



Turn Data into Corporate Assets.

Make Data Available for Reuse.

Secure Compliance and Data Integrity.

ZONTAL Allotrope Fall – Dr. Christof Gaenzler - Nov-20-2024

From Electronic Document to Executable Method: USP's Journey to Digitalizing the USP NF



THE LIFE SCIENCE DATA PLATFORM

AGENDA

DIGITAL LABORATORY

DATA PRESERVATION

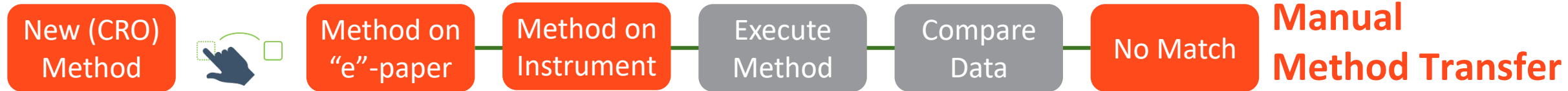
LIFE SCIENCE ANALYTICS

- ZONTAL Methods Hub
- Cross Platform Chromatography Method Integration
- ZONTAL Chromatography Solution
- USP NF

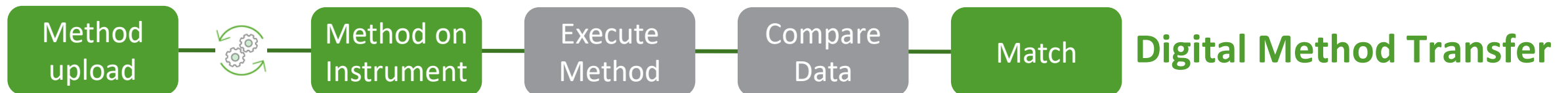
Securing Digital Sustainability

Value Prop: Methods Hub

Problem Statement: What happens when you cannot replicate a method?



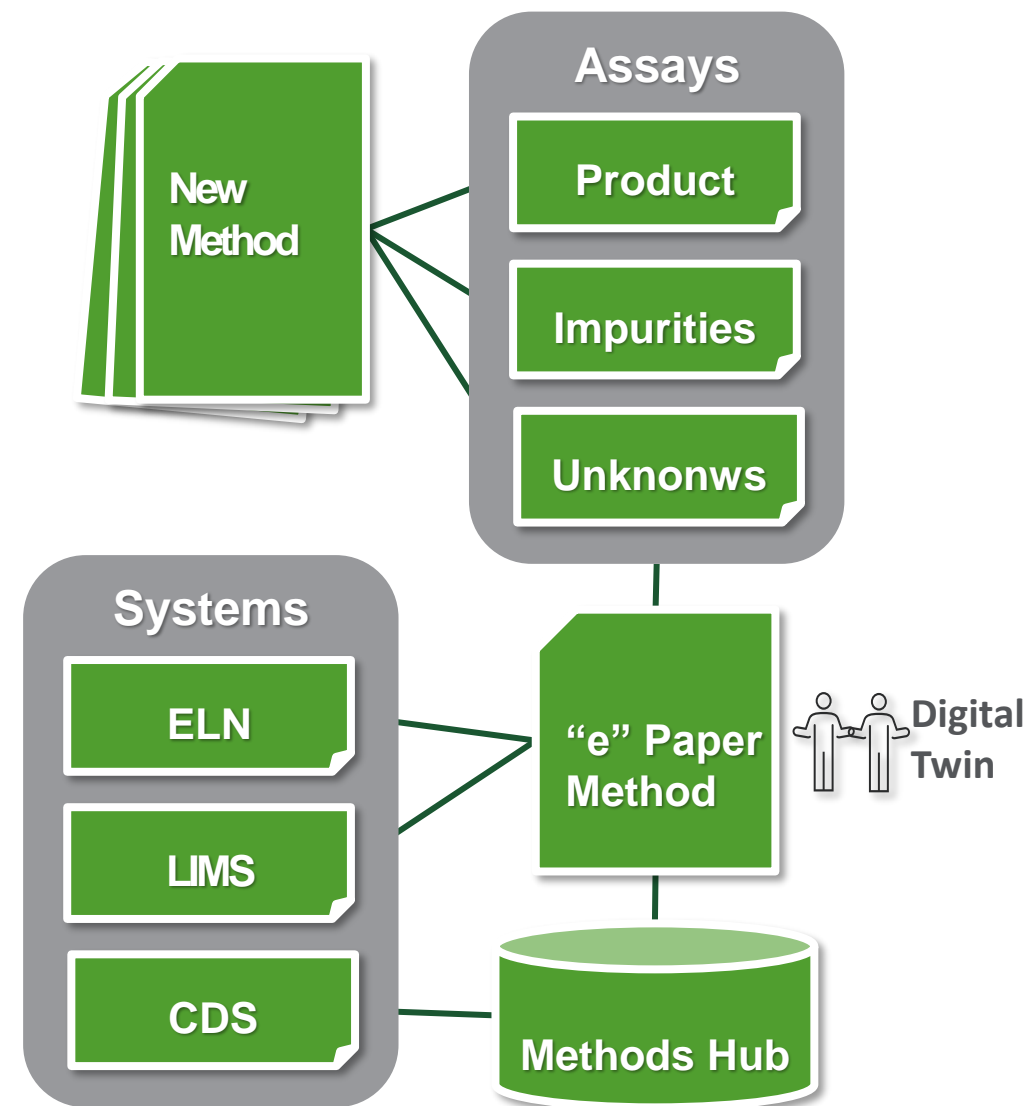
- Method by sharing electronic protocols, procedure manuals, and articles etc.
- Methods are interpreted and placed internal documentation
- Instrument specific methods are created on the individual CDS
- New method from CRO does NOT show same results → cumbersome root cause analysis
- Difference in “hidden” settings between instruments
- Digital method includes all settings



Value Prop: Methods Hub

ROI and Soft Benefits

- Methods Hub accounts for differences in the instruments (“hidden settings”)
- Improves Instrument Method Transfer
 - Reduction / Elimination of
 - Manual setting of CDS parameters
 - Human error
 - Resolution of failures
 - Reduction of
 - Documentation effort
 - Validation effort
 - Automation of parameter “translation” across different instrument types



Methods Hub properties mapped to AFO*

20

Addendum Methods Hub properties mapped to AFO

Auto Sampler

| | | |
|---|---------------------|--|
| http://purl.allotrope.org/ontologies/result-AFR_0001815 | Duration (stoptime) | duration setting A duration setting is a setting that specifies the duration of a planned process or when a situation should trigger. [Allotrope] |
| http://purl.allotrope.org/ontologies/result-AFR_0000941 | Injection section | action specification synonyms: 2017-05-03 remove subclass of event [OSTHUS], command, instruction |

21

Addendum Methods Hub properties mapped to AFO

Pump (1/2)

| | | |
|---|---------------------|---|
| http://purl.allotrope.org/ontologies/result#AFR_0001815 | Duration (stoptime) | duration setting A duration setting is a setting that specifies the duration of a planned process or when a situation should trigger. [Allotrope] |
| http://purl.allotrope.org/ontologies/equipment#AFP_0001850 | Piston target | piston A piston is a component of reciprocating engines, reciprocating pumps, gas compressors and pneumatic cylinders, among other similar mechanisms. It is the moving component that is contained by a cylinder and is made gas-tight by piston rings. [Wikipedia] |

22

Addendum Methods Hub properties mapped to AFO

Pump (2/2)

| | | |
|---|------------------------------------|--|
| http://purl.allotrope.org/ontologies/result#AFR_0000941 | Section for various configurations | action specification synonyms: 2017-05-03 remove subclass of event [OSTHUS], command, instruction A directive information entity that describes an action the bearer will take. [IAO] |
| http://purl.allotrope.org/ontologies/result#AFR_0000945 | Timetable with members | linear procedure specificationsynonyms: linear procedure specification, event table, sequence specification A procedure specification with a linear ordered collection of action specifications. [Allotrope] |
| http://purl.allotrope.org/ontologies/result#AFR_0002033 | Timetable index | temporal index A temporal index is an index that follows temporal order of the list items or the processes that the items are about. [Allotrope] |
| http://purl.allotrope.org/ontologies/process#AFP_0003289 | Timetable specification | mobile phase delivery Mobile phase delivery is a process performed by a liquid chromatography system in which the solvent of the liquid phase are mixed and transported through the instrument for separation and detection. [Allotrope] |
| http://purl.allotrope.org/ontologies/process#AFP_0001135 | Mixing information | mixing synonyms: mixing material The combining of components, particles or layers into a more homogeneous state. The mixing may be achieved manually or mechanically by shifting the material with stirrers or pumps or by revolving or shaking the container. The process must not permit segregation of particles of different size or properties. Homogeneity may be considered to have been achieved in a practical sense when the sampling error of the processed portion is negligible compared to the total error of the measurement system. [CHMO] |
| http://purl.allotrope.org/ontologies/material#AFM_0000403 | Solvent target | liquid A liquid is a nearly incompressible fluid that conforms to the shape of its container but retains a (nearly) constant volume independent of pressure. [Wikipedia] |

23

Addendum Methods Hub properties mapped to AFO

Column Compartment

| | | |
|---|-------------------------------|--|
| http://purl.allotrope.org/ontologies/result#AFR_0001815 | Duration (stoptime) | duration setting A duration setting is a setting that specifies the duration of a planned process or when a situation should trigger. [Allotrope] |
| http://purl.allotrope.org/ontologies/result#AFR_0001805 | Mode setting (chromatography) | test mode setting (chromatography) synonyms: test mode The test mode determines the measurements collected during the device execution, e.g. Injection Time only or Dispense Volume and Injection Time). [Allotrope] |

24

Addendum Methods Hub properties mapped to AFO

PDA/DAD detector (1/2)

| | | |
|---|--------------------------------|--|
| http://purl.allotrope.org/ontologies/result#AFR_0001815 | Duration (stoptime) | duration setting A duration setting is a setting that specifies the duration of a planned process or when a situation should trigger. [Allotrope] |
| http://purl.allotrope.org/ontologies/result#AFR_0001250 | Detector sampling rate (Hertz) | detector sampling rate setting synonyms: acquisition rate, detection sampling rate, sampling frequency, sampling rate, detector rate setting, sampling rate setting A detector setting parameter that specifies the rate at which the detector changes its |

*List with PURLs in addendum

Methods in Allotrope Format

LC-UV Method

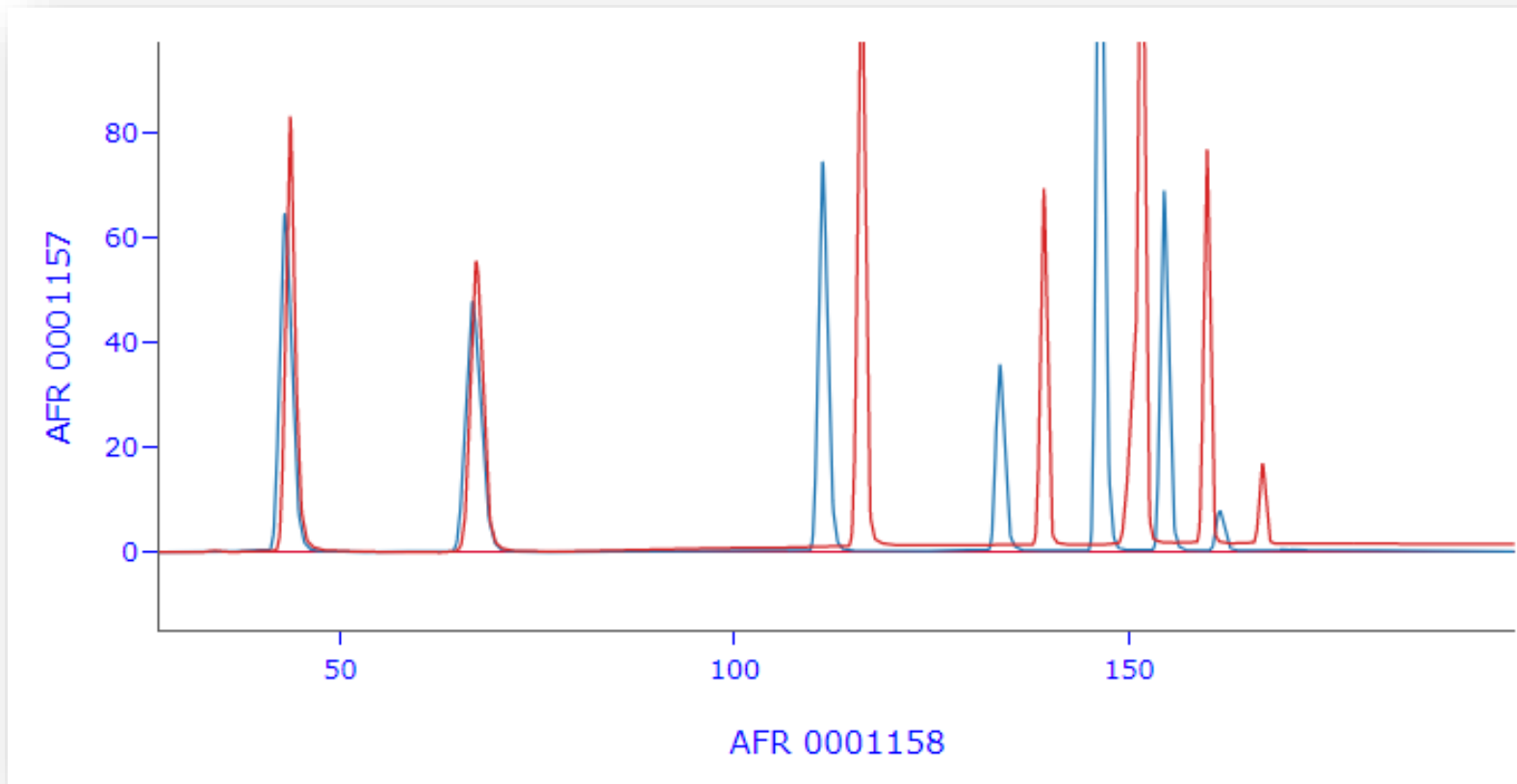
- Impact of Allotrope Format
 - Standardized across all instruments and vendors
 - Drivers for each current and future instrument have identical source
- Initially ADF now ASM
 - Standardized method descriptions of a Liquid Chromatography - Ultraviolet detection experiment to allow a unified method import and export across different instruments
 - Only Pros and No Cons of representing chromatographic methods in ASM vs ADF
 - ASM can hold all parameters and is linked to AFO
 - Lowers barrier to integrate
 - Human readable format is easy to access and verify



Cross Platform Chromatography Method Integration

Pistoia – Methods Hub (1/3)

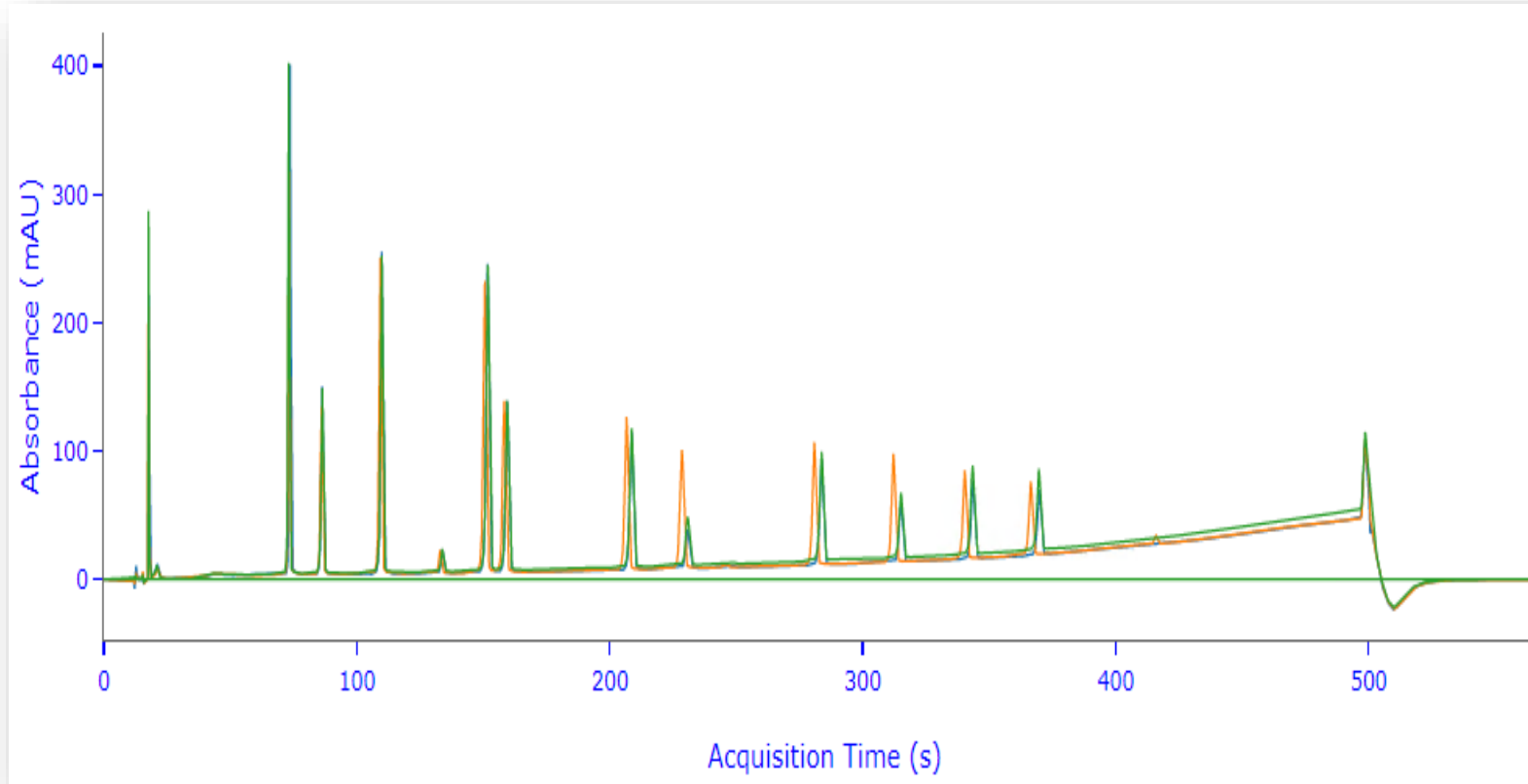
Transferring Empower Method from MERCK to ZONTAL to GSK



Method's transfer on Agilent 1290

Pistoia – Methods Hub (2/3)

Transferring Method From OpenLab to ZONTAL to Empower



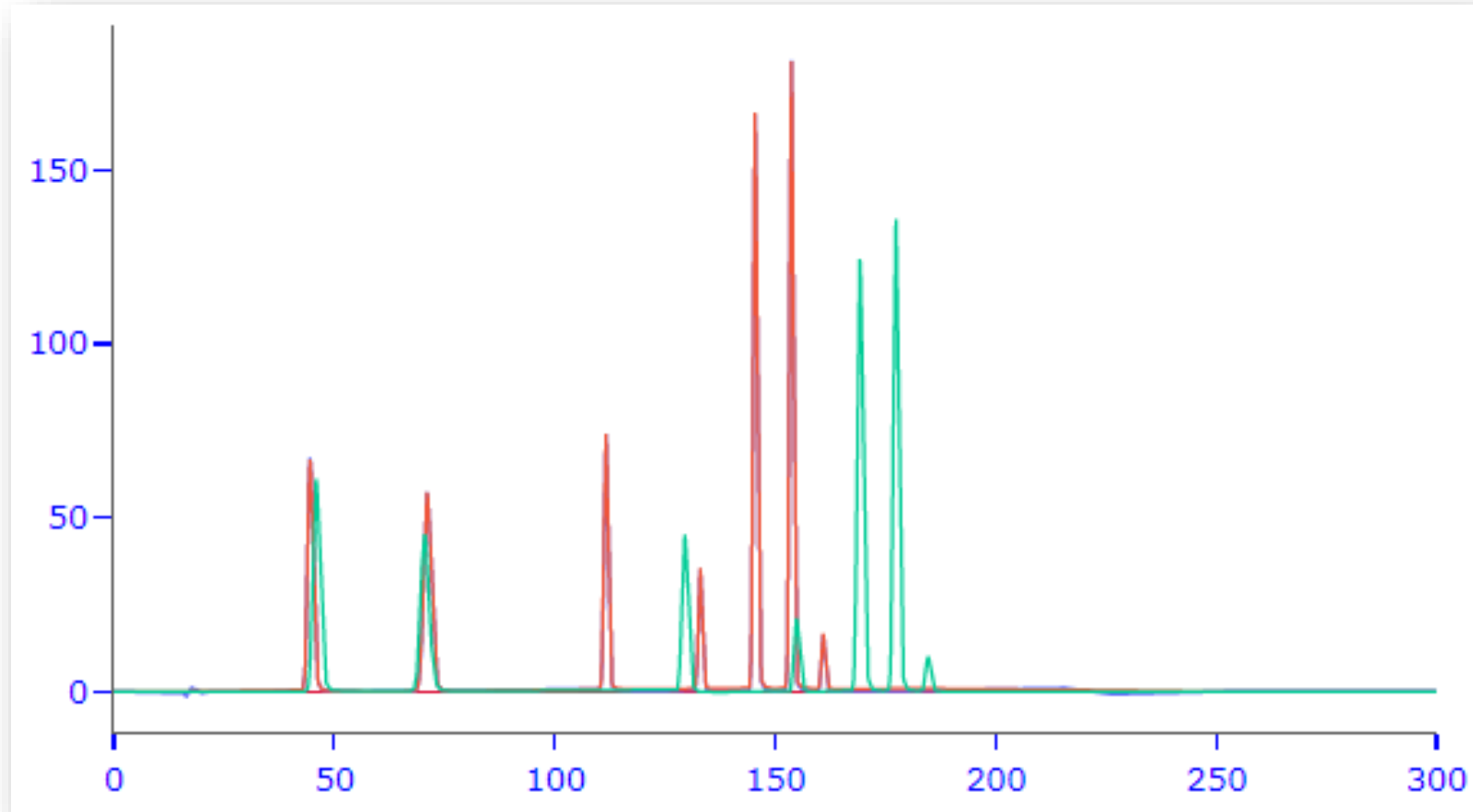
— Agilent

— Waters™

Expected slight difference in peak height and retention time due to different lots of standards and mobile phases.

Pistoia – Methods Hub (3/3)

Transfer Methods between Different Control Software, Instruments, and Companies



Dwell Volume = 137 μ l



Dwell Volume = 357 μ l



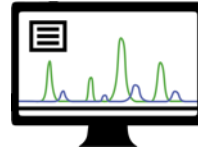
ZONTAL Chromatography Solution

ZONTAL Chromatography Solution

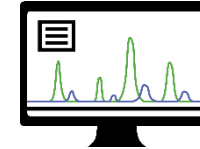
Cross Platform Chromatography Data Management



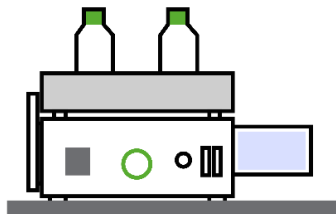
Method Viewer



Overlay Viewer



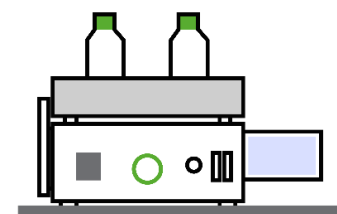
Result Viewer



Openlab

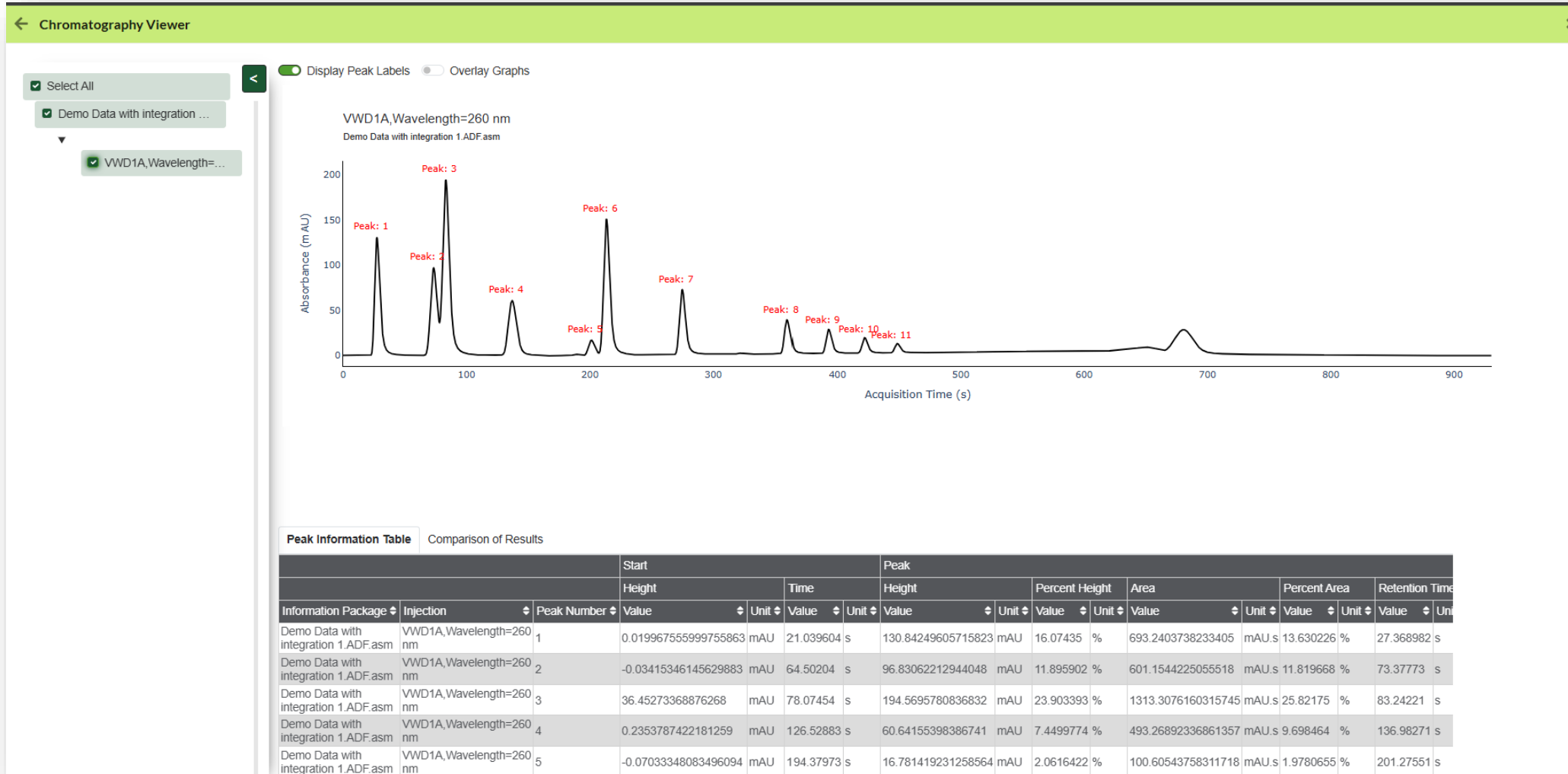


Empower



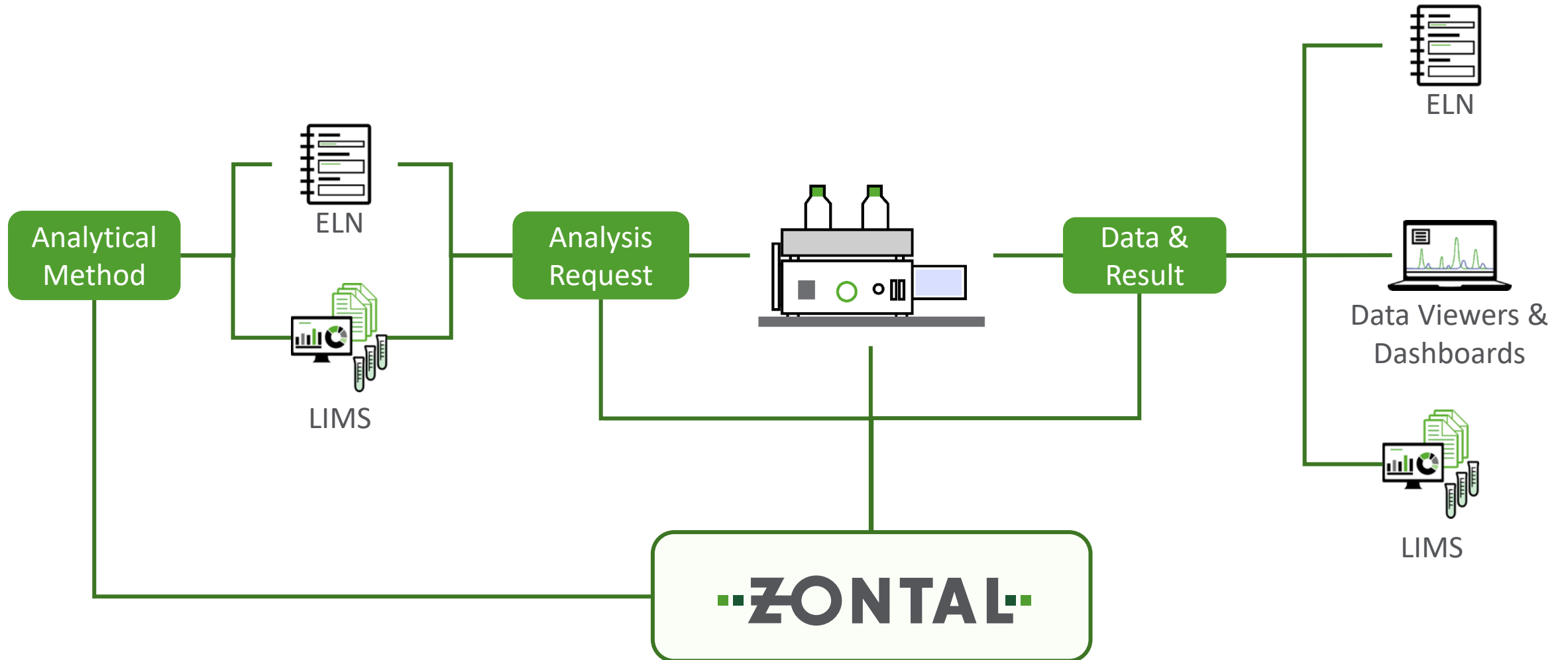
Chromeleon

ZONTAL Platform Data Viewer for Chromatography



Chromatography Workflow

Eliminates Issues in Instrument Method Transfer



ZONTAL Chromatography Solution

Methods Storage & Transfer

Z ← LC-UV Viewer ✕

Q Instrument Method

| | | | |
|-------------|----------------------|--------------|------|
| Autosampler | Diode Array Detector | Liquid, Pump | Oven |
| Autosampler | Diode Array Detector | Liquid, Pump | Oven |

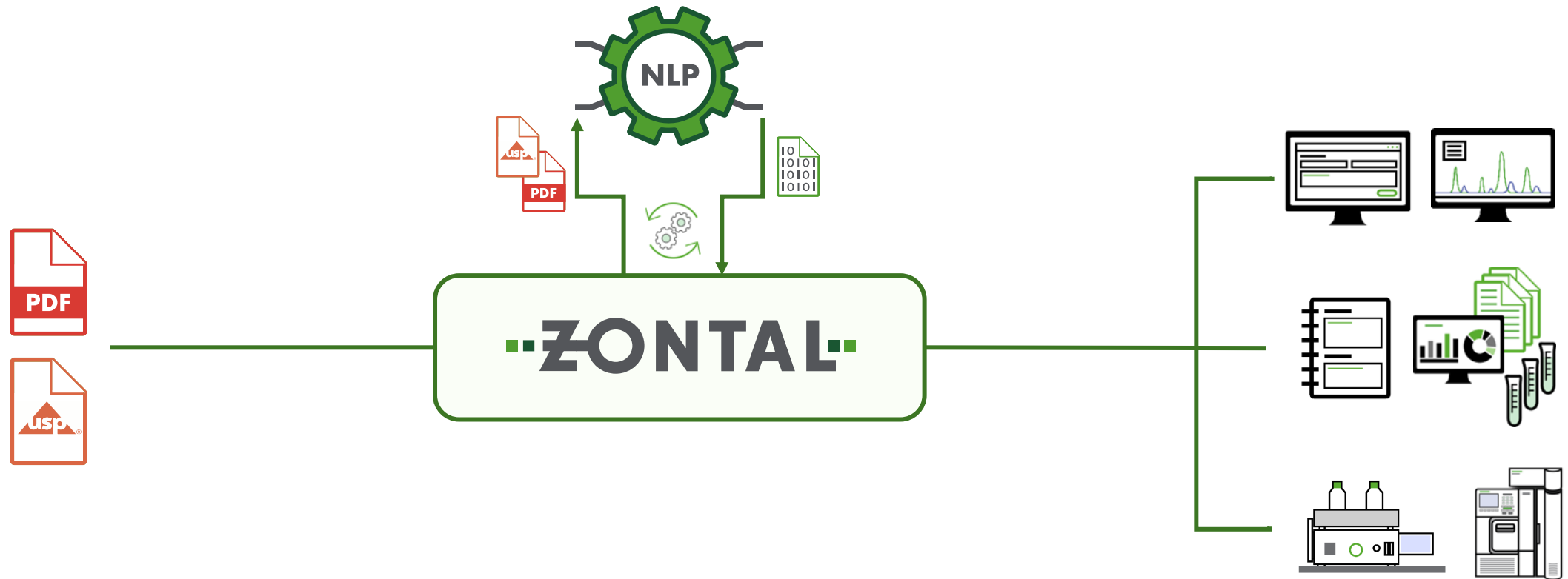
☁ Difference Viewer (6/75)

| | | | |
|-------------------|-----------------------------|----------------------------|------------|
| Autosampler (2/5) | Diode Array Detector (0/20) | Liquid, Pump (4/43) | Oven (0/7) |
|-------------------|-----------------------------|----------------------------|------------|

| | |
|--|---|
| Compressibilityfactor: 75.0 DimensionlessMicroPerBar | Compressibilityfactor: 50.0 DimensionlessMicroPerBar |
| Solvent Channel: B | Solvent Channel: A |
| Compressibilityfactor: 45.0 DimensionlessMicroPerBar | Compressibilityfactor: 100.0 DimensionlessMicroPerBar |
| Solvent Channel: A | Solvent Channel: B |

Digitalization of Analytical Methods

Eliminates Issues in Manual Transcription of Analytical Methods & Monographs



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Addendum Methods Hub properties mapped to AFO

| Auto Sampler | | |
|---|-------------------------------------|---|
| http://purl.allotrope.org/ontologies/result - AFR_0001815 | Duration (stoptime) | duration setting A duration setting is a setting that specifies the duration of a planned process or when a situation should trigger. [Allotrope] |
| http://purl.allotrope.org/ontologies/result - AFR_0000941 | Injection section | action specification synonyms: 2017-05-03 remove subclass of event [OSTHUS], command, instruction A directive information entity that describes an action the bearer will take. [IAO] |
| http://purl.allotrope.org/ontologies/result - AFR_0001556 | Device method | device method synonyms: instrument method A device method is a plan specification that specifies how some process is to be executed on a device. [Allotrope] |
| http://purl.allotrope.org/ontologies/process - AFP_0001611 | Injection | injection synonyms: injection, sample introduction |
| http://purl.allotrope.org/ontologies/process - AFP_0002833 | Temperature control | temperature control A temperature control is a controlling process that controls the temperature of some material. [Allotrope] |
| http://purl.allotrope.org/ontologies/result#AFR_0001255 | Column Temperature (Degree Celsius) | temperature setting synonyms: temperature parameter A temperature setting is a setting that specifies some temperature. |

Addendum Methods Hub properties mapped to AFO

Pump (1/2)

| | | |
|---|---|---|
| http://purl.allotrope.org/ontologies/result#AFR_0001815 | Duration (stoptime) | duration setting A duration setting is a setting that specifies the duration of a planned process or when a situation should trigger. [Allotrope] |
| http://purl.allotrope.org/ontologies/equipment#AFE_0001850 | Piston target | piston A piston is a component of reciprocating engines, reciprocating pumps, gas compressors and pneumatic cylinders, among other similar mechanisms. It is the moving component that is contained by a cylinder and is made gas-tight by piston rings. [Wikipedia] |
| http://purl.allotrope.org/ontologies/result#AFR_0001660 | Flow rate (Milliliter per minute) | flow rate setting A flow rate setting is a setting that specifies some flow rate configuration. [Allotrope] |
| http://purl.allotrope.org/ontologies/result#AFR_0001548 | Maximum flow ramp (Milliliter per minute squared) | maximum flow rate change setting synonyms: maximum flow gradient, pump maximum flow rate change setting Maximum flow rate change setting is a control setting that sets the maximum rate at which the pump is allowed to change the % of solvents being flowed. [Allotrope] |
| http://purl.allotrope.org/ontologies/result#AFR_0001918 | Pressure (Bar) | pressure synonyms: pressure datum, pressure (datum) |
| http://purl.allotrope.org/ontologies/result#AFR_0001269 | Solvent mixing ratio (Percent) | pump mobile phase ratio setting A pump parameter specification that specifies the mobile phase ratio in the eluent. [Allotrope] |
| http://purl.allotrope.org/ontologies/result#AFR_0001270 | Flow change | pump flow rate setting A pump parameter specification that specifies the total flow rate of the combined mobile phases (eluent). [Allotrope] |
| http://purl.allotrope.org/ontologies/result#AFR_0001625 | Timetable entry time (Second) | delay synonyms: time offset |
| http://purl.allotrope.org/ontologies/result#AFR_0001635 | Timetable entry | control command synonyms: set command A control command is an action specification that specifies a setting to be set by a controlling process. [Allotrope] |

Addendum Methods Hub properties mapped to AFO

Pump (2/2)

| | | |
|---|------------------------------------|--|
| http://purl.allotrope.org/ontologies/result#AFR_0000941 | Section for various configurations | action specification synonyms: 2017-05-03 remove subclass of event [OSTHUS], command, instruction A directive information entity that describes an action the bearer will take. [IAO] |
| http://purl.allotrope.org/ontologies/result#AFR_0000945 | Timetable with members | linear procedure specificationsynonyms: linear procedure specification, event table, sequence specification A procedure specification with a linear ordered collection of action specifications. [Allotrope] |
| http://purl.allotrope.org/ontologies/result#AFR_0002033 | Timetable index | temporal index A temporal index is an index that follows temporal order of the list items or the processes that the items are about. [Allotrope] |
| http://purl.allotrope.org/ontologies/process#AFP_0003289 | Timetable specification | mobile phase delivery Mobile phase delivery is a process performed by a liquid chromatography system in which the solvent of the liquid phase are mixed and transported through the instrument for separation and detection. [Allotrope] |
| http://purl.allotrope.org/ontologies/process#AFP_0001135 | Mixing information | mixing synonyms: mixing material The combining of components, particles or layers into a more homogeneous state. The mixing may be achieved manually or mechanically by shifting the material with stirrers or pumps or by revolving or shaking the container. The process must not permit segregation of particles of different size or properties. Homogeneity may be considered to have been achieved in a practical sense when the sampling error of the processed portion is negligible compared to the total error of the measurement system. [CHMO] |
| http://purl.allotrope.org/ontologies/material#AFM_0000403 | Solvent target | liquid A liquid is a nearly incompressible fluid that conforms to the shape of its container but retains a (nearly) constant volume independent of pressure. [Wikipedia] |

Addendum Methods Hub properties mapped to AFO

Column Compartment

| | | |
|---|---|--|
| http://purl.allotrope.org/ontologies/result#AFR_0001815 | Duration (stoptime) | duration setting A duration setting is a setting that specifies the duration of a planned process or when a situation should trigger. [Allotrope] |
| http://purl.allotrope.org/ontologies/result#AFR_0001805 | Mode setting (chromatography) | test mode setting (chromatography) synonyms: test mode The test mode determines the measurements collected during the device execution, e.g. Injection Time only or Dispense Volume and Injection Time). [Allotrope] |
| http://purl.allotrope.org/ontologies/result#AFR_0000941 | Section for various configurations | action specification synonyms: 2017-05-03 remove subclass of event [OSTHUS], command, instruction A directive information entity that describes an action the bearer will take. [IAO] |
| http://purl.allotrope.org/ontologies/process#AFP_0002833 | Temperature control | temperature control A temperature control is a controlling process that controls the temperature of some material. [Allotrope] |
| http://purl.allotrope.org/ontologies/result#AFR_0001255 | Temperature (Degree Celsius) | temperature setting synonyms: temperature parameter A temperature setting is a setting that specifies some temperature. |
| http://purl.allotrope.org/ontologies/equipment#AFE_0000528 | Temperature controller | temperature controller synonyms: temperature control, temperature control device, thermostat A device used to control the temperature in a compartment. [Allotrope] |
| http://purl.allotrope.org/ontologies/common#AFC_0000021 | Range for not-ready mode (Degree Celsius) | range A range is an interval of values with a lower and/or upper limit. [Allotrope] |
| http://purl.allotrope.org/ontologies/equipment#AFE_0000270 | Valve | column selection valve A valve used to select a column if multiple columns are part of the column compartment. [Allotrope] |

Addendum Methods Hub properties mapped to AFO

PDA/DAD dectector (1/2)

| | | |
|---|---------------------------------|--|
| http://purl.allotrope.org/ontologies/result#AFR_0001815 | Duration (stoptime) | duration setting A duration setting is a setting that specifies the duration of a planned process or when a situation should trigger. [Allotrope] |
| http://purl.allotrope.org/ontologies/result#AFR_0001250 | Detector sampling rate (Hertz) | detector sampling rate setting synonyms: acquisition rate, detection sampling rate, sampling frequency, sampling rate, detector rate setting, sampling rate setting A detector setting parameter that specifies the rate at which the detector changes its output signal. It is limited by the actual physical/chemical process of detection and the detector electronics. Often the sample rate is set lower than the maximum sampling rate so that adjacent data points can be averaged to provide better signal to noise. [Allotrope] |
| http://purl.allotrope.org/ontologies/result#AFR_0001253 | Signal bandwidth (Nanometer) | electronic absorbance bandwidth setting synonyms: detector bandwidth setting A electronic absorbance detector setting parameter that specifies the bandwidth of a particular signal to be measured by the device. |
| http://purl.allotrope.org/ontologies/result#AFR_0001254 | Signal wavelength (Nanometer) | electronic absorbance wavelength setting synonyms: detector wavelength setting A electronic absorbance detector setting parameter that specifies the nominal wavelength of a particular signal to be measured by the device. |
| http://purl.allotrope.org/ontologies/result#AFR_0001251 | Reference bandwidth (Nanometer) | electronic absorbance reference bandwidth setting synonyms: detector reference bandwidth setting A electronic absorbance detector setting parameter that specifies the bandwidth of the reference signal that is subtracted from a particular signal of the device in order to compensate for background signal and noise. |

Addendum Methods Hub properties mapped to AFO

PDA/DAD dectector (2/2)

| | | |
|---|-----------------------------------|---|
| http://purl.allotrope.org/ontologies/result#AFR_0001252 | Reference wavelength (Nanometer) | electronic absorbance reference wavelength setting synonyms: detector reference wavelength setting A electronic absorbance detector setting parameter that specifies the nominal reference wavelength of the reference signal that is subtracted from a particular signal of the device in order to compensate for background signal and noise. |
| http://purl.allotrope.org/ontologies/process#AFP_0000246 | UV absorbance measurement | ultraviolet absorbance measurement synonyms: ultraviolet detection, UV detection, ultra-violet detection, UV measurement, ultra-violet measurement, ultraviolet measurement Ultraviolet absorbance measurement is electronic absorbance measurement of light in the wavelength region of 190-350 nm. [Allotrope] |
| http://purl.allotrope.org/ontologies/process#AFP_0000896 | UV spectrophotometry | ultraviolet spectrophotometry synonyms: ultraviolet spectrometry, UV spectrophotometry, UV spectroscopic measurements, UV spectroscopy, ultra-violet spectrometry, ultra-violet spectrophotometry, ultra-violet spectroscopy, ultraviolet spectroscopy Spectroscopy where the sample absorbs radiation from the ultraviolet region (190-400 nm) resulting in electronic transitions within the sample. [CHMO] |
| http://purl.allotrope.org/ontologies/result#AFR_0001542 | UV spectra scan range (Nanometer) | detector scan range setting synonyms: scan range setting A detector scan range setting is a detector setting that sets the wavelength range of scans as well as the increment between different scans. [Allotrope] |