

Creating an Allotrope file format

ADFExport for OpenLab

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, a standardized framework developed by the Allotrope Foundation, 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 detailed information please visit the website <https://www.allotrope.org>.

This technical overview describes OpenLab CDS and OpenLab ChemStation features that enable the export of chromatography data to the Allotrope Data Format (ADF) and outlines the information stored in the ADF file.

Saving Data in the Allotrope Data Format

ADFExport for OpenLab enables the export of single sample or sequence data to ADF. It is available as an Add-on for workstations and client/server systems of OpenLab CDS revision 2.6, 2.5 and 2.4 and OpenLab ChemStation revision C.01.10 and C.01.09 Update 2. ADFExport supports the export of LC-UV data acquired with Agilent instruments including HPLC and SFC systems. Depending on the CDS system there are different ways to export data to ADF.

With **OpenLab CDS** the user set up automated ADF export by using a suitable processing method in Data Acquisition or during reprocessing in Data Analysis. Users can define “ADF Export” as post processing plugin in the processing method (Figure 1). For each injection in a result set (single run or sequence) one ADF file is created. In case of a sequence with multiple injections the data is exported to multiple ADF files without storing the sequence context.

Additionally, a sequence or single sample result set can be exported manually to ADF by using the ribbon command “Export ADF” in Data Analysis application. Only one ADF file is generated for the entire result set. A sequence with multiple injections is exported to a single ADF file and the sequence context is kept.

OpenLab ChemStation allows to export data automatically to ADF by using a post-run or a post-sequence command/macro. Defining the post-run command/macro in the run time checklist (Figure 2) results in one or multiple ADF files either based on the injection of a single run or based on every injection of a sequence.

By using a post-sequence command/macro from the OpenLab ChemStation sequence parameters (Figure 3) the entire result set is exported to one single ADF file keeping the sequence context.

Alternatively, to export existing ChemStation data manually into ADF run the export tool via Windows command prompt defining a *.D folder or a sequence folder as input path. Specifying ADF files generated with previous revisions of ADFExport for OpenLab as target the ADFExport executable allows to update these to the current format.

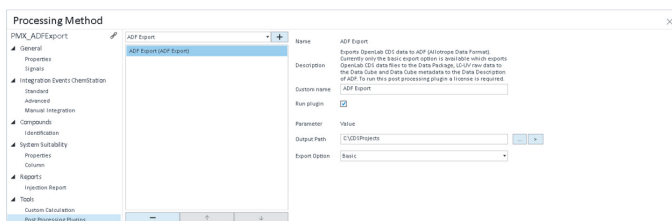


Figure 1. Configure “ADF Export” as post processing plugin in the processing method of Data Analysis.

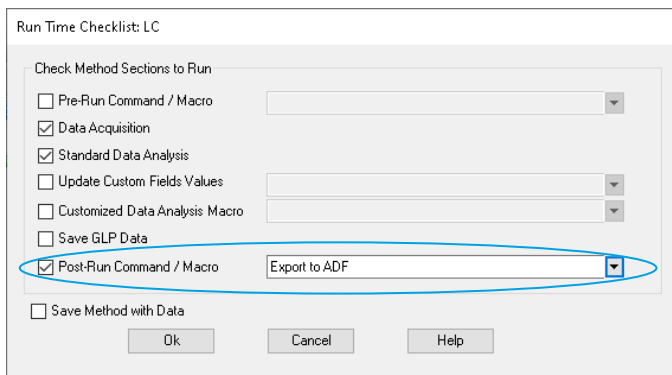


Figure 2. Configure “Export to ADF” as post-run command/macro in the run time checklist of OpenLab ChemStation.

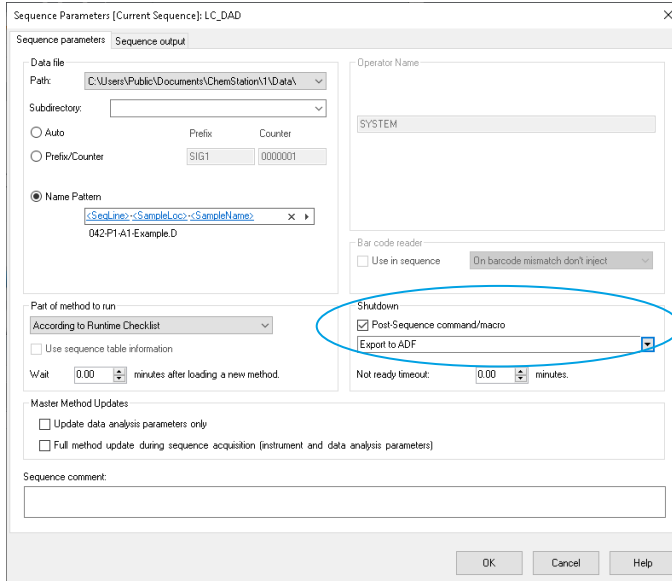


Figure 3. Configure “Export to ADF” as post-sequence command/macro in Sequence Parameters of OpenLab ChemStation.

Allotrope Data Format – File Content

The Allotrope Data Format (ADF) is a binary format. It is based on HDF5, a platform independent file format and is divided into the following three parts: Data Description, Data Cube and Data Package as shown in Figure 4.

The **Data Description** is based on semantic web technology and linked data concepts using the W3C standardized RDF format (see <https://www.w3.org/RDF>) to store analytical metadata as data graph in a standardized and structured way. The metadata include information about the run, such as the system (HPLC/SFC instrument, including module and column information), the submitter, the sample, the injection, the sequence, and the software the data was acquired with. Furthermore, information on chromatograms and UV spectra as well as acquisition and processing method names and peak results are stored.

The **Data Cube** contains analytical raw data: For every chromatogram and the corresponding UV spectra a data cube item is available.

The **Data Package** is a universal data container filled with the original CDS files. For OpenLab CDS this includes *.dx, *.acaml, *.amx, *.pmx (if available) and *.sqx files (if available). For OpenLab ChemStation the whole sequence folder or the *.D folder of the current injection with all files and subfolders is stored.

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.

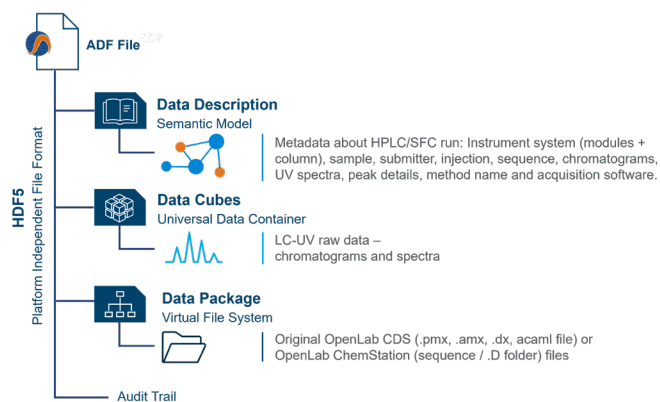


Figure 4. Schematic representation of the Allotrope Data Format and its content.

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 for OpenLab provides an ADF export functionality for chromatography data. Currently LC-UV data from Agilent HPLC or SFC systems acquired with OpenLab CDS or OpenLab ChemStation can be stored in the Allotrope Data Format. Plans are underway to support additional techniques and more contextual metadata in future software releases.

To learn more about OpenLab CDS visit,

www.agilent.com/chem/openlab-cds.

To learn more about OpenLab ChemStation visit,

www.agilent.com/chem/openlab-chemstation

To learn more about the Allotrope Foundation visit,

<https://www.allotrope.org>.

[**www.agilent.com/chem**](http://www.agilent.com/chem)

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