Allotrope Connect Workshop

New release of ADFExport for OpenLab -
Demo of an example ADF viewer tool to read created ADF

2020 May - Virtual Allotrope Connect Workshop
Abstract

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 different Allotrope members.

Fulfilling the aims of the Allotrope Foundation, Agilent has started in 2018 with delivering commercial products for basic ADF export functionality for OpenLab CDS and ChemStation based on the Allotrope Framework.

Agilent is releasing a new product combining the ADF export for OpenLab CDS and ChemStation in a single commercial product focusing on metadata export applying the knowledge graph according to the LC-UV data model: **ADFExport for OpenLab**
Engagement and Product Vision
Ralph Mueller
Problem Statement

Goal: end-to-end workflow supported by Allotrope

- Long-term archiving in a proprietary data format → not able to view data in 10-20 years
- Along the workflow no re-use of data because of data silos & different terminologies
- Not possible to efficiently exchange data with: external contract labs/ vendor proprietary formats
Engagement of Agilent with the Allotrope Foundation

- **2014**: Agilent joined Allotrope as Partner Member
- **2015**: Prototype development
- **2016**: Collaboration with Allotrope members: Prototypes available as beta; installed in laboratory of different pharma companies;
- **2017**: Prototype enhancement; Contribution to LC, GC and MS data model
- **2018**: 1st commercial product release: ADFExport for OpenLab CDS ChemStation
- **2019**: ADFExport for OpenLab CDS
- **2020**: ADFExport for OpenLab
A vision for OpenLab….

ADFExport

OpenLab CDS

OpenLab ChemStation

ADF

OpenLab ECM

long-term storage

ECM import

ECM import

Vendor A

Vendor B

ADF

ADFConverter

ECM

Search

Semantic data

Upload

“Smart data lake”

Instrument utilization

Asset Management

Trend Charts

… and AI would then be a next thinkable step

Semantic Layer

For Research Use Only
ADFExport for OpenLab – Revision 1.2
Henrike Gehring
**What’s new?**

**LC UV metadata available in ADF Data Description**
- Data structure according to standardized data model released by the Allotrope Foundation Mar 2020

**Combined product release**
- One product including both add-ons, one for ChemStation and one for OpenLab CDS
- One single product license

**Improved performance of ADF file generation**
- Current version of the Allotrope Framework 1.4.10 is used (including the performance fix)
- Audit trail is activated at the end of ADF file generation
What’s new?

• **CDS specific features**
  • Export of ChemStation data is supported from Data Analysis.

• **ChemStation specific features**
  • Distributed system support
  • Export of ChemStation data acquired during sequence operation
  • Data can be exported to a network share
  • Data Migration
ADFExport for OpenLab – revision 1.2

Supported Features / File Content

- Export of LC-UV data acquired with OpenLab CDS / OpenLab CDS ChemStation
- Export of data to a local file directory or a network share
- Basic export mode, which writes the following content into the ADF file:

  - Metadata about LC-UV data: HPLC run, system, column, sample, submitter, injection, chromatogram, spectrum, peak details and method name information.
  - CDS LC-UV raw data (chromatograms + UV spectra).
  - Original CDS files (.pmx, .amx, .dx, acaml file) or ChemStation files (sequence / .D folder).
ADFExport for OpenLab – revision 1.2

Compatibility

Supported CDS versions

• OpenLab CDS ChemStation Edition
  – C.01.09 Update 2
  – C.01.10

• OpenLab CDS
  – 2.4
  – 2.5

Supported Data

• LC-UV data acquired with Agilent instruments
• ChemStation: Existing data acquired with ChemStation C.01.01 or later (via cmd line tool)
• OpenLab CDS: Existing data acquired with OpenLab CDS 2.0 or later, existing data acquired with ChemStation C.01.01 or later; (re-load to DA)
ADFExport for OpenLab
ChemStation Workflows

1. ADF file generation via windows command line

Export existing ChemStation single sample or sequence data (run by run or sequence based)

Migrate existing ADF files

ADFExport 1.0

ADFExport 1.2
ADFExport for OpenLab
ChemStation Workflows

2. Export single run or sequence data automatically to ADF via post-run / post sequence macro

Post-run macro
“Export to ADF”

Post-sequence macro
“Export to ADF”
ADFExport for OpenLab
OpenLab CDS Workflows

1. Export manually via ribbon command
ADFExport for OpenLab
OpenLab CDS Workflows

2. Export automatically via post-processing plugin defined in the processing method

“Unattended” processing in Acquisition

Processing/ reprocessing in Data Analysis

acquire, analyze and export data
archive
Demo of LC Data Viewer using high level API’s in CDS products and ECM products

Heiko Fessenmayr
All Agilent ADFExport written LC ADF content can be read via this API

- Reading of ADF content via Allotrope low-level ADF API requires learning of semantic web skills not every developer can afford
- To lower this hurdle Allotrope Foundation has worked on a LC high-level API to ease reading of LC ADFs
- Agilent has contributed to this so that all Agilent ADFExport written LC ADF content can be read via this API
- LC ADF content written by all vendors following the LC ADF standard will readable through this common API

LC ADF consumer (e.g. ADF viewer) → LC ADF high-level API → ADF low-level API

standardized SPARQL queries for LC data

Provides classes for
- instrument
- injection date/time
- sample / submitter
- chromatograms
- uv spectra
- peak details
LC ADF Viewer
based on Allotrope LC-UV High-Level API

- Visualize LC-UV data for single samples and sequence ADFs
- Visualize Instrument, sample, submitter, chromatogram, uv spectra, Peak details information
- Windows 10 desktop app
- Can be linked to .ADF file extension as "Default App" in windows OS
- Can be used as LC ADF viewer for Agilent OpenLab ECM 3.X and ECM XT
- Agilent will license the source code of this viewer to Allotrope community
Thanks!
HPLC System

- Pump
- Sampler
- Oven
- Column
- Detector

HPLC Chromatograph

- Global Identifier, Local identifier (name)
- Identifier, Date/Time
- Actual Injection Volume

Injection

Mobile Phase Delivery

- Mobile Phases
- Actual Gradient Table
- Temperatur control
- Actual Temp. Gradient Table
- Temperature Control

UV Spectrum

Chromatogram(s)

- Identifier
- Description
- Actual Wavelength,
- Temperature Control
- Baseline (metadata + data cube)

Chromatography

- Acquisition Method
- Data Processing Method
- Software agent

Integration

- Peak list
- Peak details: Retention Time, Area, Height, Baseline...
- Peak area sum
- Analyte amount sum
- Peak height sum
- Analyte amount sum
- Signal to noise

Data Processing

- UV Spectra
- Identifier, Description

Sequence

- Person Name
- Submitting
- Sample

Software agent

- Person
- Submitter, Submission, Sample

HPLC Run

- Sequence
- Identifier, Index

Manufacturer,
SerialNo,
ModelNo,
Firmware

Person

- Person Name
- Submitting
- Sample

Pump

- Method
- Injection

Sampler

- Method
- Submission

Oven

- Method
- Index

Column

- Method
- Identification

Detector

- Method
- Parameters

Chromatography

- Data Processing
- Software agent

Integration

- Calculation
- Totaling

Peak Table

- Analyte amount
- Noise
- Signal to noise

Electronic absorbance measurement

- UV Spectra
- Identifier, Description

Baseline (metadata + data cube)
1. ADF file generation via windows command line

- `i "…\MySingleSample1.D"`  ➔  SiSa_MySingleSample1.adf
- `i "…\MySequence"`  ➔  MySequence.adf
- `i "…\001-1-Sample1.D"`  ➔  MySequence_001-1-Sample1.adf
- `i "…\MyADF.adf"`  ➔  MyADF.adf