Agilent Allotrope Initiative Prototypes -> Agilent Products

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Agilent Trusted Answers

Introduction

Mission Statement – Allotrope Foundation

Driven by the pharmaceutical and biopharmaceutical industry, Allotrope Foundation consortium is developing a new common, vendor independent, standardized data format for any analytical technique with the mission to "Revolutionize the way we acquire, share and gain insights from scientific data, through a community and the framework for standardization and linked data."

Agilent's Allotrope Engagement

The Agilent Allotrope engagement started 2014, where Agilent Technologies joined Allotrope as a Partner Member followed by the development of several prototypes and the collaboration with several Allotrope members. In 2018 and 2019 Agilent released the first two commercial products based on the Allotrope Framework: ADFExport for OpenLab CDS ChemStation and ADFExport for OpenLab CDS.

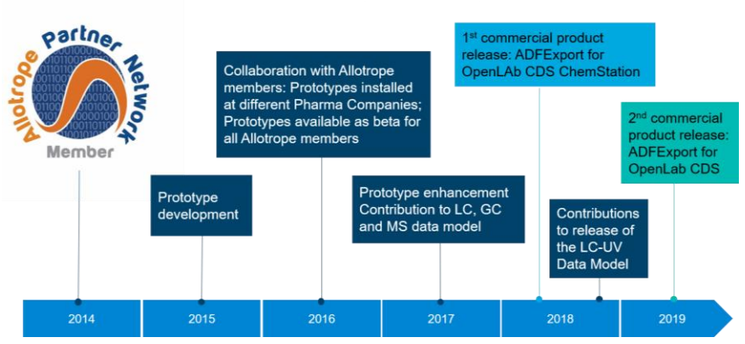

Figure 1. Timeline Agilent's Allotrope Engagement

Prototypes

Chromatography Data Systems

ADF Export Tool: Prototypes for OpenLab CDS ChemStation Edition and OpenLab CDS are available supporting the export of the following data:

- LC and GC metadata according to the prototype data model
- LC and GC chromatogram, UV spectra, instrument signal raw data
- LC and GC peak results
- ChemStation LC acquisition parameters
- ChemStation LC-MSD raw data (MS spectra, TIC)
- ChemStation Sequence data

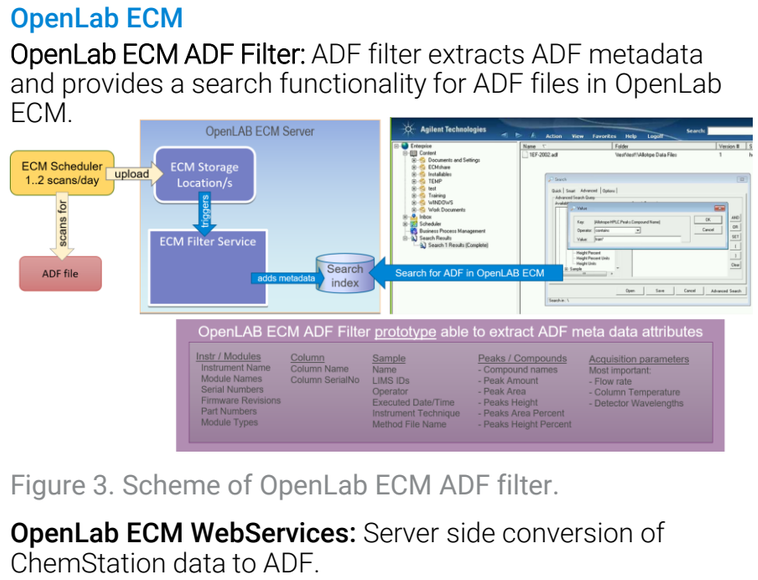

Figure 2. Metadata in Data description of ADF based on the preliminary data model.

Figure 2. Companies with installed prototypes.

OpenLab ECM

OpenLab ECM ADF Filter: ADF filter extracts ADF metadata and provides a search functionality for ADF files in OpenLab ECM.

Figure 3. Scheme of OpenLab ECM ADF filter.

OpenLab ECM WebServices: Server side conversion of ChemStation data to ADF.

Allotrope Integration Projects

Integration Project with BMS: MassHunter BioConfirm Protein Characterization Workflow

The protein characterization workflow demonstrates the ability to extract MassHunter BioConfirm data to a universal data format, the ADF. Metadata can be stored in a standardized way and subsequently be imported to an ELN or LIMS system. In this case BioBook is used as an example.

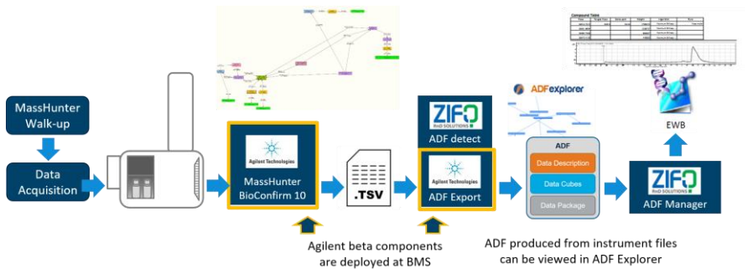

Figure 5. Protein Characterization Workflow – Complete roundtrip from data acquisition to data archiving in EWB.

Integration project with Pistoia Alliance: Method DB

Goal of this collaboration is the exchange of method information in a standardized way. Based on a preliminary data model the ADF export and import of an initial set of ChemStation acquisition method parameters is possible.

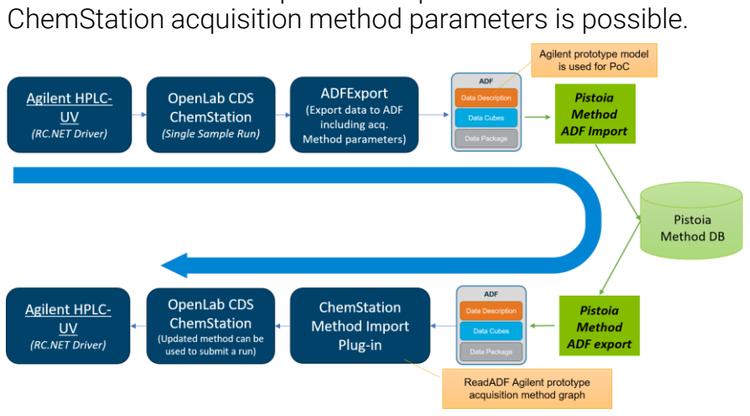

Figure 6. PoC: ADF method export/import of ChemStation acquisition method parameters.

Integration Project with GSK: Digital Lab I/O Adaptor

Method information can be read from a central graph database and modified to submit a run.

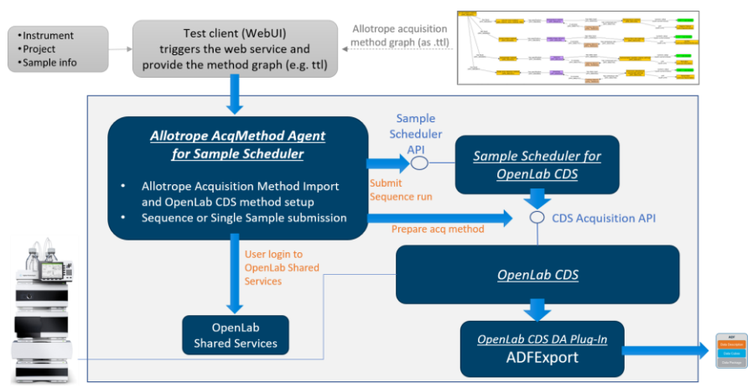

Figure 7. Allotrope Acquisition Method Agent for Sample Scheduler.

1st Commercial Product

ADFExport for OpenLab CDS ChemStation

ADFExport for OpenLab CDS ChemStation Edition provides the functionality to export ChemStation data to ADF. It supports the export of single runs of LC-UV ChemStation raw data. ADF export can be done through an automated ADF export during acquisition or manually using the windows command line. Running the ADFExport tool from command line allows the user to transfer existing ChemStation LC-UV data to ADF.

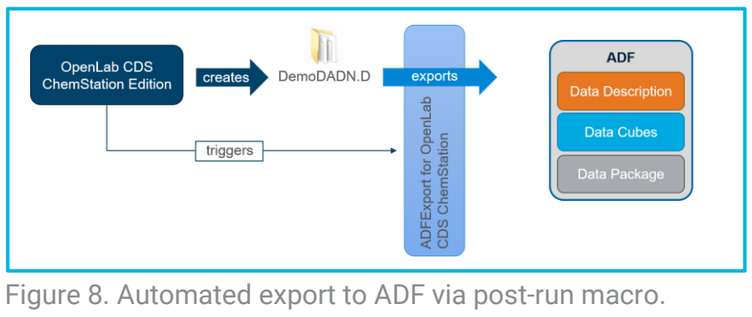

Figure 8. Automated export to ADF via post-run macro.

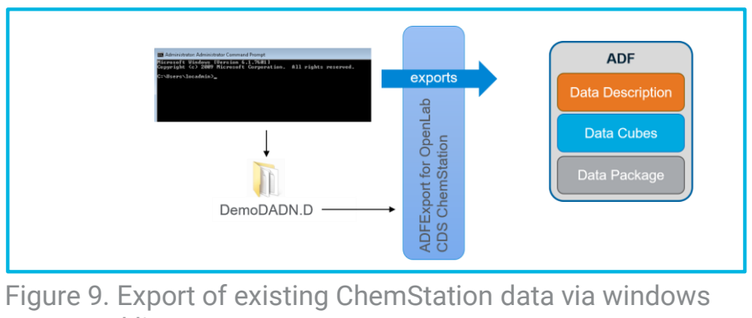

Figure 9. Export of existing ChemStation data via windows command line.

2nd Commercial Product

ADFExport for OpenLab CDS

ADFExport for OpenLab CDS provides the functionality to export OpenLab CDS single sample or sequence data to ADF. It is available as an add-on for OpenLab CDS 2.4 and supports the export of LC and LC-UV OpenLab CDS raw data. The user can do an automated ADF export by using a suitable processing method in Data Acquisition or during reprocessing in Data Analysis. One ADF file for every injection is created.

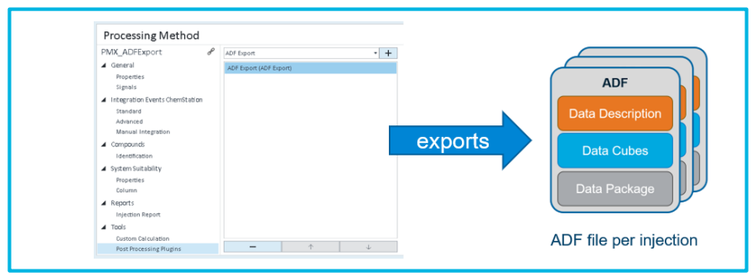

Figure 10. Automated export via post-processing plugin.

Additionally, a single sample or sequence result set can be exported manually to ADF by using the ribbon command "Export ADF" in Data Analysis. Only one single ADF file is generated for the entire result set.

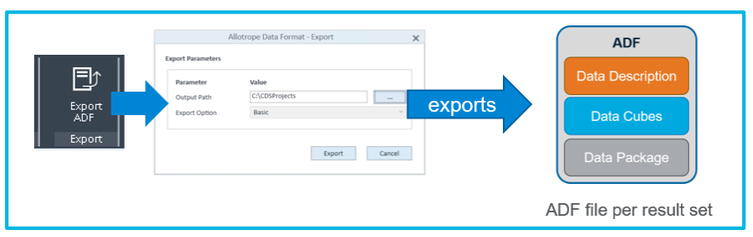

Figure 11. Manual export via ribbon command in DA.

Sequence ADF File

Entire sequence can be exported into one single ADF file.

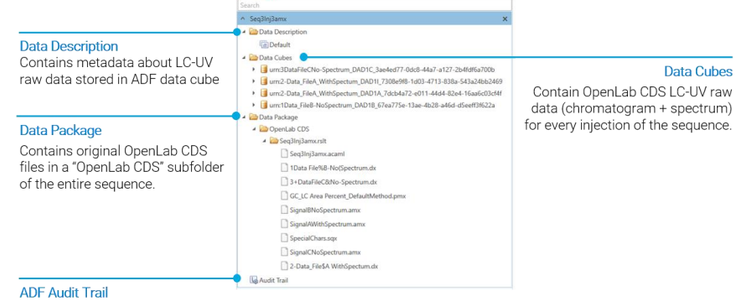

Figure 12. Content of an ADF file displayed in ADFexplorer.

Conclusions

The goal of the Allotrope Foundation in generating the Allotrope Data Format (ADF) is to standardize the collection, exchange, and storage of analytical data captured in laboratory workflows. Agilent is proactively involved in the development of this standardized data format, providing the first two products for the export of chromatography data:

- ADFExport for OpenLab CDS ChemStation
- ADFExport for OpenLab CDS

Commercial solutions in the Allotrope ecosystem are a cornerstone for the adoption across the industry and the global acceptance of the standard.

References

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