

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).

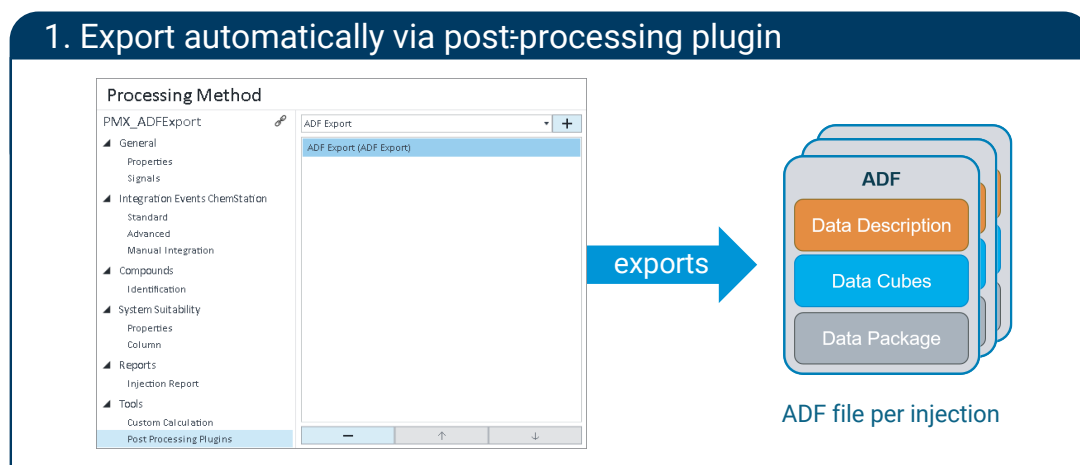


Figure 2. Workflow 1: Automated export to ADF by using a processing method having the post-processing plugin defined, either in Data Acquisition or Data Analysis.

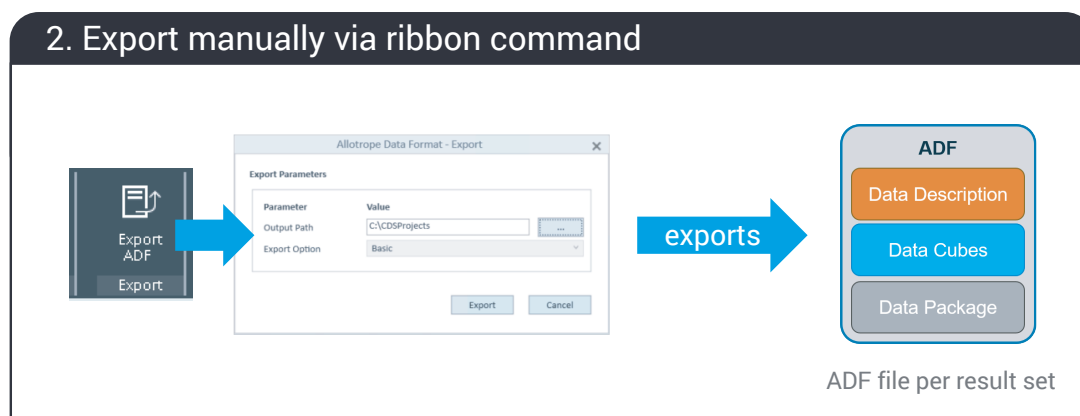


Figure 3. Workflow 2: Manual export to ADF using the ribbon command in Data Analysis.

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.

Data Description
Contains metadata about LC-UV raw data stored in ADF data cube

Data Package
Contains original OpenLab CDS files in a "OpenLab CDS" subfolder

Data Cubes
Contains OpenLab CDS LC-UV raw data (chromatogram + spectrum).

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>

This information is subject to change without notice.