

# 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

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**

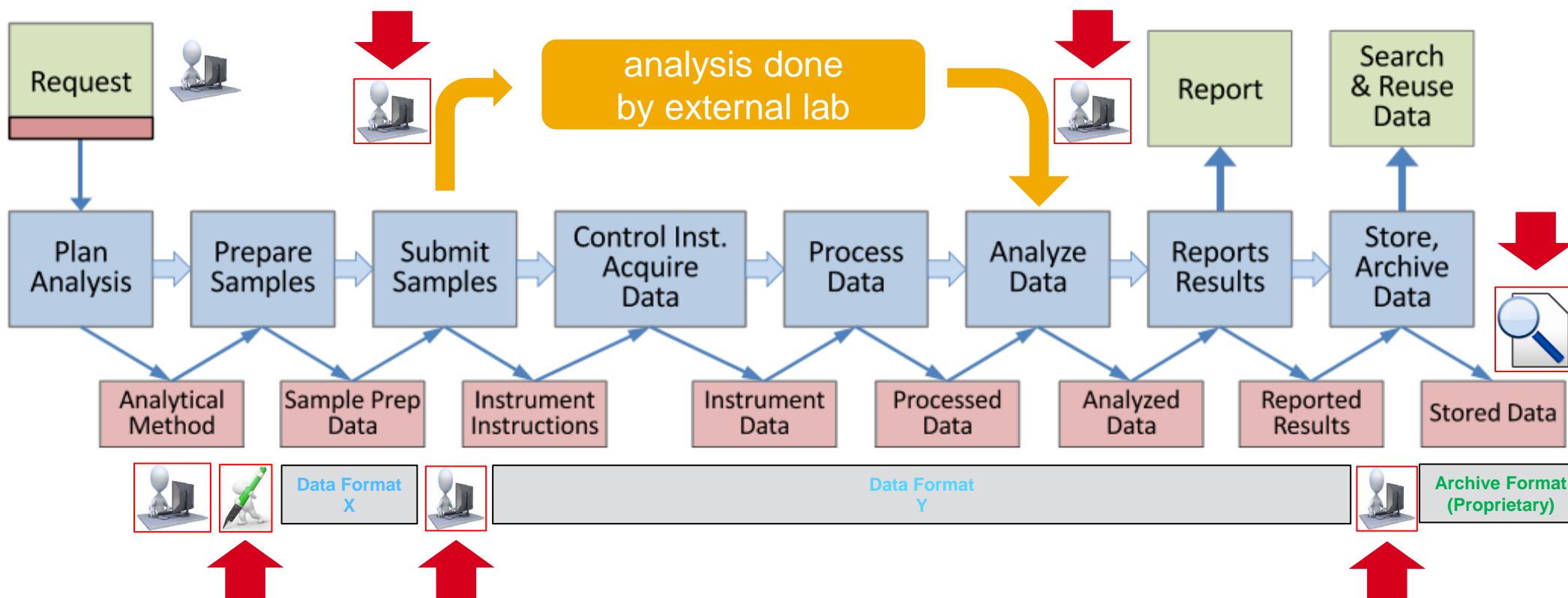
# Engagement and Product Vision

Ralph Mueller

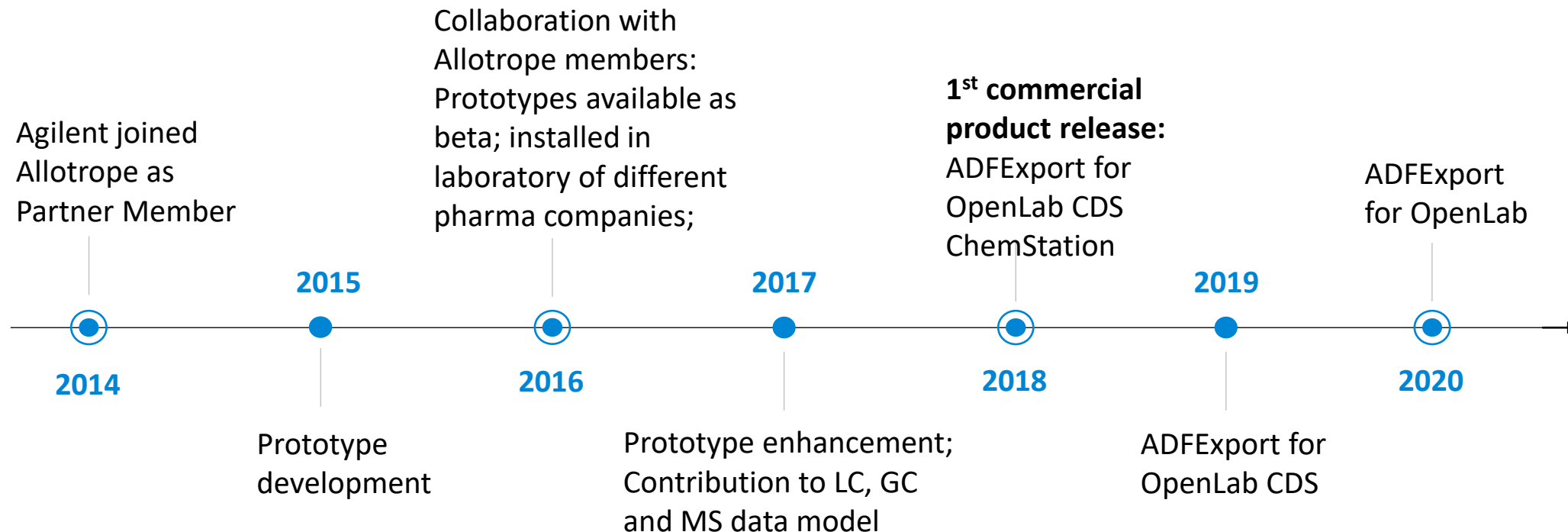
# Problem Statement

## Goal: end-to-end workflow supported by Allotrope

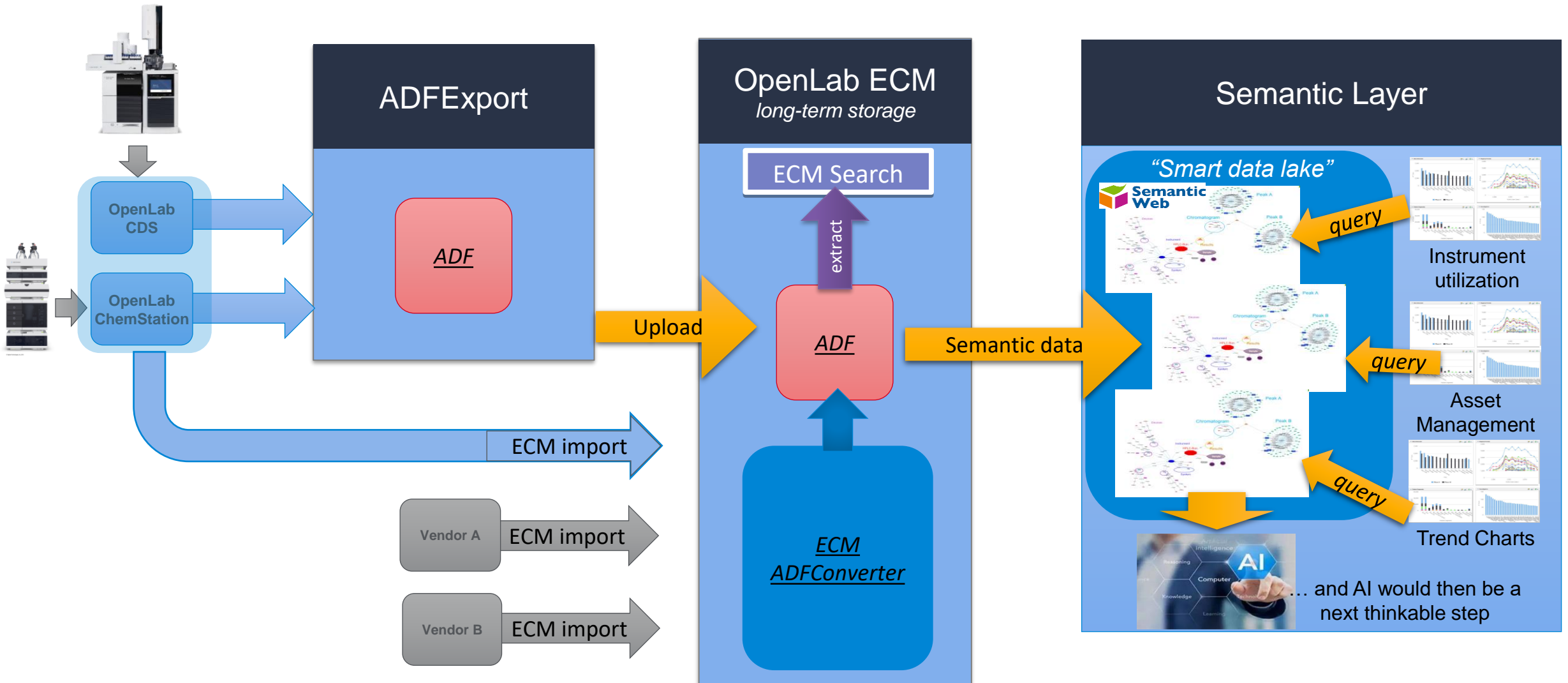
- Long-term archiving in a proprietary data format → not able to view data in 10-20 years
- Along the workflow no re-use of data because of data silos & different terminologies
- Not possible to efficiently exchange data with: external contract labs/ vendor proprietary formats



# Engagement of Agilent with the Allotrope Foundation



# A vision for OpenLab....



# ADFExport for OpenLab – Revision 1.2

Henrike Gehring

# ADFExport for OpenLab – Revision 1.2

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



# ADFExport for OpenLab – Revision 1.2

## What's new?

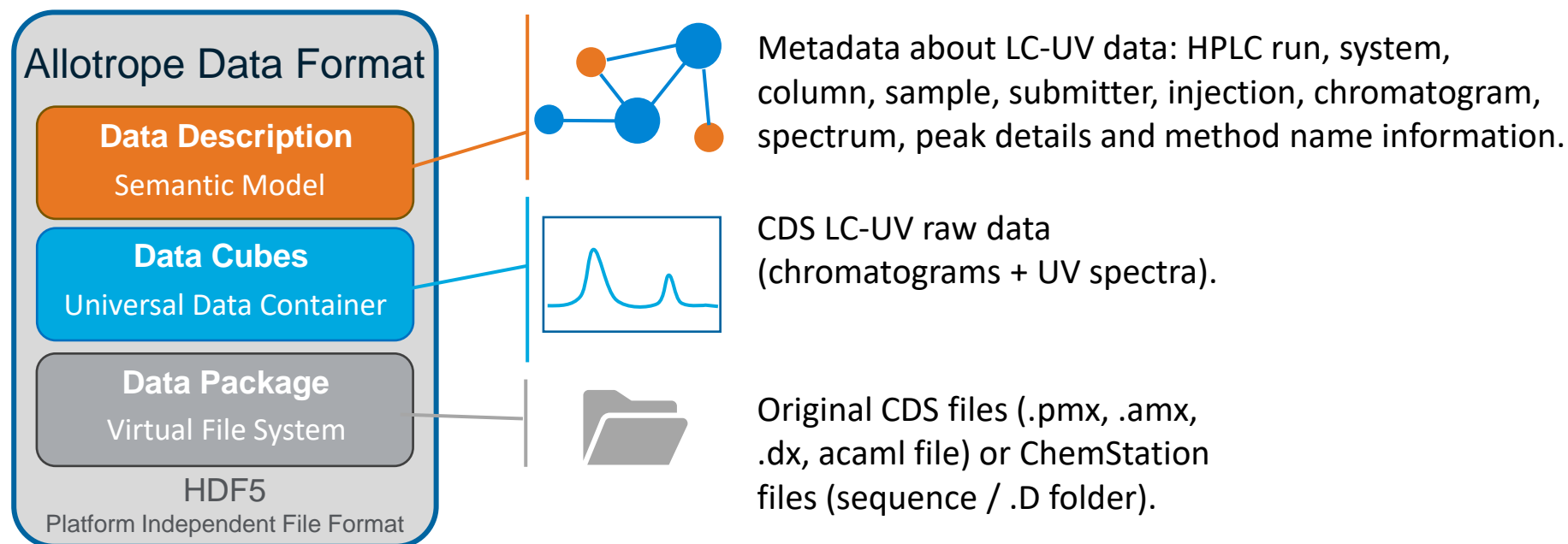


- **CDS specific features**
  - Export of ChemStation data is supported from Data Analysis.
  
- **ChemStation specific features**
  - Distributed system support
  - Export of ChemStation data acquired during sequence operation
  - Data can be exported to a network share
  - Data Migration

# 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:



# 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

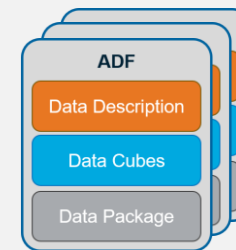
Export existing  
ChemStation single  
sample or sequence  
data (run by run or  
sequence based)



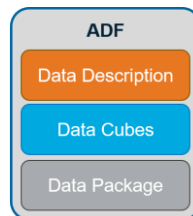
```
Administrator: Windows Command Prompt
Copyright (c) 2009 Microsoft Corporation. All rights reserved.
C:\Users\michael> cd C:\Program Files (x86)\Agilent Technologies\OpenLab\ADFExport
ADFExport -help
ADFExport for OpenLab CSE Clientation - For research use only.
Agilent OpenLab CSE Clientation 1.1.1.1211
Copyright (c) 2009 Agilent Technologies, Inc.

Required: Specify the export mode. For the first release, the
file will be saved in "ADF". With the first release, the
following control is used: C:\Program Files (x86)\Agilent Technologies\OpenLab\ADFExport
Control: Specify the ChemStation file and data. ADF data
description contains metadata about CSE run data stored in ADF
files and ADF data package contains OpenLab CSE Clientation
files.

Required: Full path to the data file that you want to export. In
some cases include all paths and special characters as necessary.
The path to the target output folder, if it is not specified, the
ADF file is stored in ... \Users\user\Documents\ADFExport.
-1 The path to the log output folder, if it is not specified, the log
output will be saved in ... \Users\user\Documents\ADFExport.
-2 If the path to the log output folder does not
exist, it is created automatically and a warning message is
displayed.
--help Display the command line parameter help. All other parameters are
ignored, and no entry is made in the log file.
```



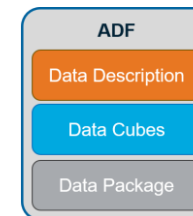
Migrate existing  
ADF files



```
Administrator: Windows Command Prompt
Copyright (c) 2009 Microsoft Corporation. All rights reserved.
C:\Users\michael> cd C:\Program Files (x86)\Agilent Technologies\OpenLab\ADFExport
ADFExport -help
ADFExport for OpenLab CSE Clientation - For research use only.
Agilent OpenLab CSE Clientation 1.1.1.1211
Copyright (c) 2009 Agilent Technologies, Inc.

Required: Specify the export mode. For the first release, the
file will be saved in "ADF". With the first release, the
following control is used: C:\Program Files (x86)\Agilent Technologies\OpenLab\ADFExport
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some cases include all paths and special characters as necessary.
The path to the target output folder, if it is not specified, the
ADF file is stored in ... \Users\user\Documents\ADFExport.
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output will be saved in ... \Users\user\Documents\ADFExport.
-2 If the path to the log output folder does not
exist, it is created automatically and a warning message is
displayed.
--help Display the command line parameter help. All other parameters are
ignored, and no entry is made in the log file.
```



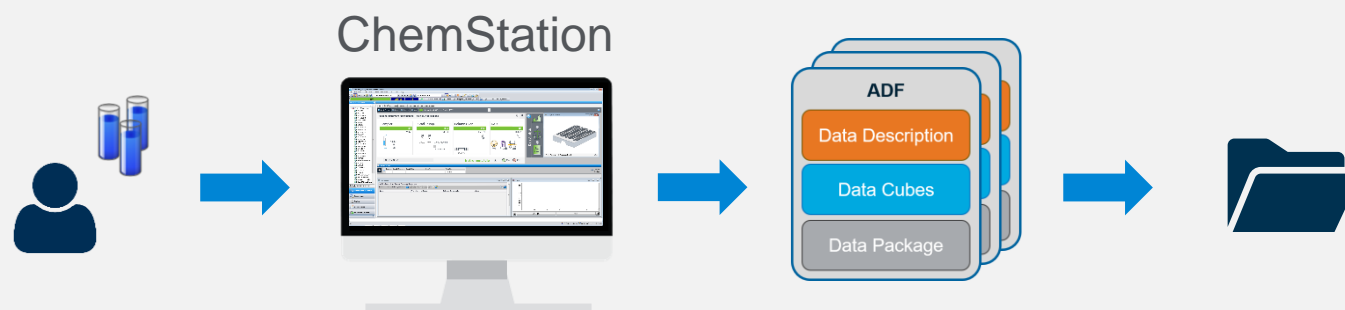
ADFExport 1.0

ADFExport 1.2

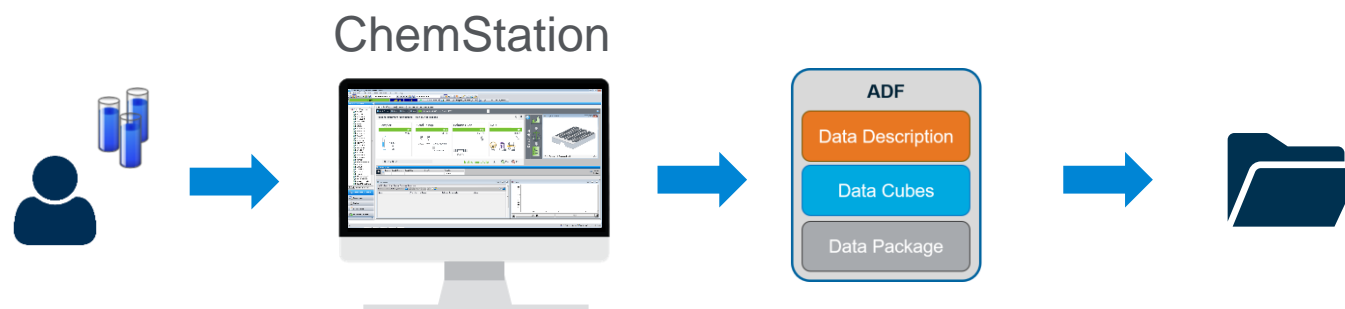
# ADFExport for OpenLab ChemStation Workflows

## 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

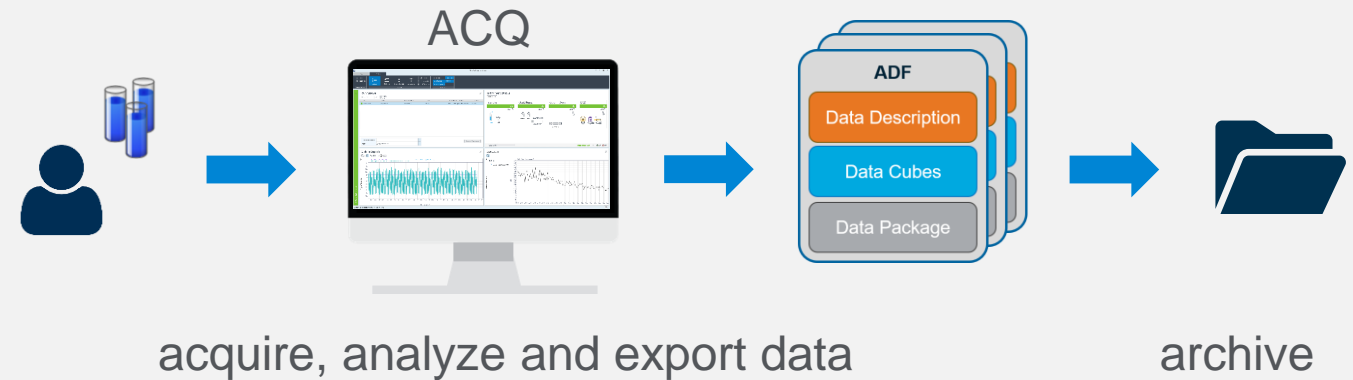


# ADFExport for OpenLab

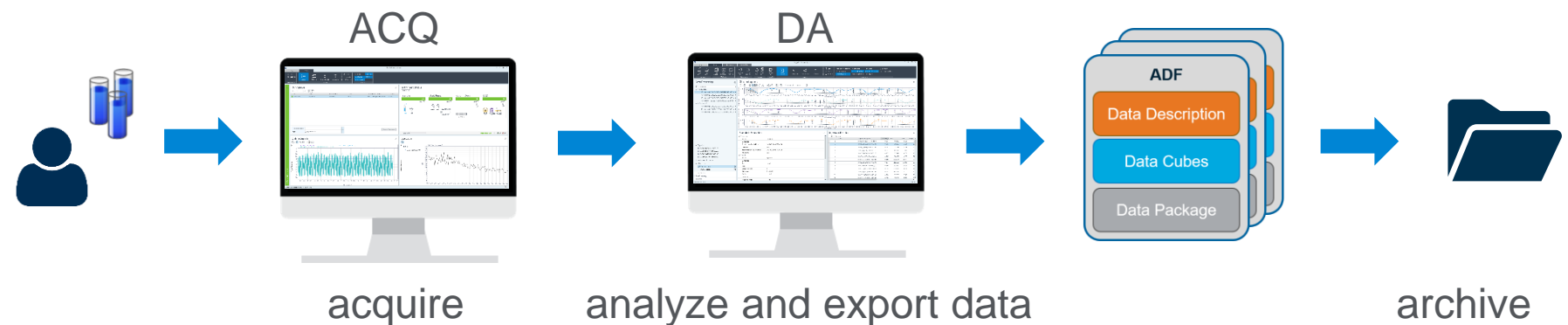
## OpenLab CDS Workflows

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

“Unattended” processing  
in Acquisition



Processing/  
reprocessing in  
Data Analysis



# Demo of LC Data Viewer using high level API's in CDS products and ECM products

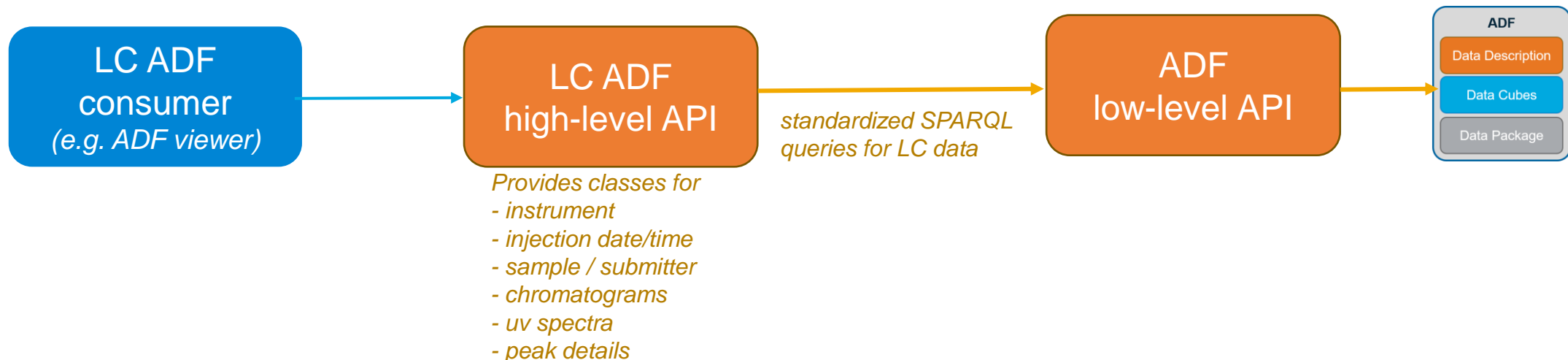
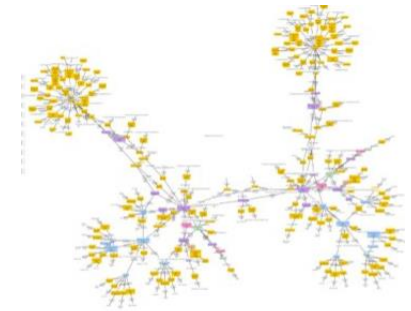
Heiko Fessenmayr



# Allotrope LC High-Level API for easy reading of LC ADF content

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 be readable through this common API



# LC ADF Viewer

## based on Allotrope LC-UV High-Level API

ADF Viewer for LC data - D:\VMWare\Shared Folder\Allotrope\Tools\LCADFViewer\def\_LC-SimuDAD-01 2016-12-06 08-02-13.ADF

**Select ADF file**

Contributed by:

Analysis run type

Single Sample(s)

Sequence

Sequence name:

def\_LC-SimuDAD-01 2016-12-06 08-02-1

**Run Information**

Sequence runs:

- Run 1: Sample 1
- Run 2: Sample 1
- Run 3: Sample 1
- Run 4: Sample 2
- Run 5: Sample 2
- Run 6: Sample 3

Sample name: Sample 1

Sample submitter: SYSTEM

Acquisition method: Demo-LC-SimuDADSequence.M

Data processing: Demo-LC-SimuDADSequence.M

Injection date/time: 12/6/16 07:02:26 +00:00

Injection volume: 1.000 [cubic millimeter]

**Used instrument**

Instrument name: LC-01 Description: <not provided>

Manufacturer	Device TypeNam	ModelNumber	SerialNumber	FirmwareVersion	WrittenName
Agilent	diode array	G4294B	DEABC50000	B.07.01 [0005]	DAD
Agilent	oven	G4294B	DEABC50000	B.07.01 [0005]	Column Oven
Agilent	autosampler	G4294B	DEABC50000	B.07.01 [0005]	Sampler
Agilent	pump	G4294B	DEABC50000	B.07.01 [0005]	Grad. Pump
	high-performance liquid chromatography column	827700-902	autoID-7		SB-C18

**Chromatograms:**

DAD1A: DAD1 A, Sig=250.100 Ref=360.100

DAD1B: DAD1 B, Sig=254.16 Ref=360.100

DAD1C: DAD1 C, Sig=210.8 Ref=360.100

DAD1D: DAD1 D, Sig=230.16 Ref=360.100

DAD1F: DAD1 F, Sig=260.16 Ref=360.100

**UV Spectra:**

DAD1UV: DAD1UV Spectra (190 - 400 nm)

**Peaktable**

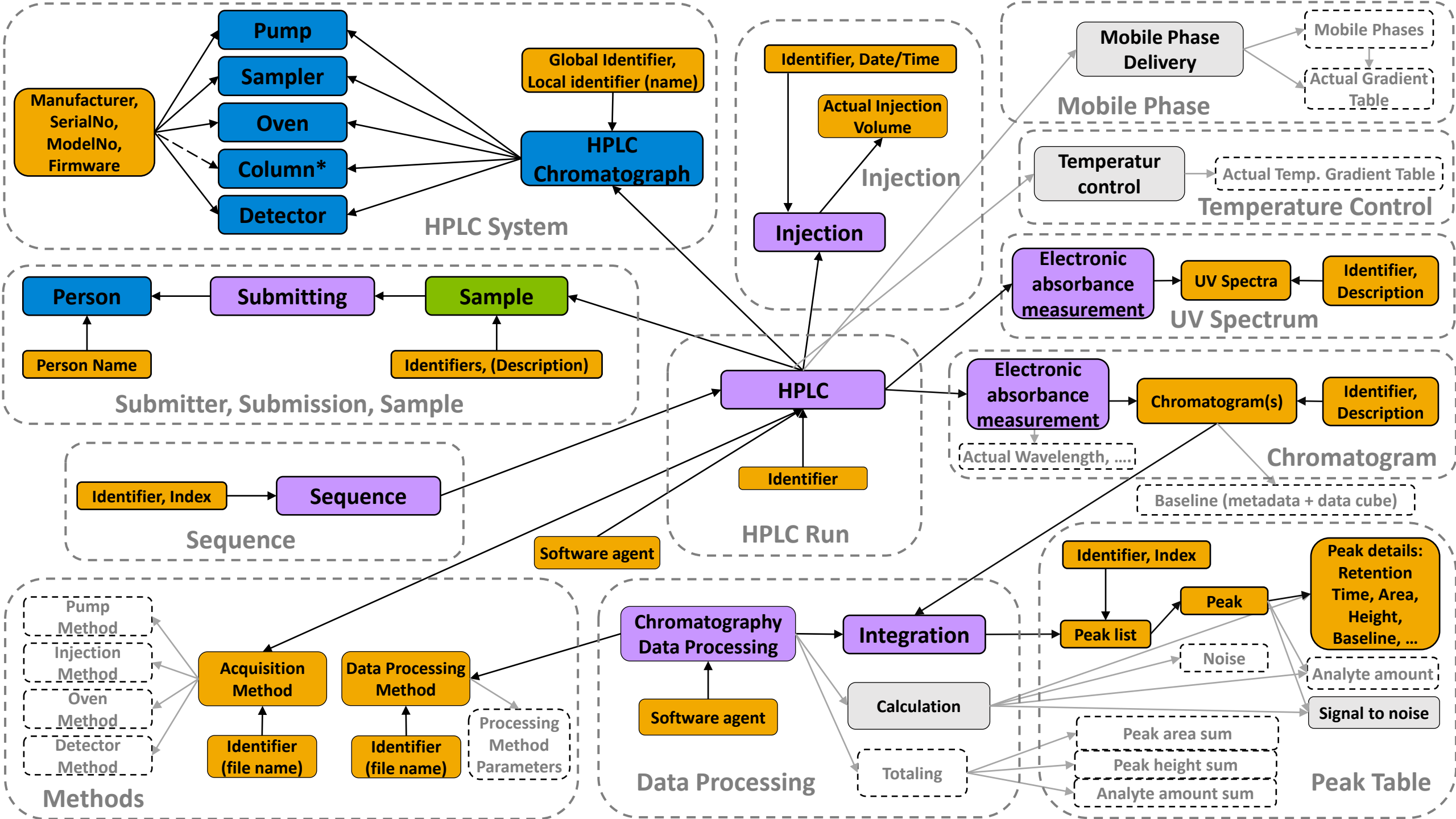
Chromatogram	Peak index	Retention Time [min]	Area [mAU*s]	Relative Area [%]	Height [mAU]	Relative Height [%]	Width At Baseline	Width At Five Percent Height	Width At Half Height	Start Time [min]	End Time [min]	Peak Value At Start Time	Peak Value At End Time
DAD1A	1	0.01302	97.19292	0.96632	86.45631	1.52923	-0.00229	0.01805	0.01805	0.00083	0.00083	-9.69505	-11.35742
DAD1A	2	0.03496	392.00177	3.89741	237.16377	4.19493	0.05212	0.02898	0.02607	0.02248	0.02248	-11.35742	-391.4302
DAD1A	3	0.10366	945.79517	9.40341	397.49176	7.03079	0.29202	0.05422	0.04089	0.05688	0.05688	-390.79184	-11.33652
DAD1A	4	0.14579	1054.67859	10.48596	458.14633	8.10365	0.09082	0.04330	0.04330	0.11354	0.11354	-11.33652	-53.07625
DAD1A	5	0.16953	554.22137	5.51025	409.17377	7.23742	0.31684	0.02337	0.02337	0.15684	0.15684	-53.07629	-10.20767
DAD1A	6	0.18962	797.79974	7.93199	412.67786	7.29940	0.52090	0.03269	0.03269	0.18021	0.18021	-10.20767	-13.02435
DAD1A	7	0.22324	204.54520	2.02321	105.89955	7.17950	17.01893	0.01610	0.01610	0.21103	0.21103	13.02435	10.47473

- 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!

# ADFExport for OpenLab

## Appendix



# ADFExport for OpenLab ChemStation Workflows

## 1. ADF file generation via windows command line

```
Administrator: Administrator Command Prompt
Microsoft Windows [Version 6.1.7601]
Copyright (c) 2009 Microsoft Corporation. All rights reserved.

C:\Users\locadmin>cd C:\Program Files (x86)\Agilent Technologies\CSADFExport
C:\Program Files (x86)\Agilent Technologies\CSADFExport>Agilent.Openlab.CSADFExp
ort.exe --help

Agilent ADFExport for OpenLab CDS ChemStation - for research use only.
Agilent.Openlab.CSADFExport.exe 1.1.0.251
Copyright c 2018-2019 Agilent Technologies, Inc.

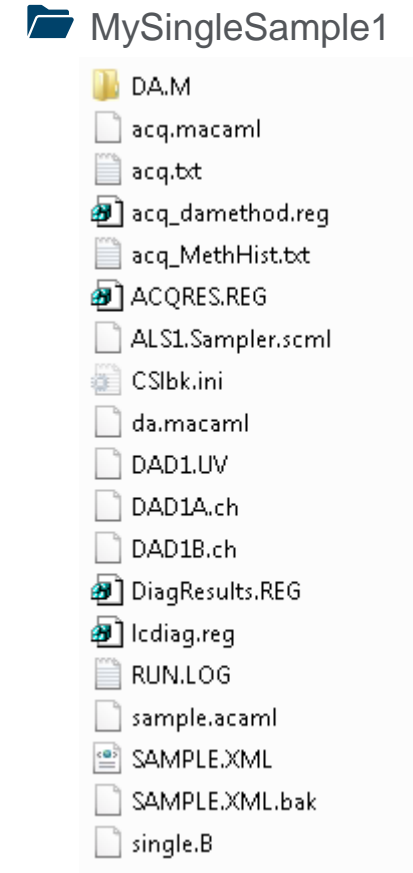
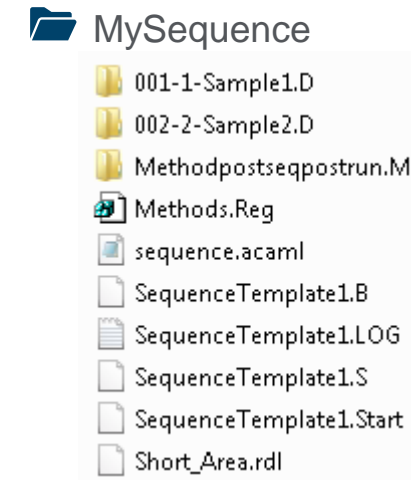
-n Required. Specifies the export mode. For the first release, the
only valid argument is "basic". Using the basic export mode the
following content is written into the ADF file: ADF data cube
contains exported OpenLab CDS ChemStation LC-UU raw data, ADF data
description contains metadata about LC-UU raw data stored in ADF
data cube and ADF data package contains OpenLab CDS ChemStation
files.

-i Required. Full path to the data file that you want to export. Be
sure to include all spaces and special characters as necessary.

-o The path to the target output folder. If -o is not specified, the
ADF file is stored in ..\Users\\Documents\CSADFExport.

-l The path to the log output folder. If -l is not specified, the log
entries are written to ..\Users\\Documents\CSADFExportLogs. If the log output folder does not
exist, it is created automatically and a warning message is
displayed.

--help Displays the command line parameter help. All other parameters are
ignored, and no entry is made in the log file.
```



- 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