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Archiving Waters Empower Data in the Allotrope File Format

ADFExport Enterprise Subscription

Introduction

The diverse analytical techniques used in today's laboratories generate an array of proprietary data formats, which can be challenging to juggle. Wouldn't you rather have a common, universal, shareable, and archive-ready format? The Allotrope Data Format (ADF) framework enables you to store data in a standardized way following the concept of semantic web and linked data.

The Allotrope Data Format is developed by the Allotrope Foundation, an international consortium of pharmaceutical, biopharmaceutical and other scientific research-intensive industries with the shared mission of a single, universal data format: *"Allotrope aims to make the intelligent analytical laboratory a reality – an automated laboratory where data, methods and hardware components are seamlessly shared among disparate platforms, and where one-click reports can be produced based on data generated by any analytical instrument with data integrity built-in by design."* - Allotrope Foundation. For more information visit the website **https://www.allotrope.org**.

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Archive Waters Empower data in OpenLab ECM in the Allotrope Data Format

Agilent OpenLab Enterprise Content Manager (ECM) allows secure and centralized management of analytical data from different manufacturers. This technical overview describes additional OpenLab ECM features providing multi-vendor laboratories the possibility to archive their data in the Allotrope Data Format.

The ADFExport Enterprise Subscription is an add-on to OpenLab ECM revision 3.6 enabling the export of Waters Empower data to ADF (Figure1). The OpenLab product portfolio allows to store Waters Empower data as SSIZip archive in OpenLab ECM. Using ACAML and the raw data stored in the SSIZip archive the export to ADF is performed and the created ADF file is stored next to the SSIZip file.

ADFExport Enterprise Subscription consists of two components, a Windows service and the ADFExportAgent. The ADFExport Windows service reads the files from ECM and exports the data to ADF. The ADFExportAgent is used to set up the ADFExport system and to trigger the service. This can be done either manually or by setting up a periodical task in the Microsoft Task Scheduler.
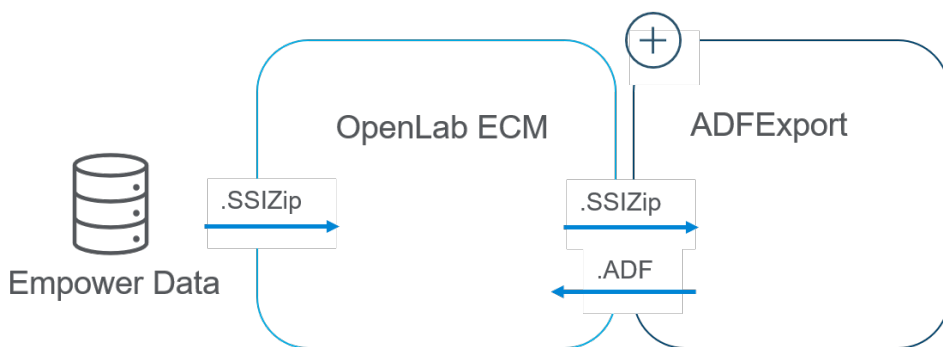

Figure 1. Schematic representation of an OpenLab ECM system with the ADFExport Add-on.

Configuring ADFExport Enterprise Subscription

ADFExport uses specific user-defined attributes in OpenLab ECM. In a first initialization step the user-defined keys *ADFExport_AltVersion, ADFExport_Details* and *ADFExport_Status* are added to the ECM system (Figure 2). The keys are used to enable fast searching, and to maintain the state for the export process including information which files shall be exported or have been exported successfully.

To make the user-defined keys available in OpenLab ECM they need to be configured by using a dedicated ECM user for ADFExport. Storing the user credentials in the Microsoft Credential Manager and initializing the keys, is accomplished by calling the ADFExportAgent via the Windows command prompt.

The keys *ADFExport_Status* and *ADFExport_Details* are linked to every specific ECM Location, Cabinet, Drawer or Folder that may contain data the user wants to export to ADF. "Ready_for_conversion" is set as default value for the *ADFExport_Status* key as shown in Figure 3. For every uploaded SSIZip archive the default value is set allowing an automated export to ADF.
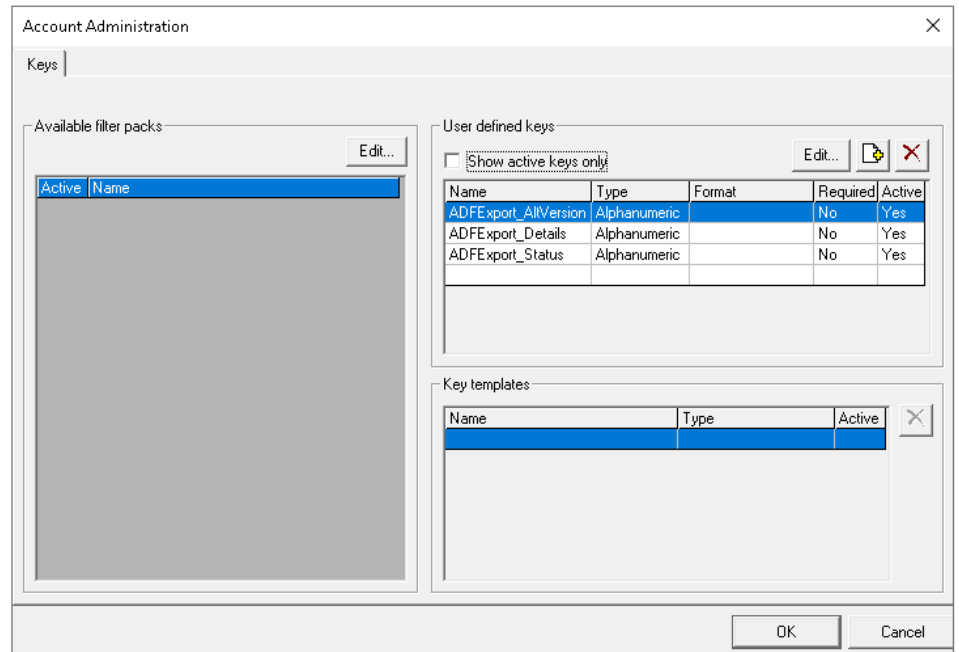

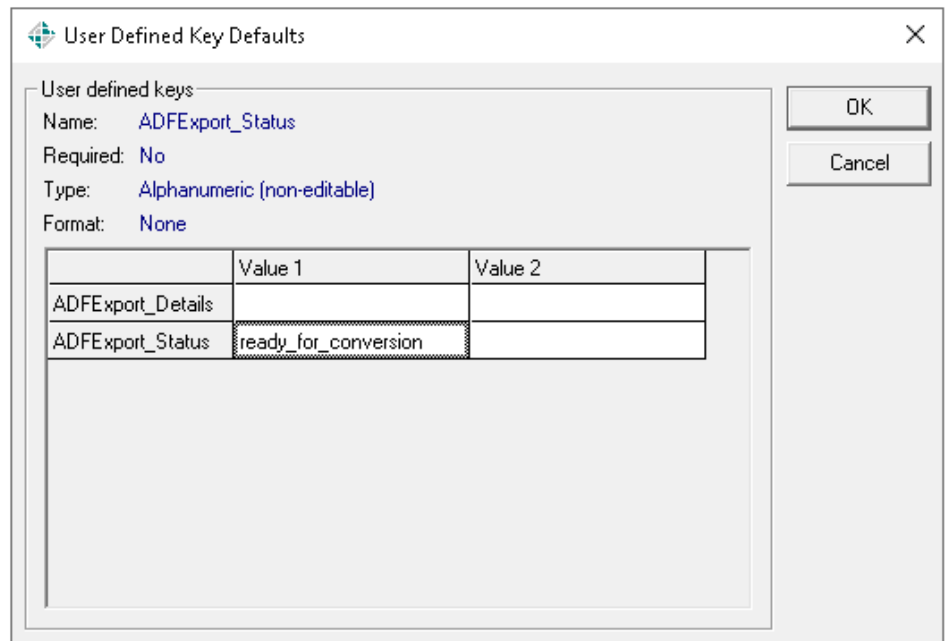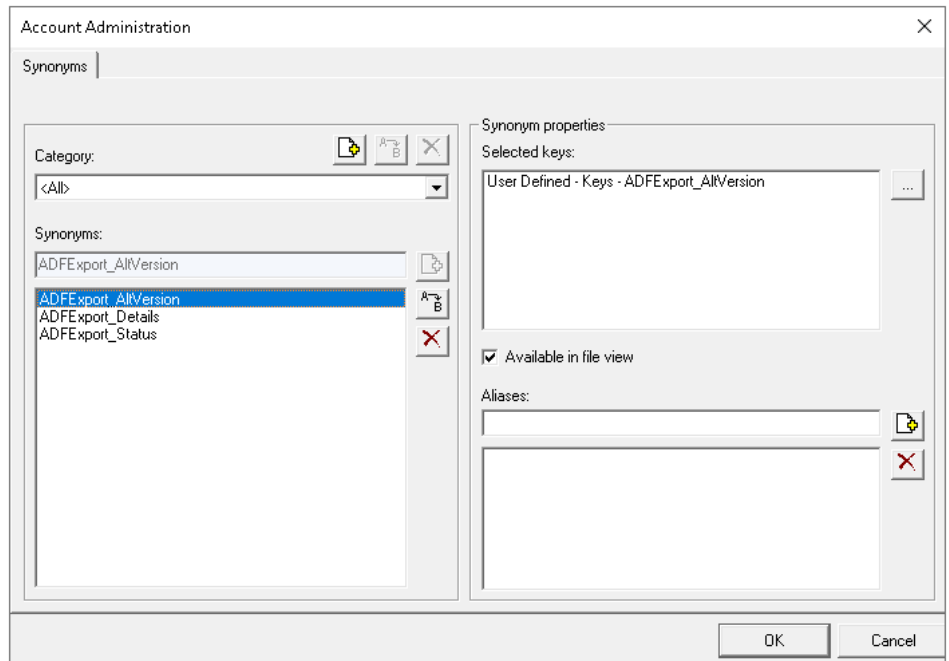**Figure 2.** Initialize ADFExport specific user defined keys in OpenLab ECM.

Figure 3. Configure user defined keys and their default values for any ECM Location, Cabinet, Drawer or Folder that may contain data to be exported to ADF.

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Once the user-defined keys are activated, the respective synonyms are created to be able to view the values of the ADFExport specific attributes in OpenLab ECM. In the Administration tab of OpenLab ECM, the user can create synonyms for all ADFExport specific user-defined keys. Figure 4 shows that the name of the user-defined key is used also as name for the synonym.

By changing the display settings on folder level of OpenLab ECM (see Figure 5), the columns *ADFExport_AltVersion, ADFExport_Details* and *ADFExport_Status* get displayed.
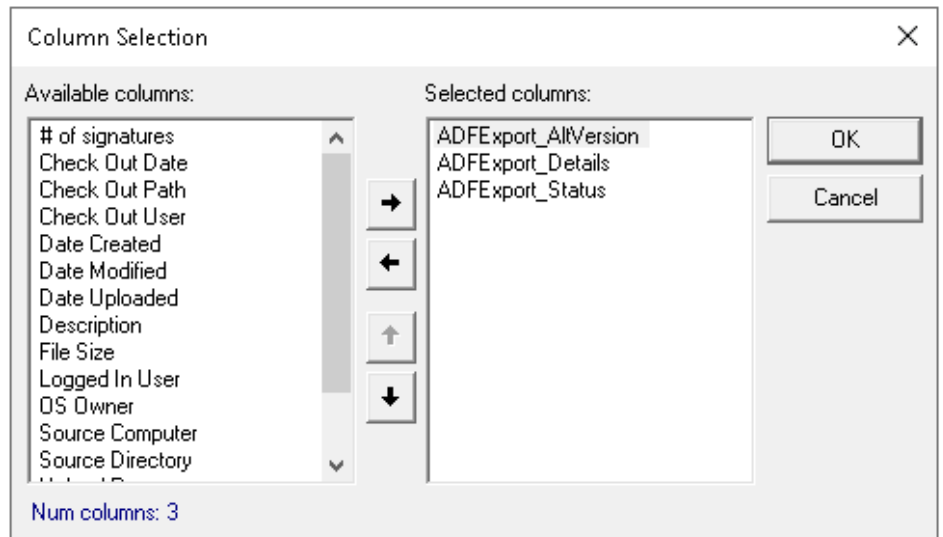
Figure 5. Change the display settings for a selected folder in OpenLab ECM so that the columns for the user-defined keys ADFExport_AltVersion, ADFExport_Details and ADFExport_Status are displayed.


Figure 4. Create synonyms for the ADFExport specific user-defined keys.

Export SSIZip archives containing Waters Empower data to ADF

Once OpenLab ECM is configured the ADFExport Service can be triggered by the ADFExportAgent. To do this automatically on a regular basis a respective task can be configured via the Windows Task Scheduler as shown in Figure 6. Exemplary the ADFExportAgent runs every week and searches for relevant files in the selected ECM Location, Cabinet, Drawer, or Folder. All SSIZip archives marked by the user defined key *ADFExport_Status* as "ready for conversion" are submitted for export. Alternatively, the user can trigger the ADFExport service manually by calling the ADFExportAgent via a Windows command prompt.

During the export process the user defined key *ADFExport_Status* is updated from "ready_for_conversion" to "conversion_scheduled" to "conversion_completed". All changes are tracked by the ECM Audit Trail. The user-defined key *ADFExport_Details* references the exported SSIZip archive including the ECM path, revision and MD5 checksum. The target ADF file is available in the same folder as the source SSIZip archive, and the status of the created file is set to "do_not_convert" (Figure 7). In case of an SSIZip archive containing not supported data the status is set to "file_not_supported" and no ADF file is created.
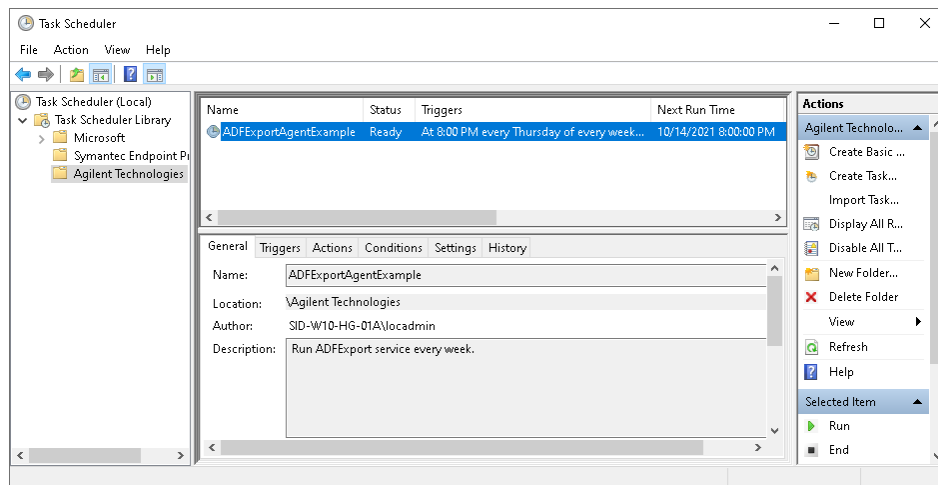
Figure 6. Setting up a task in Windows Task Scheduler on the ADFExport computer. In this example the ADFExportAgent runs periodically on every Thursday of a week at 08:00 PM.

Figure 7. OpenLab ECM folder with changed display settings to visualize the user defined keys. Two of the three example SSIZip archives are converted to ADF and the ADFExport_Status is set to "conversion_completed". For LC.Empower3.SSIZIP the export to ADF is not supported and the ADFExport_Status is set to "file_not_supported".

Allotrope Data Format – File content

The Allotrope Data Format (ADF) is a binary format. It is based on HDF5 (see https://www.hdfgroup.org/solutions/hdf5/), a platform independent file format and is divided into the following three parts: Data Description, Data Cubes and Data Package. With the current revision of the ADFExport Enterprise Subscription the following content is written into the ADF file:

The **Data Description** containing an initial set of metadata about the single run or the entire sequence. The metadata includes information about the HPLC run, such as the system (HPLC instrument, including module and column information), the submitter, the sample, the injection, and the sequence. Furthermore, information on chromatograms and UV spectra as well as acquisition and processing method names, acquisition software and peak results are stored.

The **Data Cubes** containing exported raw data (chromatograms and spectra) in a format according to the ADF data cube ontology.

The **Data Package** containing a subfolder with the original unmodified SSIZip archive data file created by the ECM Scheduler Add-in.

The ADF audit trail ensures integrity and tracks modifications to the ADF file. When creating the file an initial record containing minimal information about the creation of the file, such as date/time and user ID is stored.
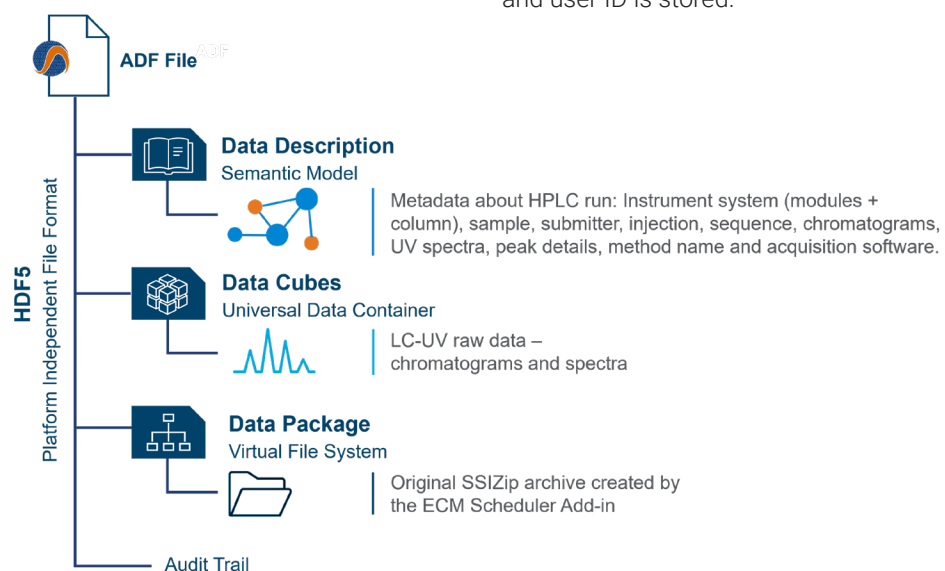
ADF File

Data Description
Semantic Model

Metadata about HPLC run: Instrument system (modules + column), sample, submitter, injection, sequence, chromatograms, UV spectra, peak details, method name and acquisition software.

Data Cubes
Universal Data Container

LC-UV raw data – chromatograms and spectra

Data Package
Virtual File System

Original SSIZip archive created by the ECM Scheduler Add-in

Audit Trail

Platform Independent File Format
HDF5

Figure 8. Schematic representation of an ADF file and its content.

Conclusion

Driven by the pharmaceutical industry, the Allotrope Foundation aims to develop a single common data format for any analytical technique. The goal is to facilitate the collection, exchange, and storage of data in the laboratory. ADFExport Enterprise Subscription provides an ADF export functionality for Waters Empower data archived in OpenLab ECM. Currently, LC-UV and SFC data can be stored in the Allotrope Data Format.

To learn more about OpenLab ECM visit,
www.agilent.com/chem/openlab-ecm

To learn more about the Allotrope Foundation visit,
https://www.allotrope.org

www.agilent.com/chem

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