raw measurement data. The retention time points and m/z values used in the measurement are defined in two lists within the **dimensions** property. The corresponding data is stored in the **points** property as a single linear list containing retention time, m/z, and count-value triplets.

Excluding Raw Data from ASM File and Empty Data Cubes

Through the web-based user interface (for details, refer to the "Configuration" section on page 39), a user can configure the application to have certain raw data excluded from the exported ASM files (e.g., for performance or data volume reasons). The following options are available:

- **Exclude raw 2D data**

  All **chromatogram data cubes** and mass chromatogram data cubes in the ASM file are empty.
- **Exclude raw 3D UV data**

  All **three-dimensional ultraviolet spectrum data cubes** in the ASM file are empty.
- **Exclude raw 3D MS data**

  All **three-dimensional mass spectrum data cubes** in the ASM file are empty.

Empty data cubes have a **cube-structure** defined but have no **data** property defined.

Processed Data (Aggregate) Document

For acquisition-only data (no post-acquisition processing performed), the ASM files do not contain a **processed data (aggregate) document**. For processed data, the ASM files include a processed data (aggregate) document.

The **processed data document** captures information related to post-acquisition data processing. This includes the **peak list**, which contains details about peaks detected during processing. If no peaks are detected, the **processed data document** is still present, but no **peak list** is included. The units used in the **peak list** correspond to the units of the associated data cube. For example, for UV-based LC detectors, **peak height** is expressed in **mAU** and **peak area** in **mAU.s**.

The **processed data document** also contains the **data processing document** section, which describes the processing method used and records when the data was processed.

The content of the ASM files reflects the current state of the data stored in ECM. Each time data is re-processed (and results are saved) in OpenLab CDS, the result files stored in ECM are updated to a newer version. Only the current version of the processing results at the time of saving is stored in the current version of the result files in ECM. Consequently, the ASM files only contain one entry in the **processed data document**. The version timestamp of the converted result file is included in the exported ASM file name (for details, refer to the "ASM File Name" section on page 31).

Data Cube Rescaling, Peak Property Rescaling and Unit Conversion

According to the ASM schema definitions, data cube and peak properties must be stored in specific units and therefore units (and corresponding values) must sometimes be rescaled and converted from the original OpenLab CDS values and units respectively. The conversion factors (and corresponding units) that can be used to back-calculate the original values present in OpenLab CDS are stored as custom information.

Data Cube Rescaling and Unit Conversion

Data cube rescaling and unit conversion information are included in the **custom information aggregate** and **custom information document** inside the **measurement document** entry. The **custom information document** contains the following properties:

- Scale_Factor_To_original_DataCube_Measure_Unit
- Original_DataCube_Measure_Unit

Peak Property Rescaling and Unit Conversion

Peak property rescaling and unit conversion information are included in the **custom information aggregate** and **custom information document** inside the **peak list**. The **custom information document** contains the following properties:

- Scale_Factor_To_Original_Peak_Height_Unit
- Scale_Factor_To_Original_Peak_Area_Unit
- Original_Peak_Height_Unit
- Original_Peak_Area_Unit

Sample Custom Parameters and Custom Calculations

Sample Custom Parameters

The OpenLab Control Panel allows you to configure **Sample Custom Parameters** that then can be defined when setting up a data acquisition experiment in OpenLab Acquisition. These Sample Custom Parameters are, if defined, exported to the **custom information document** inside the **sample document**.

Custom Calculations

OpenLab Data Analysis allows you to configure **Custom Calculations**, which are user-defined formulas applied to (processed) data to derive additional analytical results beyond the standard output. These calculations can operate at different scopes (e.g., injection-level or peak-level) and are typically used to compute domain-specific metrics, perform normalization, or combine multiple signals into a single reported value. Once defined and executed within CDS, the resulting values are included in the generated ASM files.

The results of **Custom Calculations** are written in **custom information document** sections. The exact section in which a given calculation result is stored inside a **custom information document** depends on the scope of the **Custom Calculation**. Each scope maps to a corresponding section in the ASM file as described in Table 7.

Table 7 Mapping between OpenLab CDS Custom Calculation scope and mapping section in ASM file

OpenLab CDS Custom Calculation Scope	Mapping section in ASM file
Sequence	analysis sequence document
Injection	technique document
Signal	measurement document
Peak or group	peak list / <individual peak>

Considerations for Missing, Partial, or Irrelevant data

In certain cases, there might be missing, partial, or irrelevant data in OpenLab CDS. The solution adheres to the following rules to generate ASM files:

- Only relevant signals are exported to the ASM file (one measurement document per signal per injection). Diagnostic or instrument parameter signals such as **Temperature** or **Pressure** signals are ignored and thus not exported.
- In case the injection and/or a signal are not completed successfully, a regular ASM file is generated containing all available data at the time of export. If no raw data/chromatogram data is available, no data cube is included in the export. If (partial) data is available, all available data is included in the data cube that is included in the export.
- The instrument technique (e.g., LC) is determined based on all available information such as hardware information, the units corresponding to (raw) data, etc. Only in case the instrument technique cannot be determined unequivocally and the required ASM schema cannot be selected, is the export terminated with an error.

Detailed ASM File Structure

For details regarding the ASM file structure, refer to the mapping table in the "Mapping Allotrope Foundation Terms to OpenLab CDS Properties" section on page 55.

7 Responsibilities and Regulatory Considerations

Software Classification and Customer Responsibilities

This software is classified as GAMP 5 Category 4 (Configured Software). Customers are responsible for performing validation activities appropriate to their intended use. The software is developed and maintained by Agilent under an ISO 9001–compliant Quality Management System (QMS).

User organizations are solely responsible for determining whether the software is suitable for their specific operational environment and for ensuring compliance with all applicable legal, regulatory, and quality system requirements. Agilent assumes no responsibility or liability for the use of this software in regulated or clinical environments, or in any application that is required to adhere to regulatory compliance.

Data Export and Data Security Responsibilities

The application accesses ECM to retrieve data, converts the data into ASM files, and deposits the ASM files into a customer-controlled transfer location (Amazon S3 bucket, local file system). ECM and the customer-controlled transfer location each have independent user management and permission systems and are not connected in any way.

Customers are responsible for the proper setup and configuration of both systems to ensure that data is handled securely and to prevent unintended information disclosure via the customer-controlled transfer location.

Backup and Data Retention Responsibilities

This application does not provide built-in backup or restore functionality.

Application, Configuration, and Logging Data

The application relies on OpenLab Shared Services for centralized services, including but not limited to:

- User authentication and authorization
- Security and privilege management
- Application-related configuration data
- Activity and logging information generated by the application

All configuration data and logging information generated by the application are stored in the OpenLab Shared Services database. Backup and restoration of this data are outside the scope of this application and are managed by the OpenLab platform.

Users and system administrators are responsible for ensuring that appropriate backup, restore, and disaster-recovery mechanisms are configured for OpenLab Shared Services in accordance with their organization's IT policies, data retention requirements, and applicable regulations. For details on available backup capabilities and recommended practices, refer to the official OpenLab documentation.

Agilent does not provide backup or recovery services for OpenLab Shared Services as part of this application.

Exported Data

Data produced, processed, or exported by this application are stored in internal systems (e.g., local file system) or external systems (e.g., Amazon S3) that are not managed by the application and are not part of the OpenLab Shared Services database.

Users are fully responsible for:

- Ensuring that exported data is stored in systems with appropriate backup, retention, and disaster-recovery mechanisms.
- Implementing regular and verifiable backup procedures for all externally stored data generated by the application.
- Protecting exported data against loss, corruption, or unauthorized access.
- Ensuring data availability and integrity throughout the required retention period.

Agilent assumes no responsibility for data loss, data corruption, or data unavailability resulting from missing, misconfigured, or insufficient backup procedures in internal or external systems.

Key Management and Token Persistence

The application persists its JWT signing key (jwt-signing-key.bin) in the key-ring directory (for details, refer to the "Security, Configuration, and Service Account" section on page 23). The key ring protects multiple sensitive elements, including database-stored credentials, the JWT signing key, and connection strings stored in config.json. Backup and restore procedures must treat these components as a single, consistent unit to ensure successful recovery and continued operation.

8 Appendix

Known Limitations

- Export of auxiliary channels and signals, such as temperature, pressure, and solvent curves, to ASM files is not supported.
- Currently, the **chromatography column document** within the ASM files is only populated for GC and GC/MS data. For LC and LC/MS data, the document is included to satisfy schema requirements but remains empty.
- Electron Capture Detector (ECD) measurements use a frequency-based signal (Hz) with processed peak values expressed in Hz and Hz.s. The currently released Allotrope GC schema does not define a frequency detector measurement alternative. As a result, ECD exports may fail schema validation despite containing valid detector data.
- ASM files generated from data acquired using 'clustered devices' (e.g., Pump Valve Cluster) do not fully preserve cluster membership information. The individual devices are listed in the device system document along with a placeholder cluster device indicating that a cluster device was present. For details, refer to the mapping table in the "Mapping Allotrope Foundation Terms to OpenLab CDS Properties" section on page 55.

Mapping Allotrope Foundation Terms to OpenLab CDS Properties

Table 8 Mapping of Allotrope Foundation terms to OpenLab CDS properties

Allotrope Simplified Model (ASM)		OpenLab CDS		
Property Name	**Unit**	**Component (1)**	**Property Name (2)**	**Unit**
technique document (3)				
submitter	-	Data Analysis	Sample Information > Injection > Acq. Operator	-
analyst	-	Data Analysis	Sample Information > Injection > Acq. Operator	-
device method identifier(GC, GC/MS)	-	-	Internally defined (Injections > MeasData > AcqParam > Method_ID in ACAML file)	-
<Parameter> (CI, 4)	Data dependent	Data Analysis	Injection Results > Summary > Injection > <Parameter>	Data dependent
measurement document				
measurement identifier	-	Data Analysis	Signals > Signal name	-
measurement time (5)	Date/Time	Data Analysis	Sample Information > Injection > Injection time	Date/Time
<Parameter> (CI, 4)	Data dependent	Data Analysis	Injection Results > Summary > Signals > <Parameter>	Data dependent
log entry (6)				
identifier	-	Data Analysis	Internally defined (generated by Allotrope Converter)	-
observation	-	Data Analysis	Audit/E-Sign > Injection Audit Trail > Description	-
scalar timestamp datum (5)	Date/Time	Data Analysis	Audit/E-Sign > Injection Audit Trail > Date	Date/Time
author	-	Data Analysis	Audit/E-Sign > Injection Audit Trail > User name	-
category (CI)	-	Data Analysis	Audit/E-Sign > Injection Audit Trail > Category	-
entity version (CI)	-	Data Analysis	Audit/E-Sign > Injection Audit Trail > Version	
entry type (CI, 7)	-	Data Analysis	Audit/E-Sign > Audit Trail > State	-

Table 8 Mapping of Allotrope Foundation terms to OpenLab CDS properties

Allotrope Simplified Model (ASM)		OpenLab CDS		
Property Name	**Unit**	**Component (1)**	**Property Name (2)**	**Unit**
audit trail source identifier (CI)	-	Data Analysis	Audit/E-Sign > Injection Audit Trail > Host name	-
reason (CI)	-	Data Analysis	Audit/E-Sign > Injection Audit Trail > Reason	-
reviewed (CI)	-	Data Analysis	Audit/E-Sign > Injection Audit Trail > Reviewed	-
fraction document				
identifier	-	N/A	Internally defined (Injections > MeasData > TechSpec > <technique> > Fraction id in ACAML file)	-
written name	-	Data Analysis	Chromatograms > <Name of the fraction>	-
start time (5, 6, 11)	Date/Time	Data Analysis	Based on Fraction Results > Start Time	min
end time (5, 6, 11)	Date/Time	Data Analysis	Based on Fraction Results > End Time	min
Volume (11)	µL	Data Analysis	Fraction Results > Volume	ml
start trigger reason (9, 11)	-	-	Internally defined (Injections > MeasData > TechSpec > <technique> > Fraction > StartTriggerReason in ACAML file)	-
end trigger reason (9, 11)	-	-	Internally defined (Injections > MeasData > TechSpec > <technique> > Fraction > EndTriggerReason in ACAML file)	-
start volume	µL	-	Internally defined (Injections > MeasData > TechSpec > <technique> > fraction > StartVolume in ACAML file)	µL
elapsed start time (CI, 6, 10, 11)	s	-	Fraction Results > Start Time	min
elapsed end time (CI, 6, 10, 11)	s	-	Fraction Results > End Time	min
start timestamp (CI, 5, 11)	Date/Time	Data Analysis	Based on Fraction Results > Start Time	min
end timestamp (CI, 5, 11)	Date/Time	Data Analysis	Based on Fraction Results > End Time	min
volume (CI, 11)	µL	Data Analysis	Fraction Results > Volume	ml
start reason ontology (CI, 10, 11)	-	-	Internally defined (generated by Allotrope Converter)	-

Table 8 Mapping of Allotrope Foundation terms to OpenLab CDS properties

Allotrope Simplified Model (ASM)		OpenLab CDS		
Property Name	**Unit**	**Component (1)**	**Property Name (2)**	**Unit**
end reason ontology (CI, 10, 11)			Internally defined (generated by Allotrope Converter)	
location document				
Location (11)	-	Data Analysis	Fraction Results > Location	-
chromatography column document (12)				
chromatography column length	m	Data Analysis	Acquisition Setpoints > Column parameters > Length	m
chromatography column part number	-	Data Analysis	Acquisition Setpoints > Column parameters > Product number	-
column inner diameter	mm	Data Analysis	Acquisition Setpoints > Column parameters > Diameter	µm
product manufacturer	-	Data Analysis	Acquisition Setpoints > Column parameters > Manufacturer	-
chromatography column serial number	-	Data Analysis	Acquisition Setpoints > Column parameters > Serial Number	
written name	-	Data Analysis	A combination of the name of the column, the manufacturer of the column, the product number of the column and position info related to the detector. For example: "HP-5 - Agilent 19091J-113 (Inlet connection: Front inlet, Outlet connection: Front detector)"	-
sample introduction document (LC/MS, GC/MS, 13)				
sample introduction mode setting	-	-	Internally defined (**liquid injection** for LC/MS **gas injection** for GC/MS)	-
sample introduction medium	-	-	Internally defined (always **“”** [blank])	-
sample introduction description	-	-	Internally defined (**liquid chromatography** for LC/MS **gas chromatography** for GC/MS)	-
device control document (14, 15)				
device identifier	-	Acquisition	Module list > Name	-
device type	-	-	Internally defined (Based on Module > Type in ACAML file)	-

Table 8 Mapping of Allotrope Foundation terms to OpenLab CDS properties

Allotrope Simplified Model (ASM)		OpenLab CDS		
Property Name	**Unit**	**Component (1)**	**Property Name (2)**	**Unit**
model number	-	Acquisition	Module list > Part Number	-
product manufacturer	-	Acquisition	Module list > Vendor	-
equipment serial number	-	Acquisition	Module list > Serial Number	-
firmware version	-	Acquisition	Module list > Firmware Revision	-
device acquisition method written name (CI)	-	Data Analysis	Sample Information > Sample > Acq. method	-
device acquisition method version (CI)	-	Data Analysis	Acquisition Setpoints > Acquisition parameters > Method Information > Version	-
position (CI, GC, GC/MS, 16)	-	Data Analysis	Sample Information > Sample > Injector position	-
device instance (CI, 17)	-	-	Internally defined (Injections > MeasData > Signal > DetectorInstance in ACAML file)	-
sample document				
sample identifier	-	-	Internally defined (Resources > Samples > Setup id in ACAML file)	-
written name	-	Data Analysis	Sample Information > Sample > Name (if available) OR Sample Information > Injection > Data file (if Sample > Name not available)	-
description	-	Data Analysis	Sample Information > Sample > Description	-
sample role type (18)	-	Data Analysis	Sample Information > Sample > Type	-
location identifier	-	Data Analysis	Sample Information > Sample > Vial	-
batch identifier	-	Data Analysis	Sample Information > Sample > Order No AND Sample Information > Sample > Replicate (e.g., 1; 13)	-
<Parameter> (CI, 5, 19)	Data dependent	Acquisition	Sample Custom Parameters > <Parameter>	Data dependent
injection document				
autosampler injection volume setting (chromatography) (LC, LC/MS)	mm^3	Data Analysis	Sample Information > Injection > Act. Inj. volume	µL

Table 8 Mapping of Allotrope Foundation terms to OpenLab CDS properties

Allotrope Simplified Model (ASM)		OpenLab CDS		
Property Name	**Unit**	**Component (1)**	**Property Name (2)**	**Unit**
injection volume setting (GC, GC/MS)	µL	Data Analysis	Sample Information > Injection > Act. Inj. volume	µL
injection identifier	-	Data Analysis	Sample Information > Injection > Data file	-
injection time (5)	Date/Time	Data Analysis	Sample Information > Injection > Injection time	Date/time
<type> data cube				
label	-	Data Analysis	Signals > Signal description	-
processed data document				
processed data identifier	-	-	Internally defined (Injections > Result > SignalResult id in .rx ACAML file)	-
data processing document				
method identifier	-	Data Analysis	Sample Information > Injection > Proc. Method (with .pmx)	-
method name	-	Data Analysis	Processing Method > <shown method name> (without .pmx)	-
method version	-	Data Analysis	Processing Method > General > Properties > Version	-
data processing time (5)	Date/Time	-	Internally defined (Injections > Result > SignalResult > Info > LastModifiedDate in .rx ACAML file)	Date/Time
peak list				
written name	-	Data Analysis	Injection Results > Peaks > Name	-
identifier	-	-	Internally defined (Injections > Result > SignalResult > Peak id in .rx ACAML file)	-
peak height	Data dependent (e.g., mAU)	Data Analysis	Injection Results > Peaks > Height	Data dependent (e.g., mAU)
relative peak height	%	Data Analysis	Injection Results > Peaks > Height%	%
peak area	Data dependent (e.g., mAU.s)	Data Analysis	Injection Results > Peaks > Area	Data dependent (e.g., mAU.s)
relative peak area	%	Data Analysis	Injection Results > Peaks > Area%	%

Table 8 Mapping of Allotrope Foundation terms to OpenLab CDS properties

Allotrope Simplified Model (ASM)		OpenLab CDS		
Property Name	**Unit**	**Component (1)**	**Property Name (2)**	**Unit**
retention time	s	Data Analysis	Injection Results > Peaks > RT%	min
peak start	s	Data Analysis	Injection Results > Peaks > Start time	min
peak end	s	Data Analysis	Injection Results > Peaks > End time	min
peak value at start	Data dependent (e.g., mAU)	-	Calculated (Signal height at "peak start" time; without baseline correction)	Data dependent (e.g., mAU)
peak value at end	Data dependent (e.g., mAU)	-	Calculated (Signal height at "peak end" time; without baseline correction)	Data dependent (e.g., mAU)
peak selectivity (chromatography)	(unitless)	Data Analysis	Injection Results > Peaks > Selectivity	(unitless)
capacity factor (chromatography)	(unitless)	Data Analysis	Injection Results > Peaks > Capacity Factor	(unitless)
chromatographic peak resolution using peak width at half-height	(unitless)	Data Analysis	Injection Results > Peaks > Resol. JP = Injection Results > Peaks > Resol. EP	(unitless)
chromatographic peak resolution using baseline peak widths	(unitless)	Data Analysis	Injection Results > Peaks > Resol. USP	(unitless)
Chromatographic peak resolution using statistical moments	(unitless)	Data Analysis	Injection Results > Peaks > Resol. statistical	(unitless)
asymmetry factor measured at 5 % height	(unitless)	Data Analysis	Injection Results > Peaks > Tailing	(unitless)
asymmetry factor measured at 10 % height	(unitless)	Data Analysis	Injection Results > Peaks > Asymmetry 10%	(unitless)
peak symmetry factor measured at 5 % peak height	(unitless)	Data Analysis	Injection Results > Peaks > Symmetry	(unitless)
number of theoretical plates by tangent method	(unitless)	Data Analysis	Injection Results > Peaks > Plates USP	(unitless)
number of theoretical plates by peak width at half height	(unitless)	Data Analysis	Injection Results > Peaks > Plates JP = Injection Results > Peaks > Plates EP	(unitless)
number of theoretical plates measured at 4.4 % of peak height	(unitless)	Data Analysis	Injection Results > Peaks > Plates 5 sigma	(unitless)

Table 8 Mapping of Allotrope Foundation terms to OpenLab CDS properties

Allotrope Simplified Model (ASM)		OpenLab CDS		
Property Name	**Unit**	**Component (1)**	**Property Name (2)**	**Unit**
peak width at baseline	s	Data Analysis	Injection Results > Peaks > Width tangent	min
peak width at 4.4 % of height	s	Data Analysis	Injection Results > Peaks >Width 5 sigma	min
peak width at 5 % of height	s	Data Analysis	Injection Results > Peaks > Width 5%	min
peak width at 10 % of height	s	Data Analysis	Injection Results > Peaks > Width 10%	min
peak width at half height	s	Data Analysis	Injection Results > Peaks > Width 50%	min
<Parameter> (CI, 4)	Data dependent	Data Analysis	Injection Results > Peaks > <Parameter>	Data dependent
device system document				
device identifier	-	Data Analysis	Sample Information > Injection > Instrument name	-
device document (15, 20, 21, 22)				
device identifier	-	Acquisition	Module List > Name	-
device type	-	-	Internally defined (Based on Module > Type in ACAML file)	-
model number	-	Acquisition	Module List > Part Number	-
product manufacturer	-	Acquisition	Module List > Vendor	-
equipment serial number	-	Acquisition	Module List > Serial Number	-
firmware version	-	Acquisition	Module List > Firmware Revision	-
written name	-	Acquisition	Module List > Name	-
position (CI, GC, GC/MS, 16)	-	Data Analysis	Sample Information > Sample > Injector position	
device instance (CI, 17)	-	-	Internally defined (Injections > MeasData > Signal > DetectorInstance in ACAML file)	-
data system document				
ASM converter name	-	-	<Name of Allotrope Converter>	-
ASM converter version	-	-	<Version of Allotrope Converter>	-
ASM conversion time (5)	Date/Time	-	<Timestamp of conversion to ASM file>	-
ASM file identifier	-	-	<File name of generated ASM file>	-

Table 8 Mapping of Allotrope Foundation terms to OpenLab CDS properties

Allotrope Simplified Model (ASM)		OpenLab CDS		
Property Name	**Unit**	**Component (1)**	**Property Name (2)**	**Unit**
data system instance identifier	-	-	<Host name of OpenLab CDS AIC/Workstation which acquired source data> (i.e., Doc > DocInfo > ClientName in ACAML file)	-
database primary key	-	Data Analysis	Sample Information > Injection > Data file	-
electronic project record				
written name	-	Control Pane	Projects > <Project Name>	-
analysis sequence document (23)				
written name	-	Data Analysis	Sample Information > Sequence > Name	-
identifier	-	-	Internally defined (Content > SampleContexts > Setup id in ACAML file)	-
<Parameter> (CI, 4)	Data dependent	Data Analysis	Injection Results > Summary > Sequence > <Parameter>	Data dependent

(1) Defines the OpenLab CDS component where the **Property Name** is defined (e.g., Data Analysis). Certain properties are not available through the interface of an OpenLab CDS component and are marked as such.

(2) **Property Names** refer to **Property Names** in version 2.8 of the referenced OpenLab Component. **Property Names** might differ or might not be available in other versions.

(3) For sequence runs, one ASM file is generated per injection. The injection's position within the sequence is recorded in the technique document using an **@index** field (e.g., **"@index": 5** for the fifth injection).

(4) All Custom Calculations are exported to the **custom information document** inside the respective section using the exact custom calculation parameter name as defined in OpenLab.
- **Integer-**type Custom Calculations are exported as scalar double datums.
- **Double**-type Custom Calculations are exported as scalar double datums.
- **Boolean** Custom Calculations are exported as scalar Boolean datums.
- **String**-type Custom Calculations are exported as scalar string datums.

(5) Timestamps are expressed in ISO 8601 date time format. The time zone offset corresponds to the time zone of the machine and/or user that generated or last modified the data associated with the timestamp. For example, the **ASM conversion time** property includes the time zone offset of the machine on which the JSON file was generated: That machine is the system where ASM Export for OpenLab CDS (including Allotrope Converter for OpenLab CDS) is installed. When data is reprocessed in a different time zone, the **injection time** may be displayed with a different time zone offset based on the **data processing time** property. The underlying UTC timestamp is unchanged and remains correct.

(6) **Start time** and **end time** in the **fraction document** are stored as absolute timestamps. In contrast, fraction **Start Time** and **End Time** in OpenLab CDS are stored as offsets relative to the start of the injection. These original offset values are available in the **custom information document** inside the **fraction document**.

(7) Only entries from the **Injection Audit Trail** in OpenLab CDS are included as **log entries** inside the **log** section. Entries from the **Result Set Audit Trail**, **Sequence Audit Trail** or **Method Audit Trail** are not included.

(8) The **entity type** property is set to **System** for standard audit trail entries generated by OpenLab CDS and to **Manual** for audit trail entries manually entered by a user.

(9) The **start trigger reason** and **end trigger reason** are mapped according to Table 9 on page 65. The **end trigger reason** property is only present in the ASM file if defined.

(10) The properties inside the custom information document contain dummy ontology references and dummy URLs; the dummy URLs and are non-functional. The following properties are defined in case fractions are contained in a single location:
- AR_ALLO_FractionElapsedStartTime: The original offset start time as defined in OpenLab CDS (Fraction Results > Start Time)
- AR_ALLO_FractionElapsedEndTime: The original offset end time as defined in OpenLab CDS (Fraction Results > End Time)
- AR_ALLO_FractionVesselTriggerStartReason: Dummy ontology reference to the start trigger reason
- AR_ALLO_FractionVesselTriggerEndReason: Dummy ontology reference to the end trigger reason (if defined)

(11) In case a single fraction is split into subfractions across multiple locations, the fraction document contains detailed information per subfraction. The following properties are relevant:
- location document: List of all the locations across which the fraction is split
- start time: The start time of the first subfraction (timestamp)
- end time: The end time of the last subfraction (timestamp)
- volume: Total volume of the fraction (sum of the subfraction volumes)
- start trigger reason: The start trigger reason of the first subfraction
- end trigger reason: The end trigger reason of the last subfraction (if defined)
- **AR_ALLO_FractionVesselElapsedStartTime (custom information document):** The original offset start time as defined in OpenLab CDS (Fraction Results > Start Time) of the specified subfraction
- **AR_ALLO_FractionVesselElapsedEndTime (custom information document):** The original offset end time as defined in OpenLab CDS (Fraction Results > Start Time) of the specified subfraction
- **AR_ALLO_FractionVesselElapsedStartTimestamp (custom information document):** The start time of the specified subfraction (timestamp)
- **AR_ALLO_FractionVesselElapsedEndTimestamp (custom information document):** The end time of the specified subfraction (timestamp)
- **AR_ALLO_FractionVesselVolume (custom information document):** The volume of specified subfraction
- **AR_ALLO_FractionVesselTriggerStartReason (custom information document):** Dummy ontology reference to the start trigger reason of the specified subfraction
- AR_ALLO_FractionVesselTriggerEndReason (custom information document): Dummy ontology reference to the end trigger reason of the specified subfraction (if defined)
- AR_ALLO_FractionElapsedStartTime (custom information document): The original offset start time as defined in OpenLab CDS (Fraction Results > Start Time) of the first subfraction
- AR_ALLO_FractionElapsedEndTime (custom information document): The original offset end time as defined in OpenLab CDS (Fraction Results > End Time) of the last subfraction

(12) Currently, the **chromatography column document** is only populated for GC and GC/MS data. For LC and LC/MS data, the document is included to satisfy schema requirements but remains empty.

(13) The **sample introduction document** is only available in **measurement documents** representing mass spectrometry spectrum data, i.e., measurement documents that contain a **three-dimensional ass spectrum data cube.**

(14) Informs on the single detector device used to acquire the signal.

(15) Some properties might be missing for non-Agilent devices.

(16) The **position** property is not applicable to LC and LC/MS data and is therefore not included. For GC and GC/MS data, the **position** property is included only when more than one detector is configured. In such cases, the value is reported as either **front position**, **back position**, or **third position**.

(17) If more than one detector of the same type is present in a single injection, the **DetectorInstance** field value from the ACAML file is added to the custom information document (**device instance** property) for the second and subsequent detectors.

(18) The **sample role type** property is mapped according to Table 10 on page 65.

(19) All parameters defined in the **Sample Custom Parameters** section in OpenLab Acquisition are exported to the **custom information document** inside the **sample document** using the exact parameter name as defined in OpenLab.
Text-type parameters are exported as scalar string datums.
Numeric-type parameters are exported as scalar double datums.
Date-type parameters are exported as scalar timestamp datums in ISO 8601 format. **Date**-type parameters are converted from the original 12-hour (AM/PM) format to a 24-hour format.

(20) Informs on all devices/modules identified in the instrument used.

(21) If clustered devices were used in the chromatography experiment, the clustered devices are listed as regular non-clustered devices. The clustering device itself is reported as a virtual device as described in details in Table 11 on page 66.

(22) For GC and GC/MS data, if column information is available (that is, the chromatography column document is populated), each column present in the device is included as an additional **device document** entry within the **device system document.** The **device document** contains the following properties:
- device identifier: Column ID
- device type: Always "**chromatography column**"
- model number: Product number of the column
- product manufacturer: Manufacturer of the column
- equipment serial number: Serial number of the column
- written name: A combination of the name of the column, the manufacturer of the column, the product number of the column and position info related to the detector. For example: "HP-5 - Agilent 19091J-113 (Inlet connection: Front inlet, Outlet connection: Front detector)"

(23) Not available for single samples (i.e., .sirslt datasets) except if sequence-level Custom Calculations are defined and available.

(CI) The property is stored as custom information in belonging section.

(LC) The property is only available for LC.

(GC) The property is only available for GC.

(LC/MS) The property is only available for LC/MS.

(GC/MS) The property is only available for GC/MS.

Table 9 Meaning of the "start trigger reason" and "end trigger reason" properties in the ASM file

start/end trigger reason	Meaning
Unknown	Trigger reason unknown.
Peak detector	Triggered by peak collector. Fraction collection started when a detector signal crossed a defined threshold. Collection begins (ends) when Agilent's peak detection algorithm determines that this is the start/end of a peak.
Time-based (Time slices)	Time-based triggered by time slices. Fraction collection was triggered purely by retention time.
Time-based (Number of fractions)	Time-based triggered by number of fractions.
Volume-based	Triggered by collected volume. Fractions are triggered after a defined volume has passed, independent of time or signal.
Digital trigger	Fraction collection was triggered by an external digital signal. E.g., digital trigger by a mass spec detector (i.e., mass-based fraction collection).
Recovery	The fraction collector is returning to a known safe state after an interruption.
External	External trigger, e.g., manual trigger (i.e., user manually clicked **Collect** during the run).
Overfill	The fraction collector detector detected that the current vial or well is full (or about to be).

Table 10 Sample role type property mapping

OpenLab CDS / Sample type	ASM / Sample role type
<Unspecified>	unknown sample role
Sample	sample role
Blank	blank role
Double Blank	blank role
Cal. Std.	calibration sample role
QC check	quality control sample role
Spike	spiked sample role
Sys. Suit.	validation sample role

Table 11 Cluster device mapping overview

OpenLab CDS / Cluster device	ASM / device identifier	ASM / device type	ASM / model number	ASM / product manufacturer	ASM / written name
PumpValveCluster	Pump Valve Cluster	device	PumpValveCluster	Agilent	Pump Valve Cluster
Vtc	VTC	device	VTC	Agilent	VTC
TccCluster (new term) ColumnCompartmentCluster (old term)	Tcc Cluster Tcc Cluster old	device	TccCluster ColumnCompartmentCluster	Agilent	Tcc Cluster Tcc Cluster Old
HdrDad (new term) HDR-DAD CLUSTER (old term)	Hdr Dad Hdr Dad Old	device	HdrDad HDR-DAD Cluster	Agilent	Hdr Dad Hdr Dad Old
FractionCollectorCluster	Fraction Collector Cluster	device	FractionCollectionCluster	Agilent	Fraction Collection Cluster
PrepPumpCluster	Prep Pump Cluster	device	PrepPumpCluster	Agilent	Prep Pump Cluster

Supported Systems and Modules

LC, SFC and LC/MS

Agilent LC Systems

- Agilent 1100 and 1200 LC systems
- Agilent 1120 and 1220 Compact LC systems
- Agilent 1260 and 1290 Infinity LC system series
- Agilent 1260 and 1290 Infinity II LC system series
- Agilent 1260 and 1290 Infinity III LC system series

Agilent SFC Systems

- Agilent 1260 Infinity III SFC system

Agilent LC and SFC Detectors

- *Diode Array Detectors (DAD):* G1315 series, G4212 series, G4285 series, G4294 series, G7115 series, G7117 series
- *Variable Wavelength Detectors (VWD):* G1314 series, G4284 series, G4286 series, G4287 series, G4288 series, G4289 series, G4290 series, G4291 series, G4292 series, G4293 series, G7114 series
- *Multiple Wavelength Detectors (MWD):* G1365 series, G4221 series, G7165 series
- *Fluorescence Detectors (FLD):* G1321 series, G7121 series, G7123 series
- *Refractive Index Detectors (RID):* G1362 series, G7162 series
- *Evaporative Light Scattering Detectors (ELSD):* G4218 series, G4260 series, G4261 series, G7102 series
- *Single Quadrupole LC/MS Detectors:* G1946 series, G6110 series, G6120 series, G6125 series, G6130 series, G6135 series, G6140 series, G6160 series
- *Analog-to-Digital Converters:* G1390 series (Universal Interface Box, UIB)

Supported Agilent LC and SFC Modules

- *Quaternary Pumps:* G1311 series, G4204 series, G5611 series, G5654 series, G7104 series, G7111 series, G7131 series
- *Binary Pumps:* G1312 series, G4220 series, G4281 series, G4288 series, G4289 series, G4290 series, G4293 series, G4294 series, G4302 series, G4782 series, G7112 series, G7120 series, G7132 series, G7161 series
- *Isocratic Pumps:* G1310 series, G4280 series, G4286 series, G4287 series, G4291 series, G4292 series, G7110 series
- *Capillary Pumps:* G1376 series
- *Nano Pumps:* G2226 series
- *Preparative Pumps:* G1361 series
- *2DLC Pumps*
- *HDRDAD*
- *Fraction Collectors:* G1364 series, G5664 series, G7158 series, G7159 series, G7164 series, G7166 series
- *MS Flow Splitters:* G7170 series
- *Column Ovens:* G1316 series, G4283 series, G4287 series, G4289 series, G4290 series, G4291 series, G4294 series, G7116 series, G7130 series, G7169 series
- *Autosamplers:* G1313 series, G1327 series, G1329 series, G1367 series, G1368 series, G1377 series, G1378 series, G1389 series, G2258 series, G2260 series, G3167 series, G4226 series, G4282 series, G4287 series, G4290 series, G4292 series, G4293 series, G4294 series, G4303 series, G4767 series, G5667 series, G5668 series, G7129 series, G7137 series, G7157 series, G7167 series
- *Temperature Controllers:* G1330 series
- *Valves:* G1156 series, G1157 series, G1158 series, G1159 series, G1160 series, G1162 series, G1163 series, G1170 series
- *SFC Controllers:* G4301 series
- *InfinityLab Assists:* G7180 series (HTS)
- *Flexible Cube:* G4227 series

GC and GC/MS

Agilent GC Systems

- Agilent 6820 GC system
- Agilent 6850 GC system
- Agilent 6890 GC system
- Agilent 7820 GC system
- Agilent 7860 GC system
- Agilent 7890 GC system
- Agilent 8850 GC system
- Agilent 8860 GC system
- Agilent 8890 GC system
- Agilent Intuvo 9000 GC system

Agilent GC Detectors

- *Flame Ionization Detectors (FID):* supported
- *Thermal Conductivity Detectors (TCD):* supported
- *Electron Capture Detectors (ECD):* supported
- *Flame Photometric Detectors (FPD), including Dual FPD (DFPD):* supported
- *Sulfur Chemiluminescence Detectors (SCD):* supported
- *Nitrogen Chemiluminescence Detectors (NCD):* supported
- *Nitrogen-Phosphorus Detectors (NPD):* supported
- *Single Quadrupole GC/MS Detectors:* 5973 GC/MSD system, 5975 GC/MSD system, 5977 GC/MSD system

Other Agilent GC Modules

- *Autosamplers:* 3430 series, 7650 series, 7673 series, 7683 series, 7693 series, ALS Controller
- *Headspace Samplers:* G1888 series, 7697 series, 8697 series
- *Injectors:* 1513 series, 2613 series, 2913 series, 4513 series, 4567 series
- *Trays:* 2614 series, 4514 series

Other Non-Agilent GC Modules

- *Autosamplers:* PAL Auto Sampler System (PAL3)

Allotrope Converter Error Code Classification

Table 12 describes how ASM Export for OpenLab CDS classifies Allotrope Converter for OpenLab CDS exit codes. Depending on the exit code, a conversion job is either marked as failed immediately (**Fail once**) or automatically rescheduled for retry with an exponential backoff (**Retry**) when the failure is considered transient (e.g., an environmental or I/O-related condition). The classification is based on the exit code registries defined by the Allotrope Converter for OpenLab CDS.

Table 12: Allotrope Converter for OpenLab CDS Error Codes

Code	Description	Action
0	No error conversion succeeded	Success
1	Fatal error: crash, truncated/unreadable archive (EOCD missing), file lock	Retry
20	Unknown error	Retry
30	No source data found	Fail once
31	Nothing to export	Fail once
32	Invalid data	Fail once
35	Not supported (general)	Fail once
36	Device not supported	Fail once
37	Source data could not be loaded	Fail once
50	Output file could not be opened (lock/AV)	Retry
51	Error closing output file	Retry
52	Output file could not be created	Retry
53	Output file already exists	Retry
54	Staging → target move failed	Retry
55	Staging cleanup failed at launch	Retry
56	Staging file delete failed	Retry
57	Source folder does not exist	Fail once
58	Target folder does not exist	Fail once
59	No write permission on target	Fail once
60	Output file not open	Fail once
61	Corrupted data	Fail once

Code	Description	Action
62	Unit details missing	Fail once
100	No ACAML found - typically, an in-progress ECM sequence stub	Fail once
101	Multiple ACAML files found	Fail once
102	Archive (zip/ssizip) could not be opened	Fail once
103	Export preconditions not fulfilled	Fail once
150	Invalid settings	Fail once
151	Unknown option	Fail once
152	Missing required option	Fail once
153	Repeated option	Fail once
154	Parameter missing its argument	Fail once
159	Command-line error, unknown root cause	Fail once
160	Invalid `-f` format option	Fail once
161	Invalid `-m` mode option	Fail once
162	Invalid `-e` exclusion option	Fail once
163	`-i` source path does not exist	Fail once
170	Failure during precondition check	Fail once
171	Failure preparing export	Fail once
172	Acquisition method parse failure	Fail once
173	Empty storage path	Fail once
174	Technique not supported (transfer)	Fail once
175	MS signal not supported (transfer)	Fail once
176	Acquiring data system not supported (transfer)	Fail once
177	Detector type not supported (transfer)	Fail once
500	Sequence data not supported	Fail once
501	Technique not supported	Fail once
502	MS signal not supported	Fail once
503	Acquiring data system not supported	Fail once
504	OS language not supported	Fail once
505	Detector type not supported	Fail once
506	Instrument system not supported	Fail once

Code	Description	Action
507	Export mode undefined	Fail once
508	Export input data missing	Fail once
509	No fitting detector	Fail once
510	Instrument technique unknown	Fail once
700	Analysis run information missing	Fail once
701	Sample information missing	Fail once
702	Injection information missing	Fail once
703	Instrument system information missing	Fail once
704	Sample submission information missing	Fail once
705	Chromatogram information missing	Fail once
706	UV spectra information missing	Fail once
707	Instrument device information missing	Fail once
708	Sequence information missing	Fail once
709	Peak information missing	Fail once
710	Use case not supported	Fail once
711	Unit information missing	Fail once
712	Signal data type not supported	Fail once
713	Signal data unit not supported	Fail once
714	Measurement run log missing	Fail once
715	Sequence analysis run log missing	Fail once
716	Acquisition method information missing	Fail once
717	Data processing method missing	Fail once
718	Device information missing	Fail once
719	Expected signal type not found	Fail once
200-499	(currently unused error registry)	Retry
900-999	(currently unused error registry)	Retry
1000-1299	Format specific read/write errors	Fail once
≥1300	(currently unused error registry)	Retry

Version History

Version 1.0 (October 2026)

(ASM Export for OpenLab CDS: 1.0.0)

(Allotrope Converter for OpenLab CDS: 1.0.0)

- First released version

In This Book

The guide describes the following:

- Introduction
- Requirements
- Installing, Updating, and Uninstalling ASM Export for OpenLab CDS
- ASM Export for OpenLab CDS Workflow
- Web-based User Interface
- ASM Content Description
- Responsibilities and Regulatory Considerations
- Appendix

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