ADFExport for OpenLab

ADF Content Description

About This Document

This document provides detailed information on the ADF (Allotrope Data Format) file content created by Agilent's ADFExport for OpenLab revision 1.3. This includes a description of the different data sections within an ADF file: ADF data cubes, ADF data description, and the ADF data package.

This document is intended for developers to extract information from ADF files. To read out this information you need to be familiar with the Allotrope Foundation ADF API. The Allotrope Foundation ADF API SDK is available as member from the Allotrope Foundation website https://www.allotrope.org.

The ADF files created with the current ADFExport version are based on the Allotrope Framework including the following versions:

- Allotrope Data Framework (ADF) 1.5.1.0
- Allotrope Foundation Ontologies (AFO) REC/2021/03
- Allotrope Data Model (ADM) LC-UV REC/2021/04 (Results-Only data model)
- Allotrope Data Model (ADM) SFC REC/2021/04

1 ADF Data Cubes

Data cubes are universal data containers which are used to store analytical raw data. For each chromatogram and UV spectrum in the CDS data, a data cube item with one of the following labels is created (see also "ADF File: Injection vs. Sequence Context" on page 7).

- Chromatogram: adf://dc/<signal name>/<ID>
  where for OpenLab CDS and ChemStation the ID is <signal ID>, (e. g. adf://dc/DAD1A/1600062f-2e19-4f88-8795-766a2b7091b9.
- Spectrum: adf://dc/<signal name>/<ID>
  where for OpenLab CDS and ChemStation the ID is < injection ID>, (e. g. adf://dc/DAD1I/473f2829-ee12-4efe-9f83-046fb7fe60e6.

NOTE

For data cube labels of ChemStation spectra <DAD#UV> is used instead of <signal name>, where # is the DAD device number, in most cases the term used in the label is "DAD1UV".

Allowed characters for the data cube label are: 0-9, a-z, A-Z, dot, hyphen and underscore. Empty characters (for example, in the data file name) are replaced by underscores. All other characters are ignored.

Data cube label for Empower data see chapter 7.

Each data cube item is described by information stored in the ADF data description. This description contains axes (absorbance, acquisition time, wavelength) and raw data description/identifier information. For more details, refer to "ADF Data Description" on page 4.

NOTE

Instrument signals such as pump pressure or temperature are not exported to ADF data cubes, yet. They are only part of the original files stored in the ADF data package.

If blank subtraction or smoothing is applied during reprocessing the data, the transformed signals are stored instead of the raw data.

2 ADF Data Description

The data description is based on an Allotrope Foundation LC-UV (Results-Only) and SFC semantic model using the W3C standardized RDF format to store an initial set of metadata about the single run or the entire sequence as data graph. The metadata include information about the HPLC/SFC run, such as the system (HPLC/SFC instrument system, including module and column information), the submitter, the sample, the injection, and the sequence. Furthermore, information on chromatograms and UV spectra as well as acquisition and processing method names and peak results are stored.

A schematic representation of the data graph is shown in Figure 1. Depending on the data only parts of the graph can be available. For example, if data are acquired but not further processed only acquisition related parameters are stored without any information on data processing and integration including peak details.

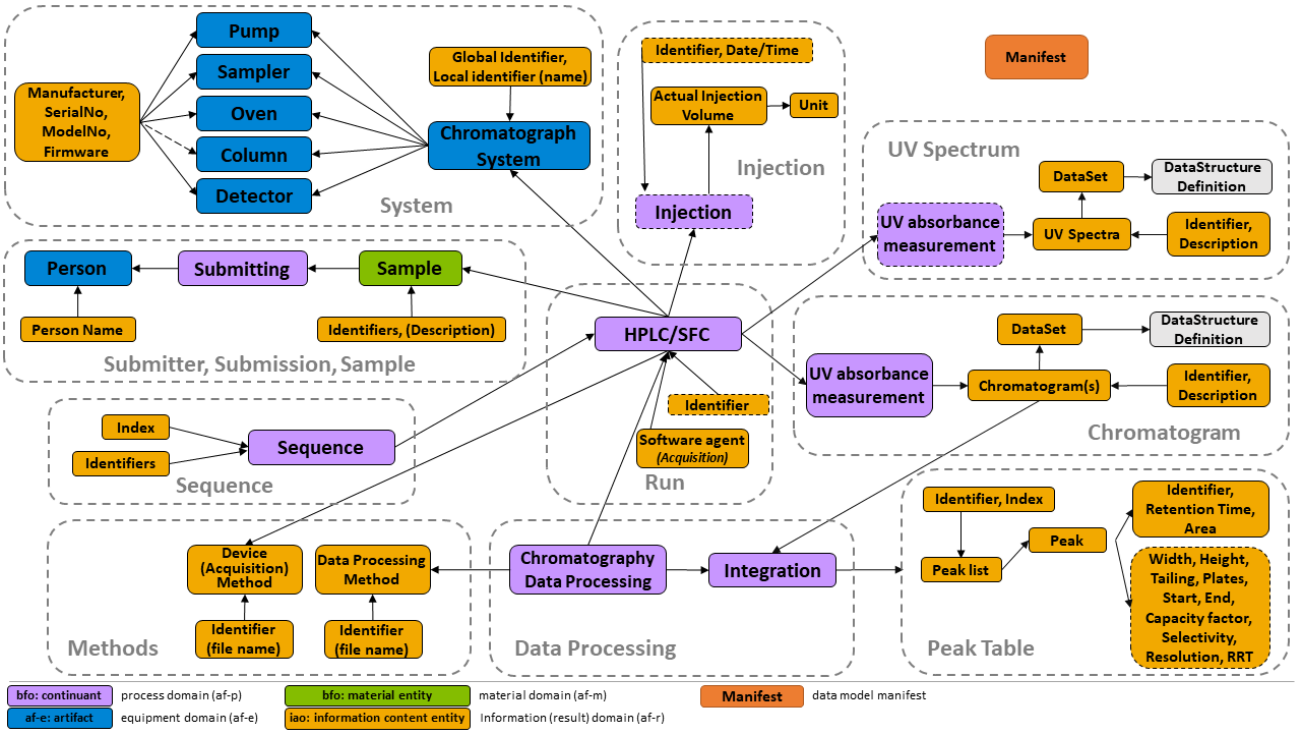

Figure 1 Schematic representation of the metadata which is available in the Data Description of a sequence ADF file.

The data cube structure for chromatograms and spectra is written into the ADF data description and linked to the respective data cube item. For more details, refer to "Data Cube Structure for Chromatograms" and "Data Cube Structure for UV Spectra" on page 5.

Water Empower data is written into the same data cube structures when converted to ADF. Waters Empower content is described in chapter 7 and 8.1.3.

A detailed list of all available parameters in the data description is documented in the "Appendix".

NOTE The data description of an ADF file contains many generated (random) IDs. Due to compression ADF files, originating from the same input data, can have different file sizes. With smaller ADF file sizes this effect becomes more and more negligible.

2.1 Data Cube Structure for Chromatograms

The LC/SFC chromatogram graph structure contains the following values and dimensions:

- Measured values (absorbance in milli absorbance units (mAU))
- Dimension (acquisition time in seconds)

A detailed description of the structure is provided in Table 2.

NOTE The chromatogram data cube structure is written once to the data description of ADF, independent of the number of chromatograms.

OpenLab CDS provides UV chromatogram rawdata time values in unit milliseconds. ADFExport converts them to the by Allotrope foundation specified time unit seconds. OpenLab ChemStation provides these values already in seconds. Therefor no conversion of the ChemStation acquisition time is required.

2.2 Data Cube Structure for UV Spectra

The UV spectra graph structure contains the following values and dimensions:

- Measured values (absorbance in milli absorbance units (mAU))
- Two dimensions (acquisition time in seconds and wavelength in nanometer)

A detailed description of the structure is provided in Figure 3.

NOTE The UV spectra data cube structure is written once to the data description of ADF, independent of the number of spectra.

OpenLab CDS provides UV spectra rawdata time values in unit milliseconds. ADFExport converts them to the by Allotrope foundation specified time unit seconds. OpenLab ChemStation provides these values already in seconds. Therefor no conversion of the ChemStation acquisition time is required.

Chromatogram Data Cube Structure Documentation

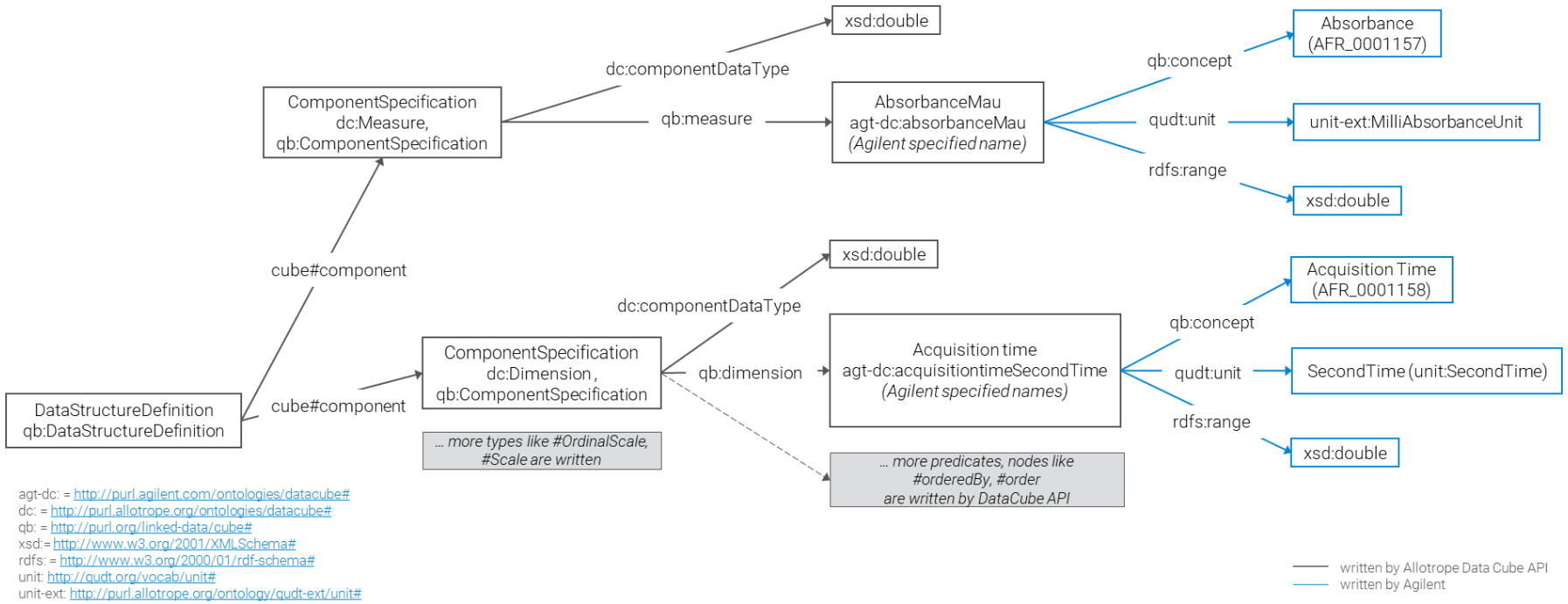

Figure 2 Chromatogram structure (absorbance / acquisition time) written into ADF data description.

UV Spectra Data Cube Structure Documentation

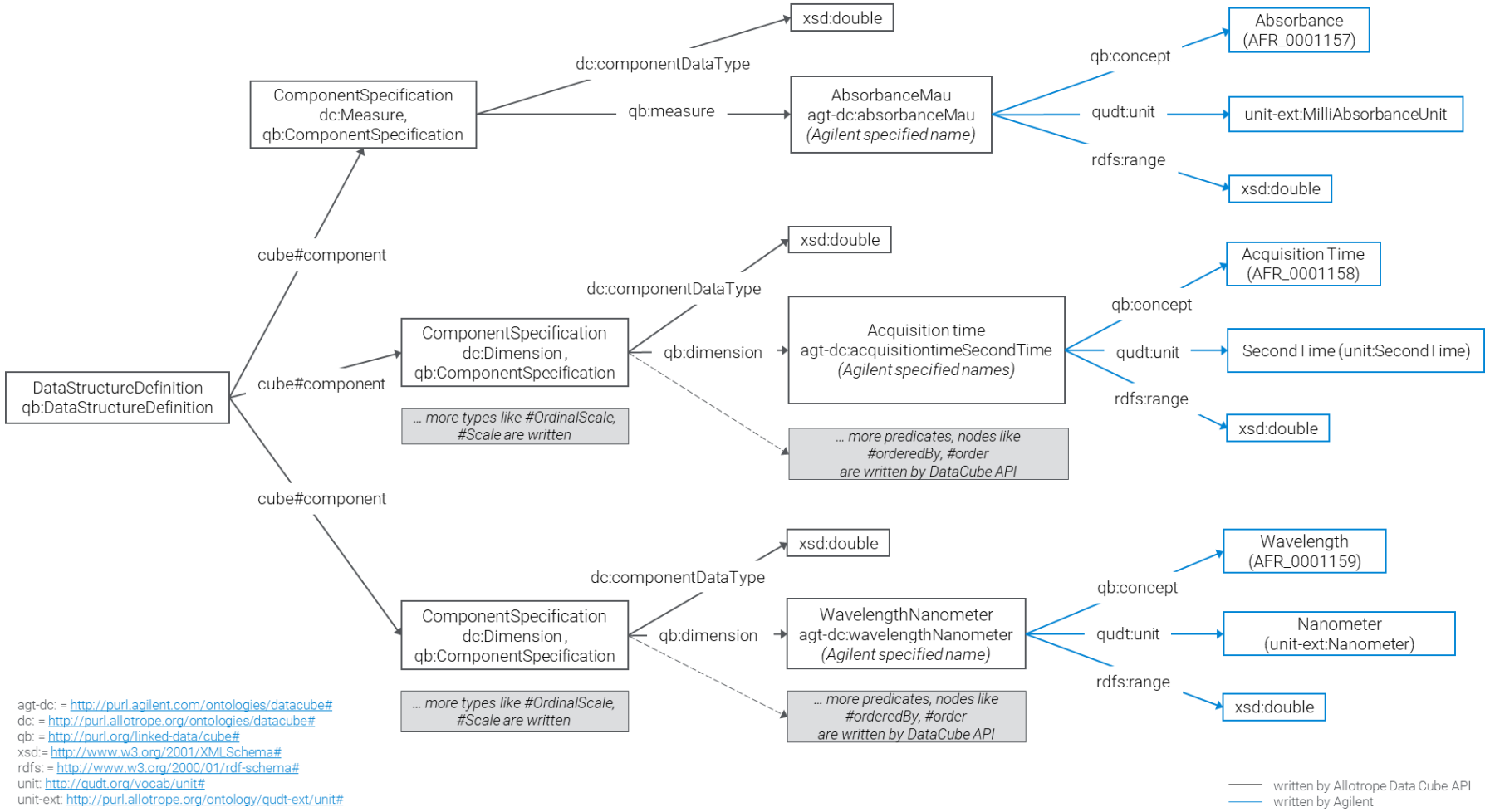

Figure 3 UV spectrum structure (absorbance / acquisition time / wavelength) written into ADF data description.

3 ADF Data Package

3.1 ChemStation

The data package contains a subfolder **ChemStation** with the original OpenLab CDS ChemStation files. For sequences, this includes the sequence folder with the .D folder of every injection, and all available files of the sequence result set folder. For single samples or sequence injections, this includes the .D folder of the current injection with all files and subfolders.

NOTE

The file content of an ADF data package created from within ChemStation using a post-run or post-sequence command compared to one created using the command-line executable (i.e. launched outside of the ChemStation with already finally persisted data) shows small differences due to the fact that in general post-run or post-sequence command is run as a second last step before ChemStation writes e.g. final activity log entries into log files. But these differences are minor and not related to rawdata or calculated results data. Following characters used for single sample or sequence result folder names are not supported: `, ^, %, #, °, ´. No ADF file is created.

3.2 OpenLab CDS

The data package contains a subfolder **OpenLab CDS** with the original CDS single sample or sequence result folder (*.sirslt or *.rslt). It includes the following files: *.dx (rawdata), *.acaml (metadata), *.amx (acquisition method), *.pmx (data processing method, if available) and *.sqx (sequence). If you export manually in Data Analysis, *.rx files are also exported.

If you export data that has been acquired with ChemStation, the original ChemStation files are exported as well.

NOTE

The *.acaml file is stored in the version of the time of export.

Following characters used for single sample or sequence result folder names will be exchanged by following % encodings:] %5D, [%5B, ^ %5E, ` %60, } %7D, { %7B,~ %7E.

3.3 OpenLab ECM Empower Scheduler Add-in provided Waters Empower data

The ADF data package for Waters Empower content is described in chapter 7.

4 ADF Audit Trail

ADF Audit Trail is a functionality provided by the Allotrope Framework and is activated at the end of ADF file generation. After activation all modifications to the ADF file are tracked and grouped into "audit records". The initial audit trail section contains minimal information about the creation of the file, such as date/time and agent (user ID) information.

NOTE To read out the ADF Audit Trail information use an Allotrope Foundation provided tool or create a *.ttl dump file of the ADF file (e.g. to get application name and version information of the tool the ADF file was created with).

5 OpenLab CDS and OpenLab ChemStation: Injection vs. Sequence based export

For OpenLab CDS and OpenLab ChemStation there are different ways to export single sample or sequence data to ADF. In a sequence injection-by-injection export only the information of a single injection is stored in an ADF file, which results in multiple ADF files for a sequence. Similar for single sample runs (for details, see "Injection Context"). In case of a sequence-based export, the whole sequence information is stored in a single ADF file (for details, see "Sequence Context").

5.1 Injection based export

An ADF file is created for the injection of a single run or for each injection of a sequence. A sequence with multiple injections exported therefore results in multiple ADF files, and no sequence context is stored in this case.

Working in a ChemStation environment, data can be exported to ADF either automatically via post-run macro within the ChemStation, or manually by running the ADFExport executable using the Windows command prompt defining a *.D folder as input path which can be a single sample folder or a sequence subfolder. For a single sample injection an ADF file with the filename *SiSa_<.D folder name>.adf* is created, where *<.D folder name>* is the name of the data file folder. For a sequence injection-by-injection export the filename is *<name of sequence result set>_<.D folder name>.adf*, where *<name of sequence result set>* is the name of the sequence folder and *<.D folder name>* is the name of the subfolder containing the data.

Using OpenLab CDS an export can be achieved via post-processing plugin either automatically at the end of data acquisition or during reprocessing in OpenLab Data Analysis. For a single sample, one ADF file with the name SiSa_<result name> is created. In case of a sequence one ADF file is created for each injection of the sequence. The files are named *<sequence name>_<injection file name>.adf*.

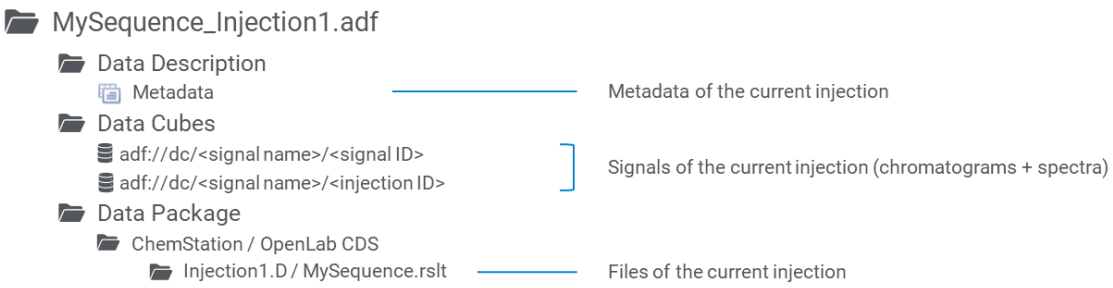

Figure 4 Exemplary data containers of an injection ADF file.

5.2 Sequence based export

The entire result set can be exported to a single ADF file. A sequence with multiple injections is exported to one ADF file, and the sequence context is kept.

Within the ChemStation environment the export can be done automatically by using a post-sequence command from the ChemStation Sequence Parameters, or manually by running the ADFExport executable using the Windows command prompt and defining a sequence folder as input path. An ADF file with the filename *<name of sequence result set>.adf* is created, where *<name of sequence result set>* is the name of the sequence folder.

Within OpenLab CDS a single sample or sequence result set (*.sirslt or *.rslt) can be exported manually to ADF in Data Analysis via the “Export ADF” button. The whole result set is stored in one single ADF file.

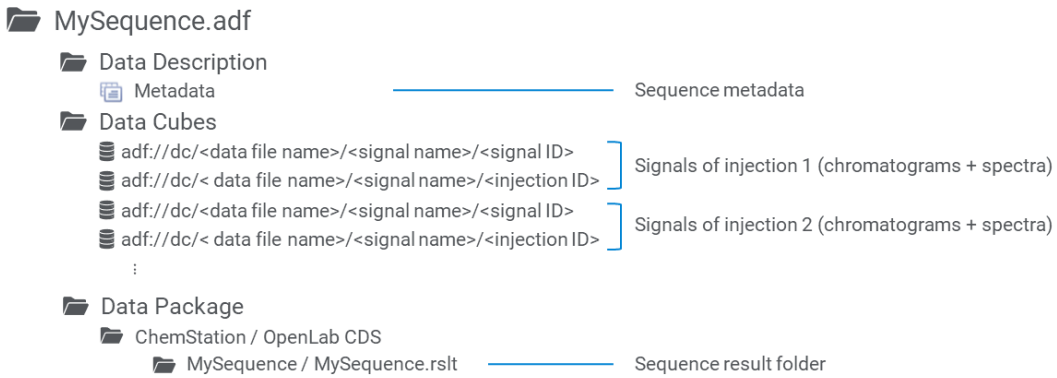

Figure 5 Exemplary data containers of a sequence ADF file.

6 Review Content of an ADF File

To browse the content of an ADF file, use the ADFexplorer or the ADFSee tool, both available from the Allotrope Foundation (https://www.allotrope.org).

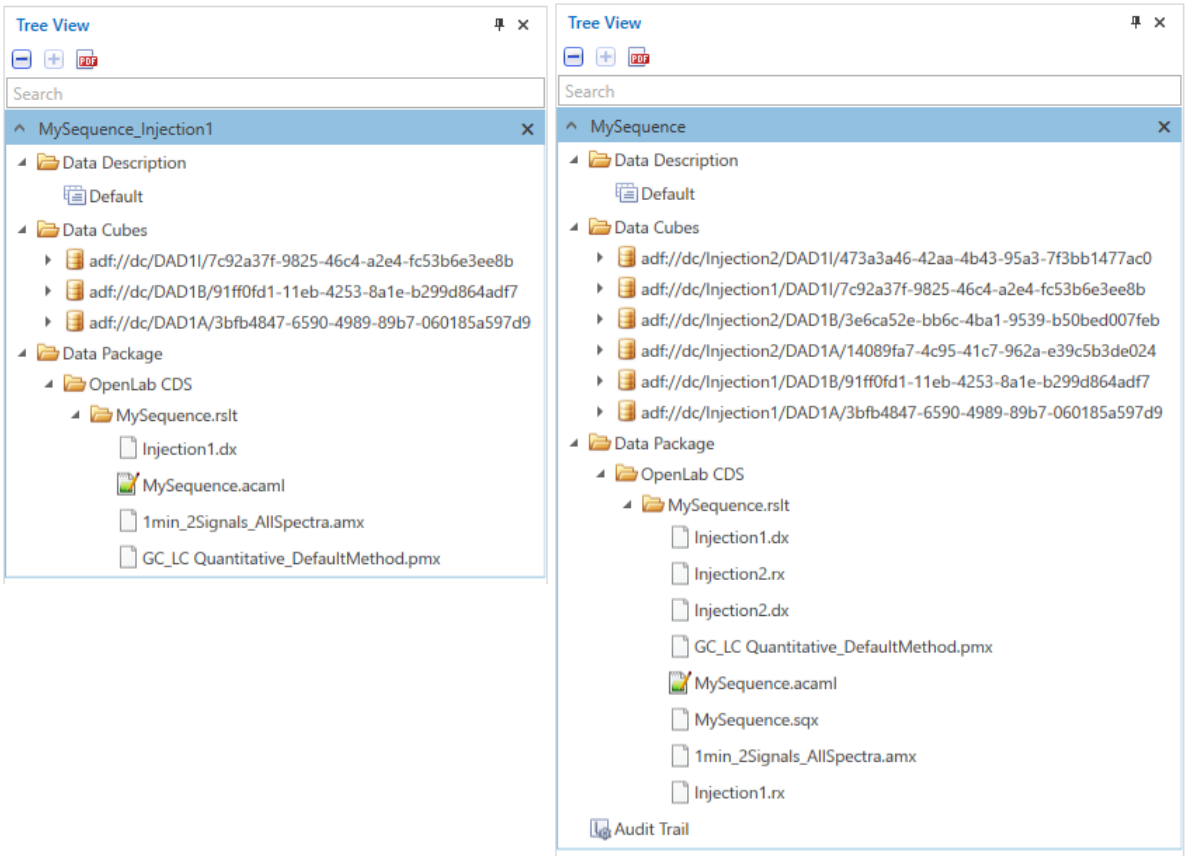

Figure 6 Tree View of ADFexplorer, showing a single injection and a sequence ADF file created with OpenLab CDS.

7 ADF file content created from Waters Empower data

OpenLab ECM Empower Scheduler Add-In provided Waters Empower data is data read by Empower Scheduler Add-In from Waters Empower systems via Waters Empower API and stored as Agilent ACAML format in an SSIzip archive in OpenLab ECM.

Supported Waters Empower data

- Sample sets
- Result sets

Not yet supported Waters Empower data

- Projects (i.e. containing multiple sample sets or result sets)
- Single injections

Basically, ADFExport exports for Waters Empower data the same information as for OpenLab CDS and OpenLab ChemStation and in the same standardized Allotrope LC-UV results-only format. But some of the information is currently not available from Waters Empower in the same granularity as for OpenLab CDS and OpenLab ChemStation:

- Agilent LC device modules: Detailed LC device module information as serial number, module number, firmware version, device type is not available. The Agilent LC is getting represented as a single HPLC instrument type w/o detailed module information.
- Waters LC device modules: Some LC device module information like device type (pump) and name (e.g. ACQ-BSM) is available, but not the serial number, module number, firmware version.

Waters Empower data acquired by following hardware can be exported:

- Agilent 11XX and 12XX LC (listed as “A1100” or as “AgilentLC”)
- Waters Acquity LC modules (listed as ACQ-XX)
  - ACQ-BSM / -QSM / -ISM (Pumps)
  - ACQ-SM / -FTN (Autosampler)
  - ACQ-PDA / -2996 / - TUV (UV detectors)
  - ACQ-CM (Oven)
  - ACQ-SO (Sample organizer)
- Other Waters LC hardware
  - W2487 / W484 / W486 / W486M1 / W487 / W490 (UV detector)
  - W2690 / W2690D / W2790 (high performance liquid chromatograph)
  - PDA / W2996 / W2996ACQ / W991M (Diode Array UV Detector)
  - PCM / W600 (Pump)
  - W710 / W712 / W715 / W717" (Autosampler)
  - TCM(Oven)
- SFC systems
  Remark: Data will be stored as HPLC runs since SFC systems cannot be identified as such with ADFExport for OpenLab rev. 1.3.

ADF Data Description

Details of ADF data description content for Waters Empower see chapter 8.1.3.

ADF Data Cube

Analogous to exported content for OpenLab CDS and OpenLab ChemStation, data cubes are stored for UV chromatograms and UV spectra if the y-axis unit is specified as (Milli-) Absorbance-Unit (mAU or AU).

Signals with other y-axis units, e.g., psi, or bar (pump pressure), °C, °F, or K (temperature), or µV, mV, or V (auxiliary trace), are not exported to ADF data cubes.

The ADF Data Cube label format for Empower data (UV chromatogram and UV spectra) has the same format as for OpenLab CDS and OpenLab ChemStation. See the definition there.

Example UV chromatogram label:

adf://dc/Injection_1290/PDA_Ch1_254nm1.2nm/eef96986-7380-4816-b3ab-d6e3cd5295e9

Example UV spectra label:

adf://dc/Injection_1290/PDA_Spectrum/f67bc217-6de3-4d5d-aee1-44ff3884c553

ADF Data Package

The created ADF data package contains a subfolder “ECM Scheduler Empower” with an identical copy of the original *.SSIzip archive.

8 Appendix

8.1 Mapping Allotrope Foundation terms to chromatography data system values

Mapping between Allotrope Foundation terms and OpenLab CDS values

Table 1 Correlation between Allotrope and OpenLab CDS parameters.

Allotrope Data Model			OpenLab CDS		
Property name	**Identifier**	**Unit**	**Name**	**Unit**	**Acaml**
Run					
Global identifier	AFR_0000918	-	Injection ID	-	<Injections><MeasData><id>
Instrument System					
Written name	IAO_0000590	-	Instrument name	-	<Instrument><Name>
Global identifier	AFR_0000918	-	Instrument ID	-	<Instrument><id>
Instrument System - Module					
Manufacturer	AFR_0001258	-	Vendor	-	<Instrument><Module><Manufacturer>
Written name	IAO_0000590	-	Name	-	<Instrument><Module><Name>
Equipment serial number	AFR_0001119	-	Serial Number	-	<Instrument><Module><SerialNo>
Model number	IAO_0000017	-	Part Number	-	<Instrument><Module><PartNo>
Firmware version	AFR_0001259	-	Firmware Revision	-	<Instrument><Module><FirmwareRevision>
Instrument System - Column					
Equipment serial number	AFR_0001119	-	Serial number	-	<SeparationMedium><Type><Column><SerialNo>
Model number	IAO_0000017	-	Product number	-	<SeparationMedium><Type><Column><ProdNo>
Written name	IAO_0000590	-	Name	-	<SeparationMedium><Name>
Manufacturer	AFR_0001258	-	-	-	-
Sample / Submitter					
Sample - written name	IAO_0000590	-	Sample name	-	<Samples><Setup><IdentParam><Name>
Description	AFR_0000922	-	Sample description	-	<Samples><Setup><IdentParam><Description>
Global identifier	AFR_0000918	-	Sample ID	-	<Samples><Setup><Id>
Submitter – written name	IAO_0000590	-	Acq. Operator	-	<Samples><Setup><Info><CreatedBy><Username>
Injection					
Global identifier	AFR_0000918		Injection ID	-	<Injections><MeasData><id>
Scalar timestamp datum	AFR_0001512		Injection Time	-	<Injections><MeasData><Info><CreatedDate>

Table 1 Correlation between Allotrope and OpenLab CDS parameters.

Allotrope Data Model			OpenLab CDS		
Property name	**Identifier**	**Unit**	**Name**	**Unit**	**Acaml**
Autosampler injection volume setting	AFR_0001267	Microliter	Injection Volume	Micro liter	<Injections><MeasData><InjectionVolume>
Sequence					
Global identifier	AFR_0000918	-	Internal parameter	-	<SampleContexts><Setup><id>
Written name	IAO_0000590	-	Sequence name	-	<SampleContexts><Setup><IdentParam><Name>
Index	AFR_0000928	-	Sequence Line	-	*(Index is defined by the acquisition order execution. First ordered by <Injection><Parent sample><OrderNumber>, then by <Injection><Replicate number>)*
Chromatogram					
Local identifier	AFR_0000919	-	Signal name	-	<Signal><Name>
Description	AFR_0000922	-	Signal description	-	<Signal><Description>
UV Spectrum					
Local identifier	AFR_0000919	-	Signal name	-	<Signal><Name>
Description	AFR_0000922	-	Signal description	-	<Signal><Description>
Acquisition Method					
Global identifier	AFR_0000918	-	Method ID	-	<Injections><MeasData><AcqParam><Method_ID>
Local identifier	AFR_0000919	-	Method name	-	<Method><BinaryData><DataItem><Name>
Processing Method					
Global identifier	AFR_0000918	-	Method ID	-	<Injections><Result><DAParam><Method_ID>
Local identifier	AFR_0000919	-	Method name	-	<Method><BinaryData><DataItem><Name>
Integration Method					
Global identifier	AFR_0000918	-	-	-	*(created and assigned by ADFExport)*
Peak Table – Peak List					
Local identifier	AFR_0000919	-	-	-	*(n/a)*
Index	AFR_0000928	-	-	-	*(set by ADFExport based on ordered peak retention time)*
Peak Table – Peak Details					
Local identifier	AFR_0000919	-	Peak ID	-	<SignalResult><Peak><id>
Retention time	AFR_0001089	Second	Retention Time	sec	<SignalResult><Peak><RetentionTime>
Peak area	AFR_0001073	Milli Absorbance Unit * Second	Peak area	mAu* sec	<SignalResult><Peak><Area>
Peak width at 5% of height	AFR_0001265	Second	Width 5%	sec	<SignalResult><Peak><Width_5Perc>
Peak width at half height	AFR_0001266	Second	Width 50%	sec	<SignalResult><Peak><Width_50Perc>
Peak width at baseline	AFR_0001264	Second	Width tangent	sec	<SignalResult><Peak><WidthTangent>
Peak height	AFR_0000948	Milli Absorbance Unit	Height	mAu	<SignalResult><Peak><Height>

Table 1 Correlation between Allotrope and OpenLab CDS parameters.

Allotrope Data Model			OpenLab CDS		
Property name	**Identifier**	**Unit**	**Name**	**Unit**	**Acaml**
Asymmetry factor measured at 5% height	AFR_0001237	-	Tailing	-	<SignalResult><Peak><TailingFactor>
Number of theoretical plates by peak width at half height	AFR_0001241	-	Plates statistical (EP, JP)	-	<SignalResult><Peak><TheoreticalPlatesEP>
Number of theoretical plates by tangent method	AFR_0001240	-	Plates statistical (USP)	-	<SignalResult><Peak><TheoreticalPlatesUSP>
Peak start time	AFR_0001178	Second	Start time	sec	<SignalResult><Peak><BeginTime>
Peak value at start	AFR_0001179	Milli Absorbance Unit	Baseline Start + Level Start	mAu	<SignalResult><Peak><BaselineStart> + <SignalResult><Peak><LevelStart>
Peak end time	AFR_0001180	Second	End time	sec	<SignalResult><Peak><EndTime>
Peak value at end	AFR_0001181	Milli Absorbance Unit	Baseline End + Level End	mAu	SignalResult><Peak><BaselineEnd> + <SignalResult><Peak><LevelEnd>
Capacity factor	AFR_0001234	-	Capacity factor	-	<SignalResult><Peak><CapacityFactor>
Peak selectivity	AFR_0001235	-	Selectivity	-	<SignalResult><Peak><Selectivity>
Relative peak height	AFR_0000949	Percent	Heigth%	%	<SignalResult><Peak><HeightPercent>
Chromatographic peak resolution using baseline peak widths	AFR_0001231	-	Resolution USP	-	<SignalResult><Peak><Resolution_USP>
Chromatographic peak resolution using peak width at half-height	AFR_0001232	-	Resolution JP, EP	-	<SignalResult><Peak><Resolution_EP>
Unadjusted relative retention time	AFR_0001175	-	RRT	-	<SignalResult><Peak><RelativeRetentionTime>
Adjusted relative retention time	AFR_0001176	-	RRT EP	-	<SignalResult><Peak><RelativeRetentionTime_EP>
Peak area (relative)	AFR_0001165	Percent	Area%	%	<SignalResult><Peak><AreaPercent>
Acquisition Software Agent					
Local identifier	AFR_0000919	-	Acquisition software	-	<Injections> <MeasData> <AcquisitionSoftware>
Manufacturer	AFR_0001258	-	Acquisiton software vendor	-	(part of <Injections> <MeasData> <AcquisitionSoftware>)
Brand name	AFR_0001680	-	Acquisition software brand name	-	<Injections> <MeasData> <AcquisitionApplication> <AgilentApp> <Name>
Software version	AFR_0001700	-	Acquisition software version	-	<Injections> <MeasData> <AcquisitionApplication> <AgilentApp> <Version>

Mapping between Allotrope Foundation terms and OpenLab ChemStation values

Table 2 Correlation between Allotrope and OpenLab ChemStation parameters.

Allotrope Data Model			ChemStation		
Property name	**Identifier**	**Unit**	**Name**	**Unit**	**Acaml**
Run					
Global identifier	AFR_0000918	-	Injection ID	-	<Injections><MeasData><id>
Instrument System					
Written name	IAO_0000590	-	Instrument name	-	<Instrument><Name>
Global identifier	AFR_0000918	-	Instrument ID	-	<Instrument><id>
Instrument System - Module					
Manufacturer	AFR_0001258	-	Vendor	-	*(set by ADFExport based on model number)*
Written name	IAO_0000590	-	Name	-	<Instrument><Module><Name>
Equipment serial number	AFR_0001119	-	Serial Number	-	<Instrument><Module><SerialNo>
Model number	IAO_0000017	-	Part Number	-	<Instrument><Module><PartNo>
Firmware version	AFR_0001259	-	Firmware Revision	-	<Instrument><Module><FirmwareRevision>
Instrument System - Column					
Equipment serial number	AFR_0001119	-	Serial number	-	<SeparationMedium><Type><Column><SerialNo>
Model number	IAO_0000017	-	Product number	-	<SeparationMedium><Type><Column><ProdNo>
Written name	IAO_0000590	-	Description	-	<SeparationMedium><Name>
Manufacturer	AFR_0001258	-	-	-	*(n/a)*
Sample / Submitter					
Sample - written name	IAO_0000590	-	Sample name	-	<SampleParams><IdentParam><Name>
Description	AFR_0000922	-	Sample description	-	<SampleParams><IdentParam><Description>
Global identifier	AFR_0000918	-	Sample ID	-	<SampleParams><IdentParam><Id>
Submitter – written name	IAO_0000590	-	Operator name	-	<Samples><MeasData><Info><CreatedBy><Username>
Injection					
Global identifier	AFR_0000918		Injection ID	-	<Injections><MeasData><id>
Scalar timestamp datum	AFR_0001512		Injection Time	-	<Injections><MeasData><Info><CreatedDate>
Autosampler injection volume setting	AFR_0001267	Microliter	Injection Volume	Microliter	<SampleParams><AcqParam><InjectionVolume>
Sequence					
Global identifier	AFR_0000918	-	Internal parameter	-	<SampleContextParams><IdentParam><id>
Written name	IAO_0000590	-	Sequence name	-	<SampleContextParams><IdentParam><Name>
Index	AFR_0000928	-	Sequence Line	-	*(Index is defined by the acquisition order execution. First ordered by <Injection><Parent*

Table 2 Correlation between Allotrope and OpenLab ChemStation parameters.

Allotrope Data Model			ChemStation		
Property name	**Identifier**	**Unit**	**Name**	**Unit**	**Acaml**
					sample><OrderNumber>, then by <Injection><Replicate number>)
Chromatogram					
Local identifier	AFR_0000919	-	Signal name	-	<Signal><Name>
Description	AFR_0000922	-	Signal description	-	<Signal><Description>
UV Spectrum					
Local identifier	AFR_0000919	-	Signal name	-	<Injections><MeasData><BinaryData><DataItem><Name>
Description	AFR_0000922	-	Signal description	-	<Injections><MeasData><BinaryData><DataItem><Name>
Acquisition Method					
Global identifier	AFR_0000918	-	Method ID	-	<InjectionParams><AcqParam><Method_ID>
Local identifier	AFR_0000919	-	Method name	-	<Method><BinaryData><DirItem><Name>
Processing Method					
Global identifier	AFR_0000918	-	Method ID	-	<InjectionParams><DAParam><Method_ID>
Local identifier	AFR_0000919	-	Method name	-	<Method><BinaryData><DirItem><Name>
Integration Method					
Global identifier	AFR_0000918	-	-	-	*(created and assigned by ADFExport)*
Peak Table – Peak List					
Local identifier	AFR_0000919	-	-	-	*(n/a)*
Index	AFR_0000928	-	-	-	*(set by ADFExport based on ordered peak retention time)*
Peak Table – Peak Details					
Local identifier	AFR_0000919	-	Peak ID	-	<SignalResult><Peak><id>
Retention time	AFR_0001089	Second	Retention Time	sec	<SignalResult><Peak><RetentionTime>
Peak area	AFR_0001073	Milli Absorbance Unit Times Second	Peak area	mAu*sec	<SignalResult><Peak><Area>
Peak width at 5% of height	AFR_0001265	Second	Width 5%	sec	<SignalResult><Peak><Width5_Perc>
Peak width at half height	AFR_0001266	Second	Width 50%	sec	<SignalResult><Peak><Width50_Perc>
Peak width at baseline	AFR_0001264	Second	Width tangent	sec	<SignalResult><Peak><WidthTangent>
Peak height	AFR_0000948	Milli Absorbance Unit	Height	mAu	<SignalResult><Peak><Height>
Asymmetry factor measured at 5% height	AFR_0001237	-	Tailing	-	<SignalResult><Peak><TailingFactor>
Number of theoretical plates by peak width at half height	AFR_0001241	-	Plates statistical (EP, JP)	-	<SignalResult><Peak><TheoreticalPlates_EP>

Table 2 Correlation between Allotrope and OpenLab ChemStation parameters.

Allotrope Data Model			ChemStation		
Property name	**Identifier**	**Unit**	**Name**	**Unit**	**Acaml**
Number of theoretical plates by tangent method	AFR_0001240	-	Plates statistical (USP)	-	<SignalResult><Peak><TheoreticalPlates_USP>
Peak start time	AFR_0001178	Second	Start time	sec	<SignalResult><Peak><BeginTime>
Peak value at start	AFR_0001179	Milli Absorbance Unit	Baseline Start + Level Start	mAu	<SignalResult><Peak><BaselineStart> + <SignalResult><Peak><LevelStart>
Peak end time	AFR_0001180	Second	End time	sec	<SignalResult><Peak><EndTime>
Peak value at end	AFR_0001181	Milli Absorbance Unit	Baseline End + Level End	mAu	<SignalResult><Peak><BaselineEnd> + <SignalResult><Peak><LevelEnd>
Capacity factor	AFR_0001234	-	Capacity factor	-	<SignalResult><Peak><CapacityFactor>
Peak selectivity	AFR_0001235	-	Selectivity	-	<SignalResult><Peak><Selectivity>
Relative peak height	AFR_0000949	Percent	Heigth%	%	<SignalResult><Peak><HeightPercent>
Chromatographic peak resolution using baseline peak widths	AFR_0001231	-	Resolution USP	-	<SignalResult><Peak><Resolution_USP>
Chromatographic peak resolution using peak width at half-height	AFR_0001232	-	Resolution JP, EP	-	<SignalResult><Peak><Resolution_EP>
Unadjusted relative retention time	AFR_0001175	-	RRT	-	<SignalResult><Peak><RelativeRetentionTime>
Adjusted relative retention time	AFR_0001176	-	RRT EP	-	<SignalResult><Peak><RelativeRetentionTime_EP>
Peak area (relative)	AFR_0001165	Percent	Area%	%	<SignalResult><Peak><AreaPercent>
Acquisition Software Agent					
Local identifier	AFR_0000919	-	Acquisition software	-	<Injections> <MeasData> <AcquisitionSoftware>
Manufacturer	AFR_0001258	-	Acquisition software vendor	-	(part of <Injections> <MeasData> <AcquisitionSoftware>)
Brand name	AFR_0001680	-	Acquisition software brand name	-	(part of <Injections> <MeasData> <AcquisitionSoftware>)
Software version	AFR_0001700	-	Acquisition software version	-	(part of <Injections> <MeasData> <AcquisitionSoftware>)

Mapping between Allotrope Foundation terms and Waters Empower values

Table 3 Correlation between Allotrope and Waters Empower parameters.

Allotrope Data Model			Waters Empower		
Property name	**Identifier**	**Unit**	**Name**	**Unit**	**Acaml / (in brackets related Waters Empower field)**
Run					
Global identifier	AFR_0000918	-	Injection ID	-	<Injections><MeasData><id> / *(n/a)*
Instrument System					
Written name	IAO_0000590	-	Instrument name	-	<Instrument><Name> / (IInjection.SystemName)
Global identifier	AFR_0000918	-	Instrument ID	-	<Instrument><id> / *(n/a)*
Instrument System - Module					
Manufacturer	AFR_0001258	-	Vendor	-	- / *(part of InstSetupClass.Type)*
Written name	IAO_0000590	-	Name	-	<Instrument><Module><Name> / (InstSetup.Name)
Equipment serial number	AFR_0001119	-	Serial Number	-	- / *(n/a)*
Model number	IAO_0000017	-	Part Number	-	- / *(part of InstSetupClass.Type)*
Firmware version	AFR_0001259	-	Firmware Revision	-	- / *(n/a)*
System - Column					
Equipment serial number	AFR_0001119	-	Serial number	-	<SeparationMedium><Type><Column><SerialNo> / (IInjection.ColumnSerialNumber)
Model number	IAO_0000017	-	Product number	-	- / *(n/a)*
Written name	IAO_0000590	-	Description	-	<SeparationMedium><Name> / (IInjection.ColumnName)
Manufacturer	AFR_0001258	-	-	-	- / *(n/a)*
Sample / Submitter					
Sample - written name	IAO_0000590	-	Sample name	-	<SampleParams><IdentParam><Name> / (IInjection.SampleName + IInjection.Vial)
Description	AFR_0000922	-	Sample description	-	<SampleParams><IdentParam><Description> / (IInjection.Comments)
Global identifier	AFR_0000918	-	Sample ID	-	<Samples><Setup><Id>/ *(n/a)*
Submitter – written name	IAO_0000590	-	Operator name	-	<Injections><MeasData><Info><CreatedBy><Username> / (IIInjection.Acquired By)
Injection					
Global identifier	AFR_0000918		Injection ID	-	<Injections><MeasData><id> / *(n/a)*
Scalar timestamp datum	AFR_0001512		Injection Time	-	<Injections><MeasData><Info><CreatedDate> / (IInjection.Date Acquired)
Autosampler injection volume setting	AFR_0001267	Microliter	Injection Volume	microliter	<Injections><MeasData><ActualInjVolume> / (IInjection.Injection Volume)
Sequence					
Global identifier	AFR_0000918	-	Internal parameter	-	<SampleContexts><Setup><id> / *(n/a)*
Written name	IAO_0000590	-	Sequence name	-	<SampleContextParams><IdentParam><Name> / (SampleSet Name)

Table 3 Correlation between Allotrope and Waters Empower parameters.

Allotrope Data Model			Waters Empower		
Property name	**Identifier**	**Unit**	**Name**	**Unit**	**Acaml / (in brackets related Waters Empower field)**
Index	AFR_0000928	-	Sequence Line	-	*(Index is defined by the acquisition order execution. First ordered by <Injection><Parent sample><OrderNumber>, then by <Injection><Replicate number>)*
Chromatogram					
Local identifier	AFR_0000919	-	Signal name	-	<Signal><Name> / (Channel.Channel)
Description	AFR_0000922	-	Signal description	-	<Signal><Description>/ (Channel.ChannelDescription)
UV Spectrum					
Local identifier	AFR_0000919	-	Signal name	-	<Signal><Name> / (Channel.ChannelName)
Description	AFR_0000922	-	Signal description	-	<Signal><Description> / (Channel.ProcessedChanDesc)
Acquisition Method					
Global identifier	AFR_0000918	-	Method ID	-	<InjectionParams><AcqParam><Method_ID> / *(n/a)*
Local identifier	AFR_0000919	-	Method name	-	<Method><name> (of <InjectionParams><AcqParam><Method_ID>) / (Injection - Acquisition Method Set→Method.Name)
Processing Method					
Global identifier	AFR_0000918	-	Method ID	-	<InjectionParams><DAParam><Method_ID> / *(n/a)*
Local identifier	AFR_0000919	-	Method name	-	<Method><name> (of <InjectionParams><DAParam><Method_ID>) / (Result.Processing Method)
Integration Method					
Global identifier	AFR_0000918	-	-	-	*(created and assigned by ADFExport)*
Peak Table – Peak List					
Local identifier	AFR_0000919	-	-	-	*(n/a)*
Index	AFR_0000928	-	-	-	*(set by ADFExport based on ordered peak retention time)*
Peak Table – Peak Details					
Local identifier	AFR_0000919	-	Peak ID	-	<SignalResult><Peak><id> / *(n/a)*
Retention time	AFR_0001089	Second	Retention Time	sec	<SignalResult><Peak><RetentionTime> / (IPeak. RetentionTime)
Peak area	AFR_0001073	Milli Absorbance Unit Times Second	Peak area	mAu*sec	<SignalResult><Peak><Area> / (IPeak.Area)
Peak width at 5% of height	AFR_0001265	Second	Width 5%	sec	<SignalResult><Peak><Width5_Perc> / (IPeak.WidthAt5Pct)
Peak width at half height	AFR_0001266	Second	Width 50%	sec	<SignalResult><Peak><Width50_Perc> / (IPeak. WidthAt50Pct)
Peak width at baseline	AFR_0001264	Second	Width tangent	sec	<SignalResult><Peak><WidthTangent> / (IPeak. WidthAtTangent)
Peak height	AFR_0000948	Milli Absorbance Unit	Height	mAu	<SignalResult><Peak><Height> / (IPeak.Height)
Asymmetry factor measured at 5% height	AFR_0001237	-	Tailing	-	<SignalResult><Peak><TailingFactor> / (IPeak. USPTailing)

Table 3 Correlation between Allotrope and Waters Empower parameters.

Allotrope Data Model			Waters Empower		
Property name	**Identifier**	**Unit**	**Name**	**Unit**	**Acaml / (in brackets related Waters Empower field)**
Number of theoretical plates by peak width at half height	AFR_0001241	-	Plates statistical (EP, JP)	-	<SignalResult><Peak><TheoreticalPlates_EP> / (IPeak.EPPlateCount / IPeak.JPPlateCount [same as EP])
Number of theoretical plates by tangent method	AFR_0001240	-	Plates statistical (USP)	-	<SignalResult><Peak><TheoreticalPlates_USP> / (IPeak. USPPlateCount)
Peak start time	AFR_0001178	Second	Start time	sec	<SignalResult><Peak><BeginTime> / (IPeak. Start Time)
Peak value at start	AFR_0001179	Milli Absorbance Unit	Baseline Start + Level Start	mAu	*<SignalResult><Peak><BaselineStart> + <SignalResult><Peak><LevelStart> / (not written by now)*
Peak end time	AFR_0001180	Second	End time	sec	<SignalResult><Peak><EndTime> / (IPeak.End Time)
Peak value at end	AFR_0001181	Milli Absorbance Unit	Baseline End + Level End	mAu	*SignalResult><Peak><BaselineEnd> + <SignalResult><Peak><LevelEnd> / (not written by now)*
Capacity factor	AFR_0001234	-	Capacity factor	-	<SignalResult><Peak><CapacityFactor> / (IPeak.K Prime)
Peak selectivity	AFR_0001235	-	Selectivity	-	<SignalResult><Peak><Selectivity> / (IPeak.Selectivity)
Relative peak height	AFR_0000949	Percent	Heigth%	%	<SignalResult><Peak><HeightPercent> / (IPeak.PctHeight)
Chromatographic peak resolution using baseline peak widths	AFR_0001231	-	Resolution USP	-	<SignalResult><Peak><Resolution_USP> / (IPeak.USPResolution)
Chromatographic peak resolution using peak width at half-height	AFR_0001232	-	Resolution JP, EP	-	<SignalResult><Peak><Resolution_EP> / (IPeak.Resolution)
Unadjusted relative retention time	AFR_0001175	-	RRT	-	(n/a)
Adjusted relative retention time	AFR_0001176	-	RRT EP	-	(n/a)
Peak area (relative)	AFR_0001165	Percent	Area%	%	<SignalResult><Peak><AreaPercent> / (IPeak.PctArea)
Acquisition Software Agent					
Local identifier	AFR_0000919	-	Acq SW Version	-	<Injections> <MeasData> <AcquisitionSoftware> or "Waters Empower" if the entry is missing / (Channel.AcqSWVersion)
Manufacturer	AFR_0001258	-	Acq SW manufacturer	-	(part of <Injections> <MeasData> <AcquisitionSoftware> or “Waters” if entry is missing) / (n/a)

Brand name	AFR_0001680	-	Acq SW brand name	-	(part of <Injections> <MeasData> <AcquisitionSoftware> or <Doc> <DocInfo> <CreatedByApplication> <CommonApp> <Name> "Agilent ECM Empower Scheduler Add-In") / (n/a)
Software version	AFR_0001700	-	Acq SW Version	-	(part of <Injections> <MeasData> <AcquisitionSoftware> or empty if entry is missing / (Channel.AcqSWVersion)

8.2 ADFExport content history

ADFExport 1.3 vs. ADFExport 1.2

New content:

- Added manifests:
- LC-UV results only: http://purl.allotrope.org/manifests/lc-uv/REC/2021/04/lc-uv-results-only.manifest
- SFC: http://purl.allotrope.org/manifests/sfc/REC/2021/04/sfc.manifest
- Added "acquisition software agent" information linked to "HPLC / SFC Run"
- Added supercritical-fluid chromatography support: "SFC system" (AFE_0002223) and "supercritical-fluid chromatography" (AFP_0000253)

Units:

- For all Data Cube time axis values and peak detail values the time unit is now "seconds" (could be milliseconds, seconds and minute before).
  Reason: Allotrope foundation specified to use in chromatography data models from Dec 2020 onwards, to always use "seconds".
- Injection volume changed Unit from QudtUnit.CubicMillimeter to QudtExt.Microliter (Remark: CubicMillimeter equals Microliter).
  Reason: Allotrope foundation specified to use the new unit term.

Instrument System:

- "LC System" (AFE_0002197) instead of "high-performance liquid chromatograph" (AFE_0000224).
  Reason: Allotrope corrected term class inconsistency. Backward breaking change.

Chromatograms:

- Subclass "electromagnetic radiation chromatogram" (AFR_0000308) instead of parent class: "chromatogram" (AFR_0000236).
  Reason: Use a more precise term of same class family.

Methods:

- Acquisition method. Subclass "device method" (AFR_0001556) instead of parent class: "plan specification" (AFR_0001501). Reason: Use a more precise term is same class family.
- Data processing method. Subclass "data processing method" (AFR_0002175) instead of parent class: "plan specification" (AFR_0001501).
  Reason: Use a more precise term is same class family.

www.agilent.com

Edition 09/2021

Document No: D0005429

Agilent