

Creating an Allotrope file format

ADFExport for OpenLab CDS



Figure 1. Word cloud: Allotrope Data Format.

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. Additional benefits include increased data integrity, improved scientific reproducibility, and reduced manual effort especially in relation to paper-based work. This also improves the ability to find, share, and archive data. Finally, this enables data re-use in the context of the sample workflow starting at sample registration to data archiving across different software platforms.

The Allotrope Data Format is developed by the Allotrope Foundation, an international consortium of pharmaceutical, biopharmaceutical and other scientific researchintensive 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.



Saving data in the Allotrope Data Format

ADFExport for OpenLab CDS revision 1.1 enables export of OpenLab CDS single sample or sequence data to ADF. It is available for workstations and client/server systems of OpenLab CDS revision 2.4 and supports the export of LC and LC-UV OpenLab CDS raw data in different ways. User can do an automated ADF export by using a suitable processing method in Data Acquisition or during reprocessing in Data Analysis. For each injection in a result set one ADF file is generated. In case of a sequence with multiple injections the data is exported to multiple ADF files without storing the sequence context.

Additionally, a single sample or sequence result set can be exported manually to ADF by using the ribbon command "Export ADF" in Data Analysis application. Only a single ADF file is generated for the entire result set. A sequence with multiple injections is exported to one ADF file and the sequence context is kept. The Allotrope Data Format is based on HDF5, a platform independent file format and is divided into the following three parts: Data Description, Data Cube and Data Package.

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. With the current basic export option, the data description contains metadata about LC-UV raw data stored in ADF data cube.

The **Data Cube** contains analytical raw data: OpenLab CDS LC-UV chromatograms and the corresponding UV spectra.

The **Data Package** is a universal data container filled with the original OpenLab CDS files including *.dx, *.acaml, *.amx, *.pmx (if available) and *.sqx files (if available).

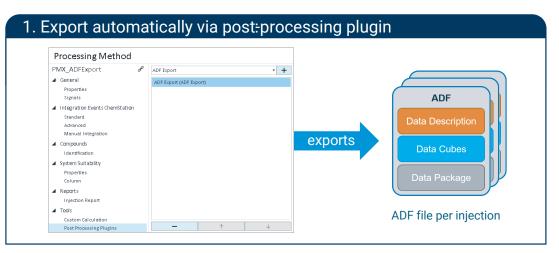


Figure 2. Workflow 1: Automated export to ADF by using a processing method having the post-processing plugin defined, either in Data Acquisition or Data Analysis.

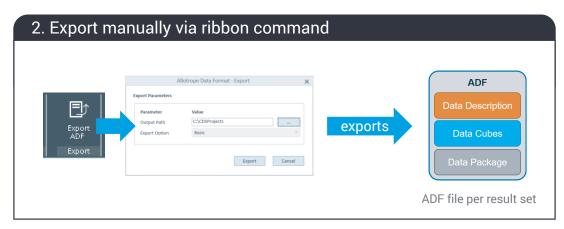


Figure 3. Workflow 2: Manual export to ADF using the ribbon command in Data Analysis.

Reviewing data with the ADFexplorer

To browse the content of the created ADF file you can use the ADFexplorer released by the Allotrope Foundation (https:// www.allotrope.org). Different views (tabular or graphical) are available to show the content of every part in more detail.

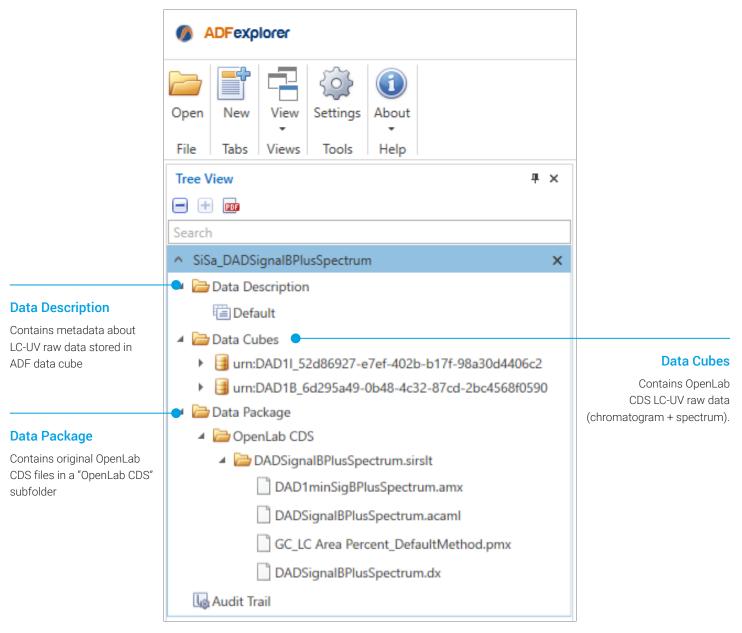


Figure 4. The content of an example ADF file SiSa_DADSignalBPlusSpectrum is displayed in the Tree View of ADFexplorer.

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 CDS provides an ADF export functionality for chromatography data. Currently LC-UV OpenLab CDS raw data 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 the Allotrope Foundation visit, https://www.allotrope.org

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