3DEXPERIENCE®

Simplifying Instrument Data Integration

Pathways to Digital Success in the Lab

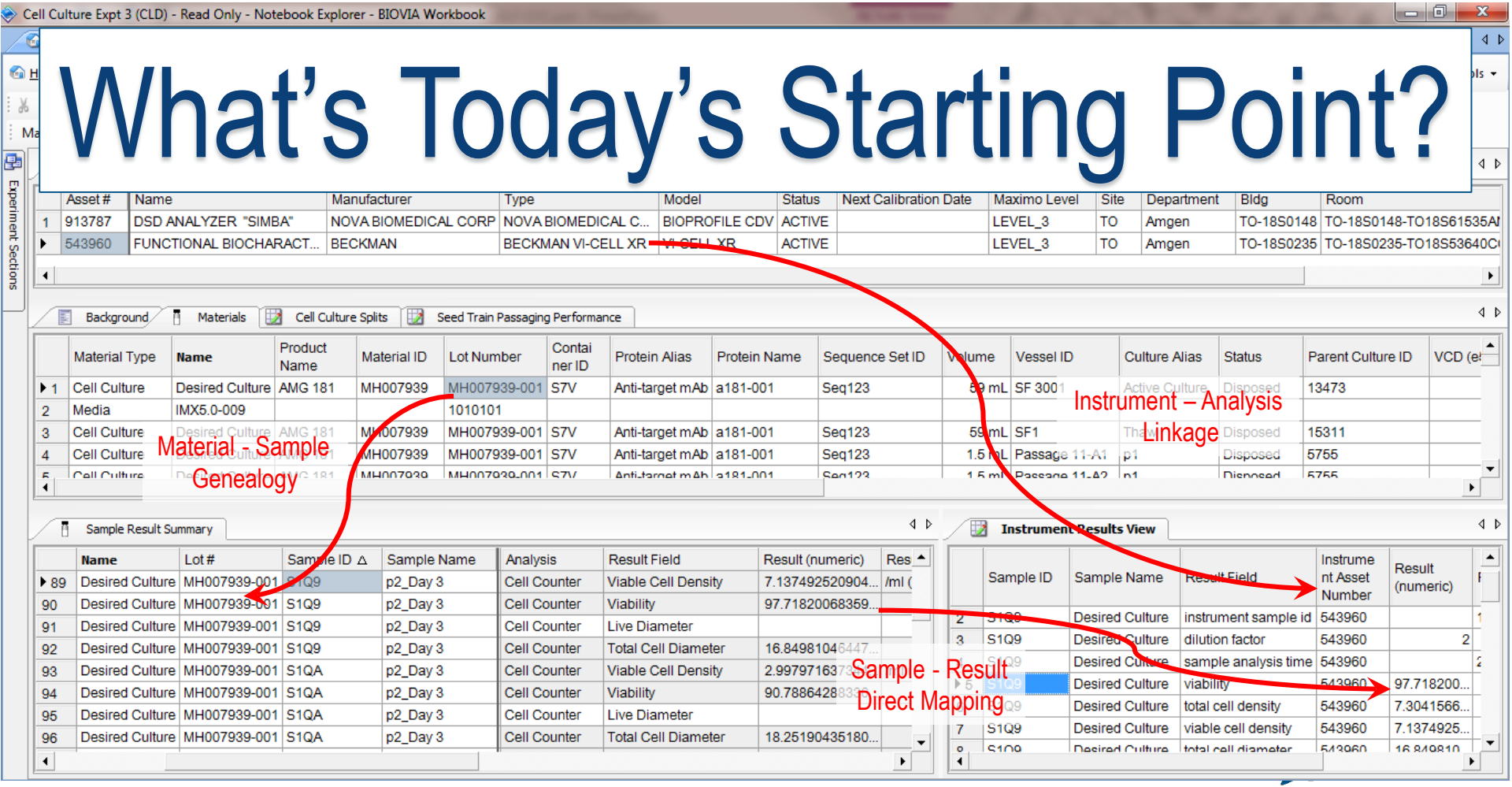
Gene Tetreault

Topics

Where we are today

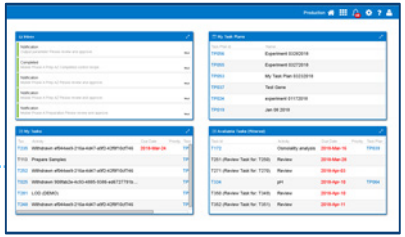
A Simplified Reference Data Configuration for Equipment Measurements

An Updated approach for Reading and Writing ADF


Cell Culture Expt 3 (CLD) - Read Only - Notebook Explorer - BIOVIA Workbook
What's Today's Starting Point?
Experiment Sections
Asset # | Name | Manufacturer | Type | Model | Status | Next Calibration Date | Maximo Level | Site | Department | Bldg | Room
1 | 913787 | DSD ANALYZER "SIMBA" | NOVA BIOMEDICAL CORP | NOVA BIOMEDICAL C... | BIOPROFILE CDV | ACTIVE | | LEVEL_3 | TO | Amgen | TO-18S0148 | TO-18S0148-TO18S61535A
543960 | FUNCTIONAL BIOCHARACT... | BECKMAN | BECKMAN VI-CELL XR | VI-CELL XR | ACTIVE | | LEVEL_3 | TO | Amgen | TO-18S0235 | TO-18S0235-TO18S53640C
Background
Materials
Cell Culture Splits
Seed Train Passaging Performance
Material Type | Name | Product Name | Material ID | Lot Number | Container ID | Protein Alias | Protein Name | Sequence Set ID | Volume | Vessel ID | Culture Alias | Status | Parent Culture ID | VCD (e
1 | Cell Culture | Desired Culture | AMG 181 | MH007939 | MH007939-001 | S7V | Anti-target mAb | a181-001 | Seq123 | 59 mL | SF 3001 | Active Culture | Disposed | 13473
2 | Media | IMX5.0-009 | | | 1010101
3 | Cell Culture | Desired Culture | AMG 181 | MH007939 | MH007939-001 | S7V | Anti-target mAb | a181-001 | Seq123 | 59 mL | SF1 | Thaw | Disposed | 15311
4 | Cell Culture | Desired Culture | AMG 181 | MH007939 | MH007939-001 | S7V | Anti-target mAb | a181-001 | Seq123 | 1.5 mL | Passage 11-A1 | p1 | Disposed | 5755
5 | Cell Culture | Desired Culture | AMG 181 | MH007939 | MH007939-001 | S7V | Anti-target mAb | a181-001 | Seq123 | 1.5 mL | Passage 11-A2 | p1 | Disposed | 5755
Material - Sample Genealogy
Instrument – Analysis Linkage
Sample Result Summary
Name | Lot # | Sample ID | Sample Name | Analysis | Result Field | Result (numeric) | Res
89 | Desired Culture | MH007939-001 | S1Q9 | p2_Day 3 | Cell Counter | Viable Cell Density | 7.137492520904... | /ml (
90 | Desired Culture | MH007939-001 | S1Q9 | p2_Day 3 | Cell Counter | Viability | 97.71820068359...
91 | Desired Culture | MH007939-001 | S1Q9 | p2_Day 3 | Cell Counter | Live Diameter
92 | Desired Culture | MH007939-001 | S1Q9 | p2_Day 3 | Cell Counter | Total Cell Diameter | 16.8498104
93 | Desired Culture | MH007939-001 | S1QA | p2_Day 3 | Cell Counter | Viable Cell Density | 2.997971637
94 | Desired Culture | MH007939-001 | S1QA | p2_Day 3 | Cell Counter | Viability | 90.7886428
95 | Desired Culture | MH007939-001 | S1QA | p2_Day 3 | Cell Counter | Live Diameter
96 | Desired Culture | MH007939-001 | S1QA | p2_Day 3 | Cell Counter | Total Cell Diameter | 18.25190435180...
Instrument Results View
Sample ID | Sample Name | Result Field | Instrument Asset Number | Result (numeric)
2 | S1Q9 | Desired Culture | instrument sample id | 543960
3 | S1Q9 | Desired Culture | dilution factor | 543960 | 2
4 | S1Q9 | Desired Culture | sample analysis time | 543960
5 | S1Q9 | Desired Culture | viability | 543960 | 97.718200...
6 | S1Q9 | Desired Culture | total cell density | 543960 | 7.3041566...
7 | S1Q9 | Desired Culture | viable cell density | 543960 | 7.1374925...
Sample - Result Direct Mapping

BIOVIA ONE Lab

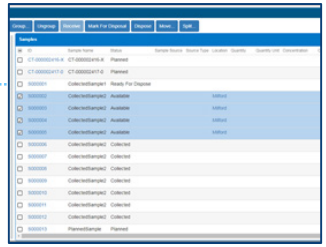
Task Planner & Samples



Lab Planning/Management

- Design and Track Studies
- Request Work
- Schedule, Review
- Confirm Requests

CISPro& Equipment



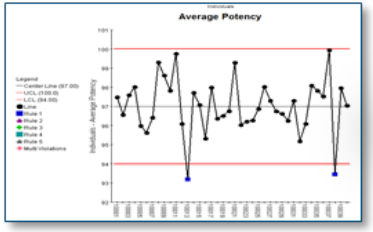
Resources

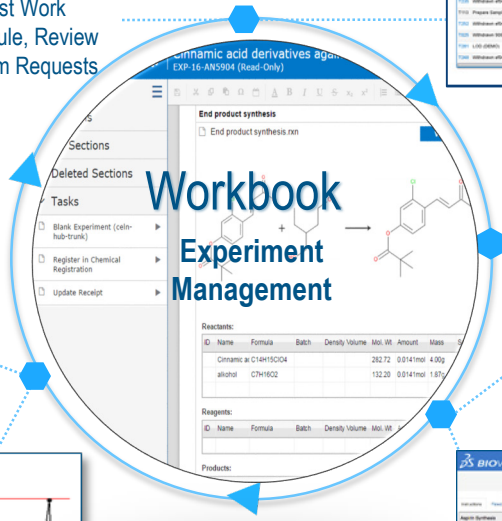
- Materials, Samples
- Personnel, Equipment

Insight & Pipeline Pilot

Reporting

- Process Monitoring
- Compile, Interpret Results
- Generate Reports
- Insights





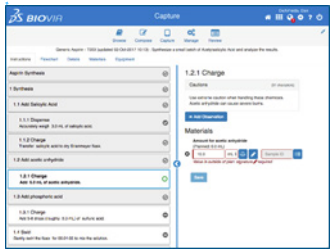
Workbook

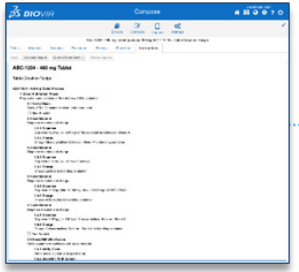
Experiment Management

Capture

Lab Execution

- Prepare Tests
- Perform Tests





Compose

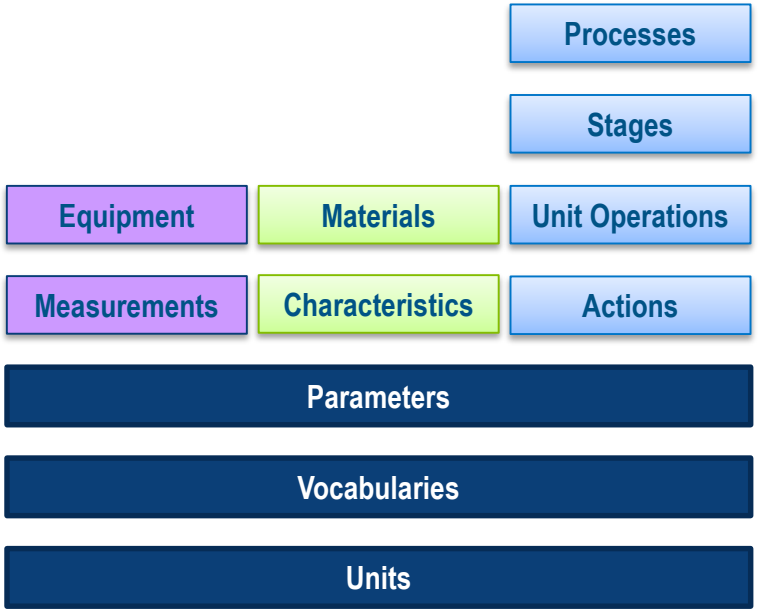
Recipes/Methods

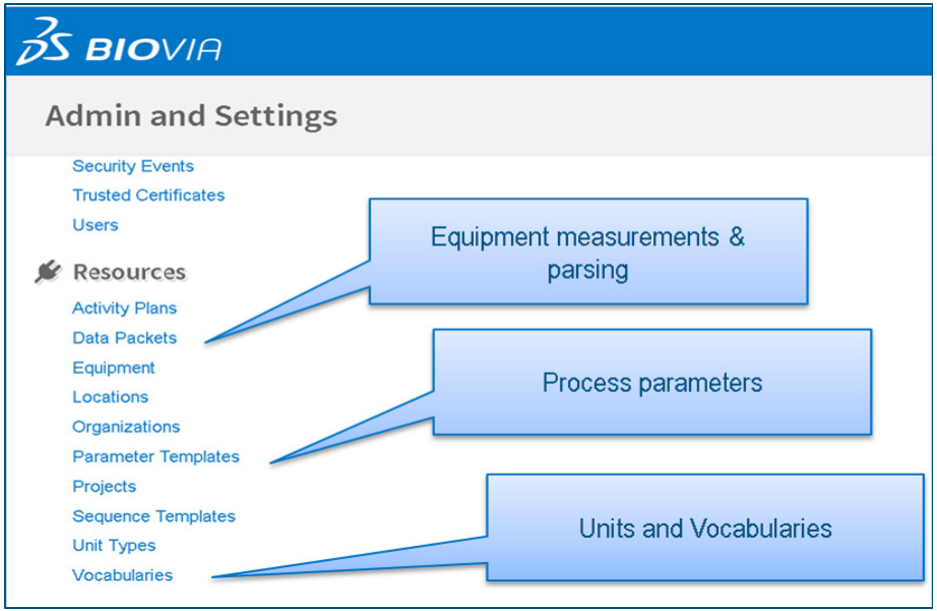
- Develop procedures
- Adapt procedures
- Manage procedures

Reference Data & Ontologies

Common master data management & reference ontologies

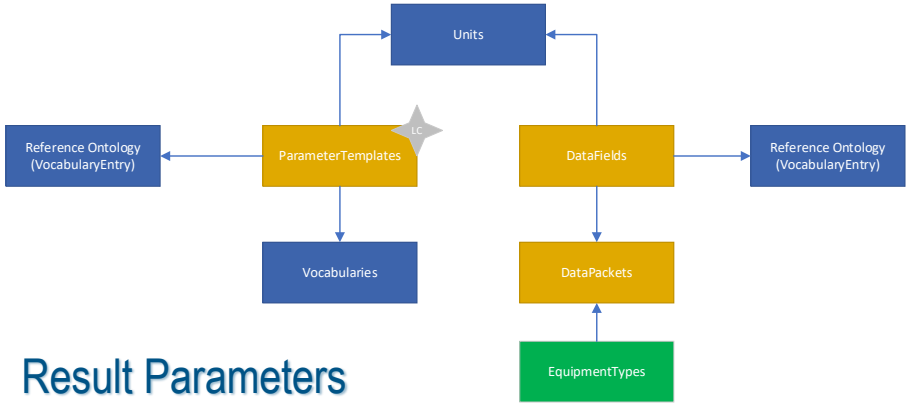
Allotrope Foundation · QUDT · ISA · Pistoia Alliance



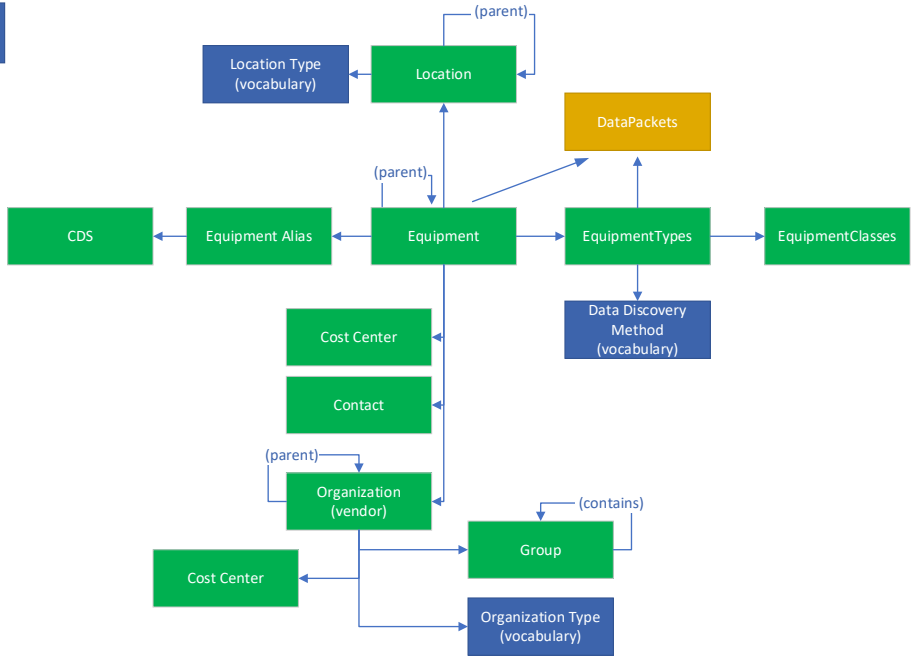


Reference Data Schematic

Units and Vocabularies



Result Parameters

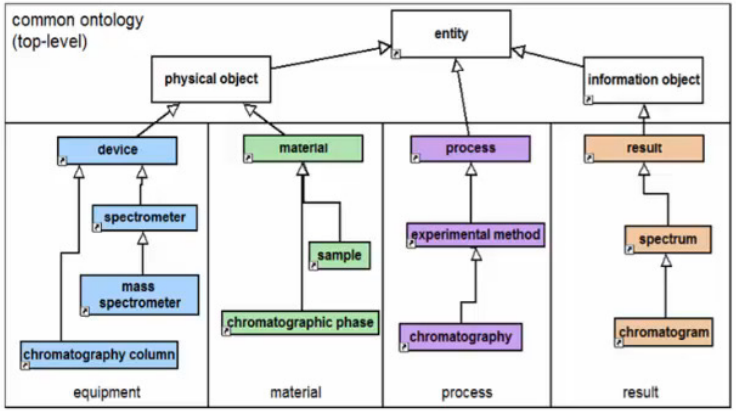


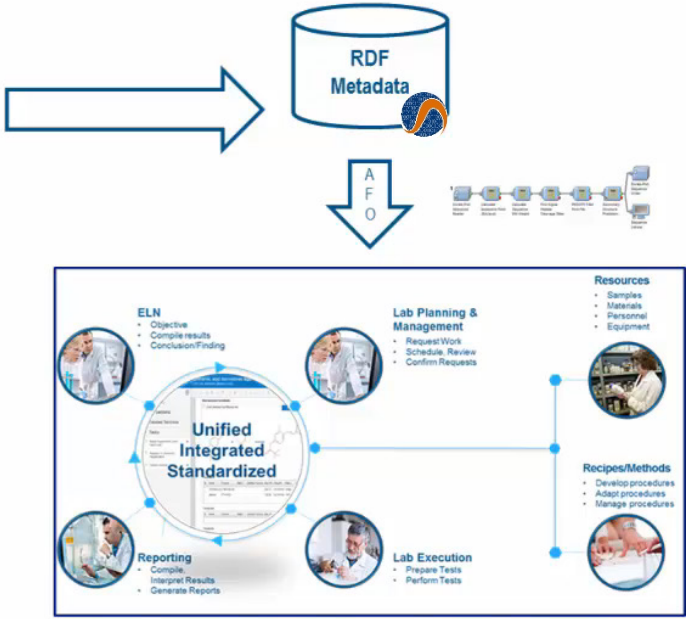
Equipment Measurements

DASSAULT SYSTEMES

Taxonomy and Ontology Synchronization

- BIOVIA ONE Lab centrally manages the ontologies
- Sync services to maintain applications usage of the vocabularies





BIOVIA ONE Lab

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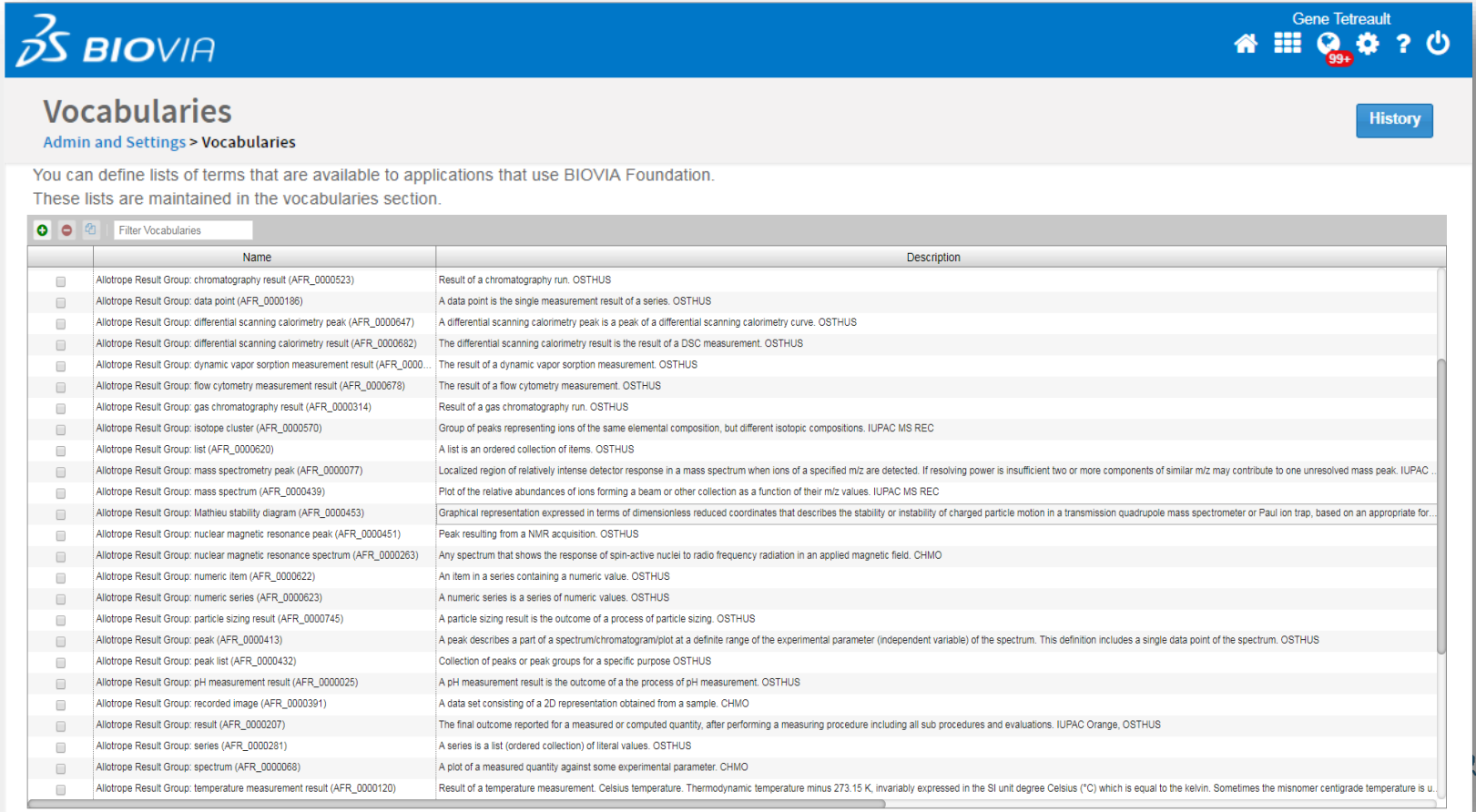
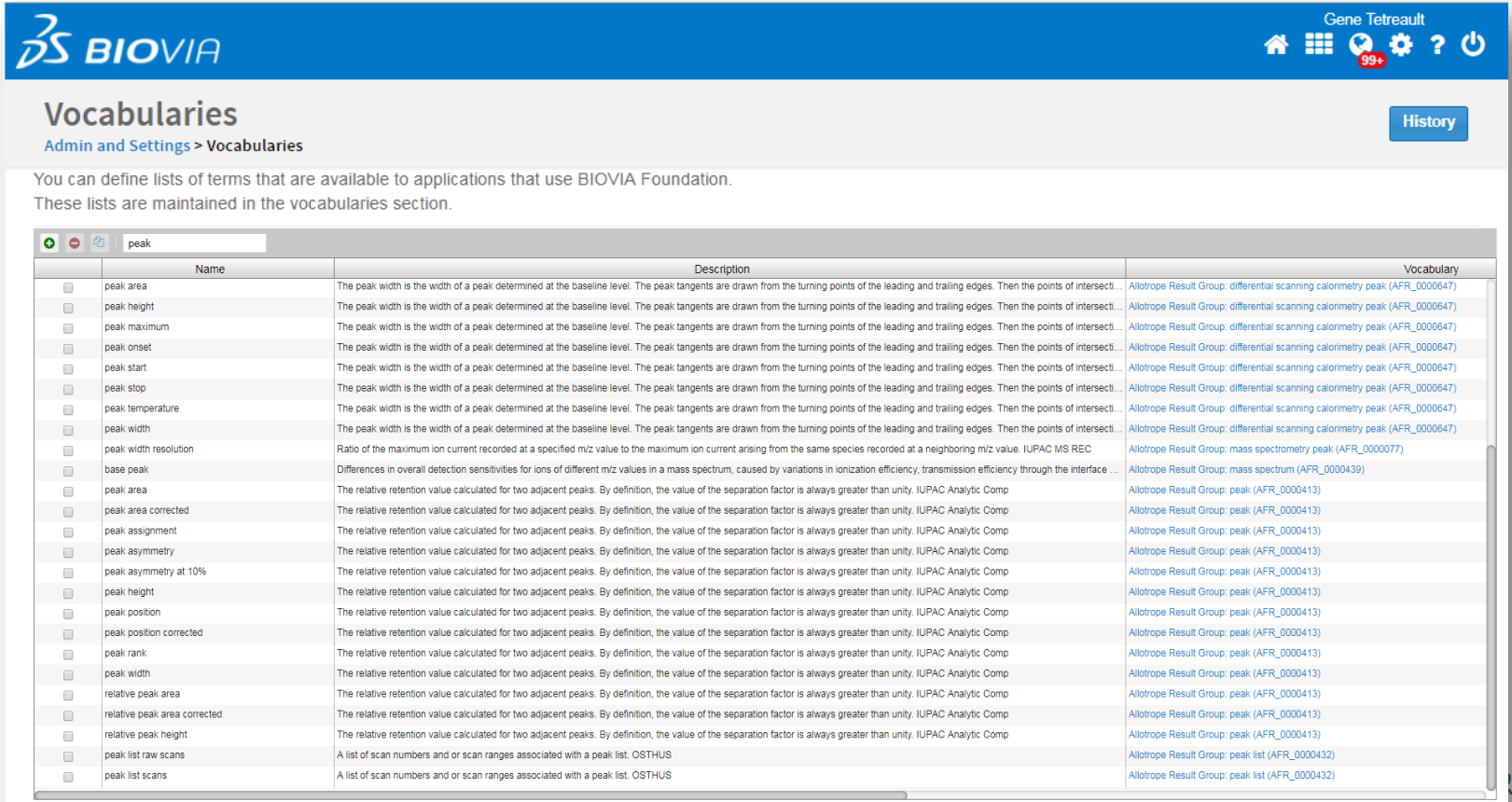
http://bcn2015.europeanbioanalysisforum.eu/wp-content/uploads/2015/12/os-2015-D2A1_3-Gerhard-Noelken.pdf

Result Groups (AFR_) as Vocabularies

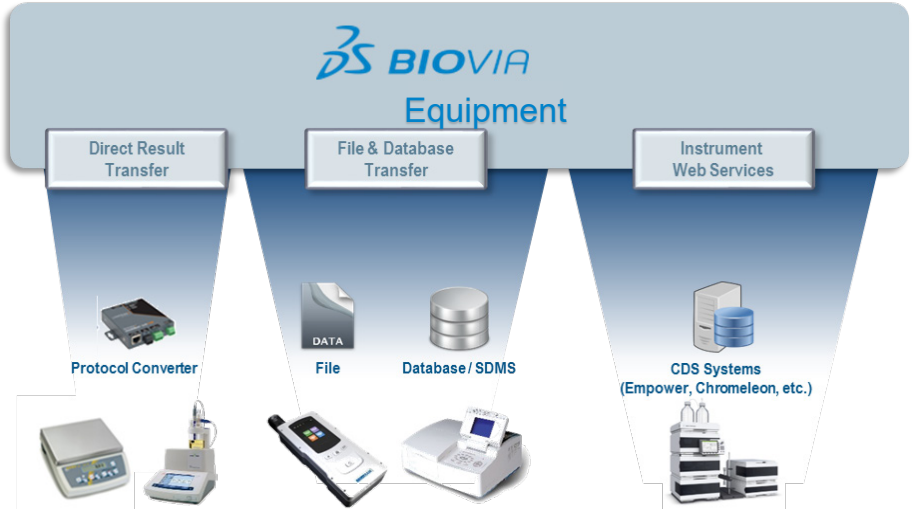


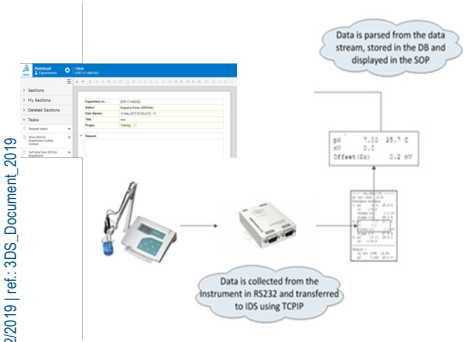
Name	Description
Allotrope Result Group: chromatography result (AFR_0000523)	Result of a chromatography run. OSTHUS
Allotrope Result Group: data point (AFR_0000186)	A data point is the single measurement result of a series. OSTHUS
Allotrope Result Group: differential scanning calorimetry peak (AFR_0000647)	A differential scanning calorimetry peak is a peak of a differential scanning calorimetry curve. OSTHUS
Allotrope Result Group: differential scanning calorimetry result (AFR_0000682)	The differential scanning calorimetry result is the result of a DSC measurement. OSTHUS
Allotrope Result Group: dynamic vapor sorption measurement result (AFR_0000...	The result of a dynamic vapor sorption measurement. OSTHUS
Allotrope Result Group: flow cytometry measurement result (AFR_0000678)	The result of a flow cytometry measurement. OSTHUS
Allotrope Result Group: gas chromatography result (AFR_0000314)	Result of a gas chromatography run. OSTHUS
Allotrope Result Group: isotope cluster (AFR_0000570)	Group of peaks representing ions of the same elemental composition, but different isotopic compositions. IUPAC MS REC
Allotrope Result Group: list (AFR_0000620)	A list is an ordered collection of items. OSTHUS
Allotrope Result Group: mass spectrometry peak (AFR_0000077)	Localized region of relatively intense detector response in a mass spectrum when ions of a specified m/z are detected. If resolving power is insufficient two or more components of similar m/z may contribute to one unresolved mass peak. IUPAC ...
Allotrope Result Group: mass spectrum (AFR_0000439)	Plot of the relative abundances of ions forming a beam or other collection as a function of their m/z values. IUPAC MS REC
Allotrope Result Group: Mathieu stability diagram (AFR_0000453)	Graphical representation expressed in terms of dimensionless reduced coordinates that describes the stability or instability of charged particle motion in a transmission quadrupole mass spectrometer or Paul ion trap, based on an appropriate for...
Allotrope Result Group: nuclear magnetic resonance peak (AFR_0000451)	Peak resulting from a NMR acquisition. OSTHUS
Allotrope Result Group: nuclear magnetic resonance spectrum (AFR_0000263)	Any spectrum that shows the response of spin-active nuclei to radio frequency radiation in an applied magnetic field. CHMO
Allotrope Result Group: numeric item (AFR_0000622)	An item in a series containing a numeric value. OSTHUS
Allotrope Result Group: numeric series (AFR_0000623)	A numeric series is a series of numeric values. OSTHUS
Allotrope Result Group: particle sizing result (AFR_0000745)	A particle sizing result is the outcome of a process of particle sizing. OSTHUS
Allotrope Result Group: peak (AFR_0000413)	A peak describes a part of a spectrum/chromatogram/plot at a definite range of the experimental parameter (independent variable) of the spectrum. This definition includes a single data point of the spectrum. OSTHUS
Allotrope Result Group: peak list (AFR_0000432)	Collection of peaks or peak groups for a specific purpose OSTHUS
Allotrope Result Group: pH measurement result (AFR_0000025)	A pH measurement result is the outcome of a the process of pH measurement. OSTHUS
Allotrope Result Group: recorded image (AFR_0000391)	A data set consisting of a 2D representation obtained from a sample. CHMO
Allotrope Result Group: result (AFR_0000207)	The final outcome reported for a measured or computed quantity, after performing a measuring procedure including all sub procedures and evaluations. IUPAC Orange, OSTHUS
Allotrope Result Group: series (AFR_0000281)	A series is a list (ordered collection) of literal values. OSTHUS
Allotrope Result Group: spectrum (AFR_0000068)	A plot of a measured quantity against some experimental parameter. CHMO
Allotrope Result Group: temperature measurement result (AFR_0000120)	Result of a temperature measurement. Celsius temperature. Thermodynamic temperature minus 273.15 K, invariably expressed in the SI unit degree Celsius (°C) which is equal to the kelvin. Sometimes the misnomer centigrade temperature is u...

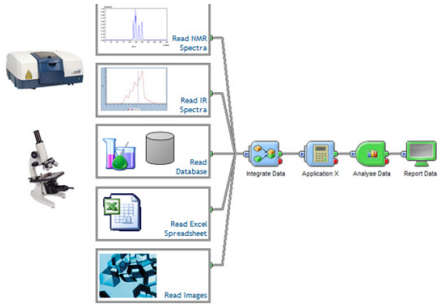
Measurements (AFX_) as Vocabulary Entries



Name	Description	Vocabulary
peak area	The peak width is the width of a peak determined at the baseline level. The peak tangents are drawn from the turning points of the leading and trailing edges. Then the points of intersecti...	Allotrope Result Group: differential scanning calorimetry peak (AFR_0000647)
peak height	The peak width is the width of a peak determined at the baseline level. The peak tangents are drawn from the turning points of the leading and trailing edges. Then the points of intersecti...	Allotrope Result Group: differential scanning calorimetry peak (AFR_0000647)
peak maximum	The peak width is the width of a peak determined at the baseline level. The peak tangents are drawn from the turning points of the leading and trailing edges. Then the points of intersecti...	Allotrope Result Group: differential scanning calorimetry peak (AFR_0000647)
peak onset	The peak width is the width of a peak determined at the baseline level. The peak tangents are drawn from the turning points of the leading and trailing edges. Then the points of intersecti...	Allotrope Result Group: differential scanning calorimetry peak (AFR_0000647)
peak start	The peak width is the width of a peak determined at the baseline level. The peak tangents are drawn from the turning points of the leading and trailing edges. Then the points of intersecti...	Allotrope Result Group: differential scanning calorimetry peak (AFR_0000647)
peak stop	The peak width is the width of a peak determined at the baseline level. The peak tangents are drawn from the turning points of the leading and trailing edges. Then the points of intersecti...	Allotrope Result Group: differential scanning calorimetry peak (AFR_0000647)
peak temperature	The peak width is the width of a peak determined at the baseline level. The peak tangents are drawn from the turning points of the leading and trailing edges. Then the points of intersecti...	Allotrope Result Group: differential scanning calorimetry peak (AFR_0000647)
peak width	The peak width is the width of a peak determined at the baseline level. The peak tangents are drawn from the turning points of the leading and trailing edges. Then the points of intersecti...	Allotrope Result Group: differential scanning calorimetry peak (AFR_0000647)
peak width resolution	Ratio of the maximum ion current recorded at a specified m/z value to the maximum ion current arising from the same species recorded at a neighboring m/z value. IUPAC MS REC	Allotrope Result Group: mass spectrometry peak (AFR_0000077)
base peak	Differences in overall detection sensitivities for ions of different m/z values in a mass spectrum, caused by variations in ionization efficiency, transmission efficiency through the interface ...	Allotrope Result Group: mass spectrum (AFR_0000439)
peak area	The relative retention value calculated for two adjacent peaks. By definition, the value of the separation factor is always greater than unity. IUPAC Analytic Comp	Allotrope Result Group: peak (AFR_0000413)
peak area corrected	The relative retention value calculated for two adjacent peaks. By definition, the value of the separation factor is always greater than unity. IUPAC Analytic Comp	Allotrope Result Group: peak (AFR_0000413)
peak assignment	The relative retention value calculated for two adjacent peaks. By definition, the value of the separation factor is always greater than unity. IUPAC Analytic Comp	Allotrope Result Group: peak (AFR_0000413)
peak asymmetry	The relative retention value calculated for two adjacent peaks. By definition, the value of the separation factor is always greater than unity. IUPAC Analytic Comp	Allotrope Result Group: peak (AFR_0000413)
peak asymmetry at 10%	The relative retention value calculated for two adjacent peaks. By definition, the value of the separation factor is always greater than unity. IUPAC Analytic Comp	Allotrope Result Group: peak (AFR_0000413)
peak height	The relative retention value calculated for two adjacent peaks. By definition, the value of the separation factor is always greater than unity. IUPAC Analytic Comp	Allotrope Result Group: peak (AFR_0000413)
peak position	The relative retention value calculated for two adjacent peaks. By definition, the value of the separation factor is always greater than unity. IUPAC Analytic Comp	Allotrope Result Group: peak (AFR_0000413)
peak position corrected	The relative retention value calculated for two adjacent peaks. By definition, the value of the separation factor is always greater than unity. IUPAC Analytic Comp	Allotrope Result Group: peak (AFR_0000413)
peak rank	The relative retention value calculated for two adjacent peaks. By definition, the value of the separation factor is always greater than unity. IUPAC Analytic Comp	Allotrope Result Group: peak (AFR_0000413)
peak width	The relative retention value calculated for two adjacent peaks. By definition, the value of the separation factor is always greater than unity. IUPAC Analytic Comp	Allotrope Result Group: peak (AFR_0000413)
relative peak area	The relative retention value calculated for two adjacent peaks. By definition, the value of the separation factor is always greater than unity. IUPAC Analytic Comp	Allotrope Result Group: peak (AFR_0000413)
relative peak area corrected	The relative retention value calculated for two adjacent peaks. By definition, the value of the separation factor is always greater than unity. IUPAC Analytic Comp	Allotrope Result Group: peak (AFR_0000413)
relative peak height	The relative retention value calculated for two adjacent peaks. By definition, the value of the separation factor is always greater than unity. IUPAC Analytic Comp	Allotrope Result Group: peak (AFR_0000413)
peak list raw scans	A list of scan numbers and or scan ranges associated with a peak list. OSTHUS	Allotrope Result Group: peak list (AFR_0000432)
peak list scans	A list of scan numbers and or scan ranges associated with a peak list. OSTHUS	Allotrope Result Group: peak list (AFR_0000432)







Existing Direct Connections

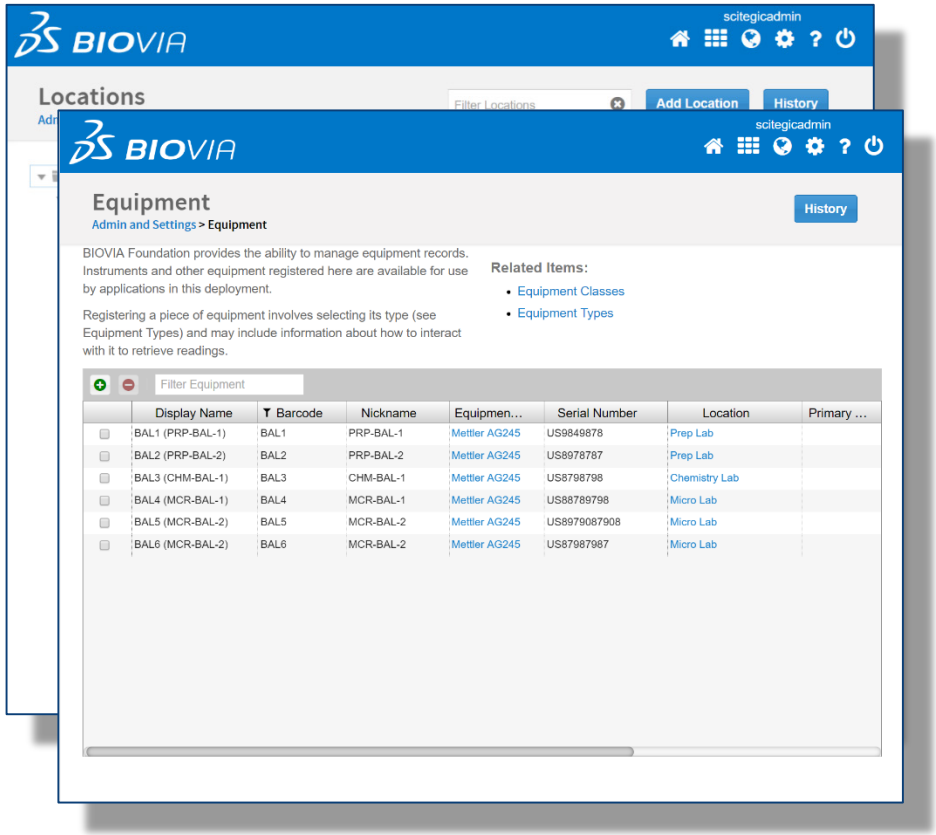
Accumet 950	Julabo MD	Mettler MX5	Mettler XP204	Photovolt Aquatest-2010	Sartorius LP1200	Thermo Orion 420A+
Accumet AR15	Kraemer Elektronik HC 97	Mettler PB1502-S	Mettler XP205	Radiometer CDM230	Sartorius LP2200S	Thermo Orion 520A+
Accumet AR20	Leica Auto ABBE	Mettler PB3001-S	Mettler XP205DR	Radiometer PHM210	Sartorius LP3200D	Thermo Orion 720A Plus
Advanced Instruments 3250	Metrohm 702SM Titrino	Mettler PB3002	Mettler XP26	Radiometer PHM220	Sartorius LP4200S	TSI 4043
Advanced Instruments 3300	Metrohm 712	Mettler PB3002-S	Mettler XP56	Radiometer PHM93	Sartorius LP5200P	Turner Quantech FM109535
Advanced Instruments 3D3	Metrohm 737 KF Coulometer	Mettler PB302	Mettler XS100S-S	Sartorius A200	Sartorius LP620S	VanKel 25-1000
AND HR-200	Metrohm 756 KF Coulometer	Mettler PB403-S	Mettler XS104	Sartorius A200-S	Sartorius M-power	Vankel VK 200
Anton Paar DMA 4500	Metrohm 780	Mettler PB602-S	Mettler XS204	Sartorius AC210S	Sartorius MSP	Vankel VK7000
Anton PaarCitizen DMA 5000	Metrohm 787 KF Titrino	Mettler PG1003-S	Mettler XS205	Sartorius AC211S	Sartorius MA40	VWR symphony SB70P
Beckman 360	Metrohm 795 Titrino	Mettler PG2002-S	Mettler XS205DU	Sartorius BP210D	Sartorius MA51	VWR symphony SB80PC
Beckman 45 pH Meter	Metrohm 831 Coulometric	Mettler PG3001-S	Mettler XS3DU	Sartorius BP211D	Sartorius MC210P	VWR symphony SP21
Brinkmann 756 KF	Metrohm 841 KF Titrando	Mettler PG4002-S	Mettler XS603-S	Sartorius BP221S	Sartorius MC210S	VWR symphony SP70P
Coulometer	Metrohm 841 Titrando	Mettler PG403-S	Mettler XS802-S	Sartorius BP3100S	Sartorius MC5	VWR symphony SR301
Brinkmann Metrohm 713	Mettler AG104	Mettler PG6002-S	Millipore Milliflex PLUS	Sartorius BP4100S	Sartorius ME215P	VWR symphony SR30I
Brookfield DVIII-LV	Mettler AG135	Mettler PM100	Mitsubishi CA-100	Sartorius CP124S	Sartorius ME215S	VWR symphony SR40C
Brookfield DVIII-RV	Mettler AG204	Mettler PM1200	Mitsubishi CA-200	Sartorius CP2201	Sartorius ME235	Wescor 5520
Buchi B-540	Mettler AG245	Mettler PM2000	Mitsubishi CAWA-100	Sartorius CP202S	Sartorius ME235P	YSI 3200
Corning 350	Mettler AT200	Mettler PM2500	Ohaus EP-412C	Sartorius CP225D	Sartorius ME235S	Zeiss MCS311
Corning 540	Mettler AT201	Mettler PR2002	OHAUS EP612C	Sartorius CP2P-F	Sartorius ME36S	
Cosa Instruments CAVA-100	Mettler AT250	Mettler PR2003	OHAUS Explorer	Sartorius ED622GS	Sartorius ME5	
Distek 2100B	Mettler AT261	Mettler PR5002	Ohaus Vt12140	Sartorius Genius	Sartorius MSA6.6S	
Dr. Schleuniger 8M	Mettler AX105	Mettler PR503	Orion 150	Sartorius L 420 S	Sartorius R160P	
Fisher Scientific AR25	Mettler AX105DR	Mettler PR8002	Orion 150A	Sartorius LA2200S	Sartorius R200-D	
Fiske 210	Mettler AX205	Mettler PR803	Orion 162A	Sartorius LA230S	Sartorius RC210S	
Fluke 1523	Mettler AX26	Mettler RE40	Orion 250A	Sartorius LA310S	Sartorius SE2	
GTB Dissoprep MX8	Mettler AX304	Mettler SB16001	Orion 350	Sartorius LC12001S	Sartorius TE612	
Hach 2100AN	Mettler DE40	Mettler SevenCompact	Orion 370	Sartorius LC2201	Shimadzu AUW1200	
Hach Ultra Mat One 3400	Mettler DL31	Mettler SevenEasy	Orion 420A	Sartorius LC220S	Sotax HT1	
Hanson Research SR8 Plus	Mettler DL36	Mettler SevenMulti	Orion 720A	Sartorius LC4200S	Stanford Research OptiMelt	
Holland C50	Mettler DL38	Mettler SR16001	Orion 920A	Sartorius LE2202S	Thermo Orion 150 A+	
Jenway 3020	Mettler HB43	Mettler UMX2	Paar DMA48	Sartorius LE225D	Thermo Orion 3 Star	
Jenway 3320	Mettler MPC227	Mettler WXSS205DU	Perkin Elmer 341	Sartorius LE26P	Thermo Orion 370	
Julabo F26MV	Mettler MT5	Mettler XP1203-S	Photovolt Aquatest - 10	Sartorius LE4202S	Thermo Orion 4 Star	

Existing Parsers

ABI 7900 HT	GUAVA EASTCYTE	Plate Reader (Envision)
ABI QuantStudio7	Headspace Analyzer FMS-1400	Plunger Inspection Device
Agilent 2100 Expert Bioanalyzer	Headspace Analyzer FMS-760	Polarimeter (Autopol V Plus)
Agilent Cary 60	iCDataCenter	PVM
AKTA Crossflow	ICP-MS	Raman Rigaku Firstguard
AKTA Explorer	Korsch XM12	Robotic Drop Tester
Analytical ultracentrifuge	Leak Detector 325	TA DSC
Barcode Labeling	Leak Detector 455	TecanMagellan
Biacore 3000	Leak Detector 655	Tecan-qPCR
BioRad ChemiDoc MP	Lyophilizer Lyostar II	Tenney Environmental Chamber
BioRad ChemiDoc ProteinGel	Lyophilizer Lyostar III	Tensiometer
Bruker B-ACS 120 NMR	Malvern Particle Sizer (Mastersizer 2000 and 3000)	Thermogravimetric Analyzer GA Q500
Bruker Vertex 70 FTIR	Micro Flow Imaging (MFI)	Tiamo KF
CARY 50	Multi-Angle static Light Scattering	Transportation Lab Environmental Chamber
Cedex	Nano Drop 1000	Tristar Surface Area
Cedex HR	Nova Biomedical Flex	Varian Cary SoloVPE
Circular Dichroism	Nova CDV	Varian Spec 4000
Compression Tester	Optical Comparator	ViCell
Digital Coordinate Measuring Machine	Particle Counter (Single) HIAC	Viscometer (Rheometer)
Dynamic Vapor Sorption	Particle Counter Auto	VMAX
Force Tester	Particle Vision System	X-Ray (Xpert Data Viewer)
Fortebio	Pendotech	XRPD

Equipment Registry

- Equipment is registered against the list of equipment types and location
- Connection information is specified for each registered equipment
- Equipment can be deactivated if they are taken out of service
- Once registered, readings may be taken from the equipment
- The list allows for filtering and quick links to related items



Equipment Model Overview

Equipment Class

Classifications make it easier for users to find equipment by grouping similar types of equipment together. Examples of classes include balances, pH meters, and HPLCs.

Equipment Type

Equipment types define the specifications for a particular make and model of equipment. Where applicable, this definition can include the data that can be acquired from the equipment and the commands to use to obtain that data.

Equipment

Instruments and equipment are registered with Foundation to make them available for use in a Foundation deployment. Registering a piece of equipment involves selecting its type and may include information about how to interact with it to retrieve readings.

Equipment Example

Equipment Class

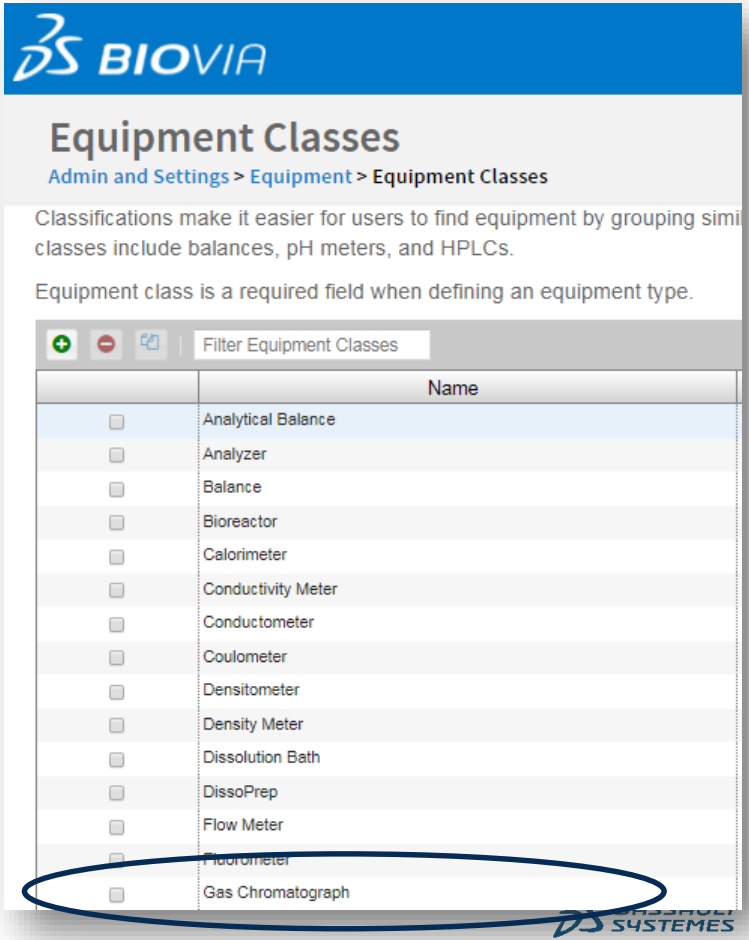
Gas Chromatograph

Equipment Type

Agilent 6890

Equipment Instance

CHM-GC-1



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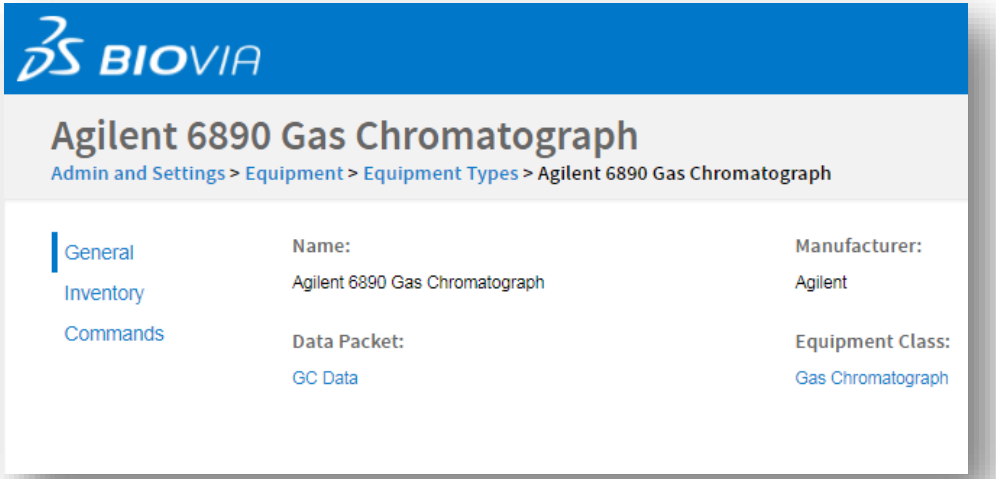

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Equipment Example

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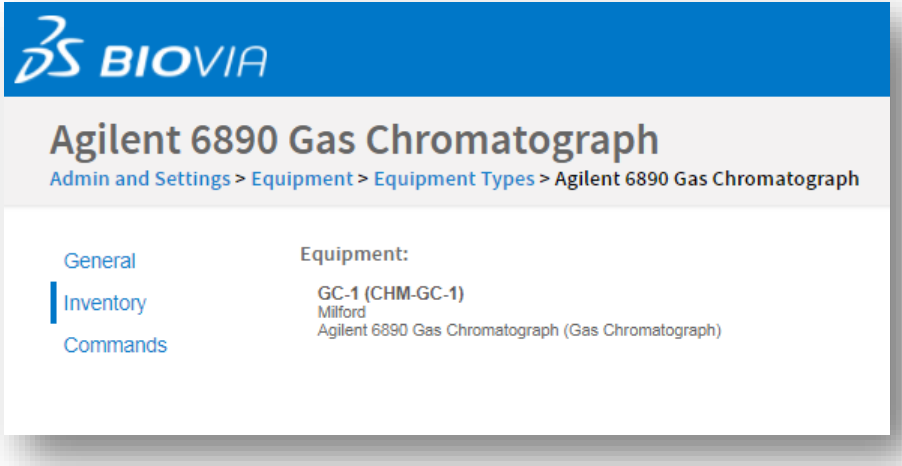
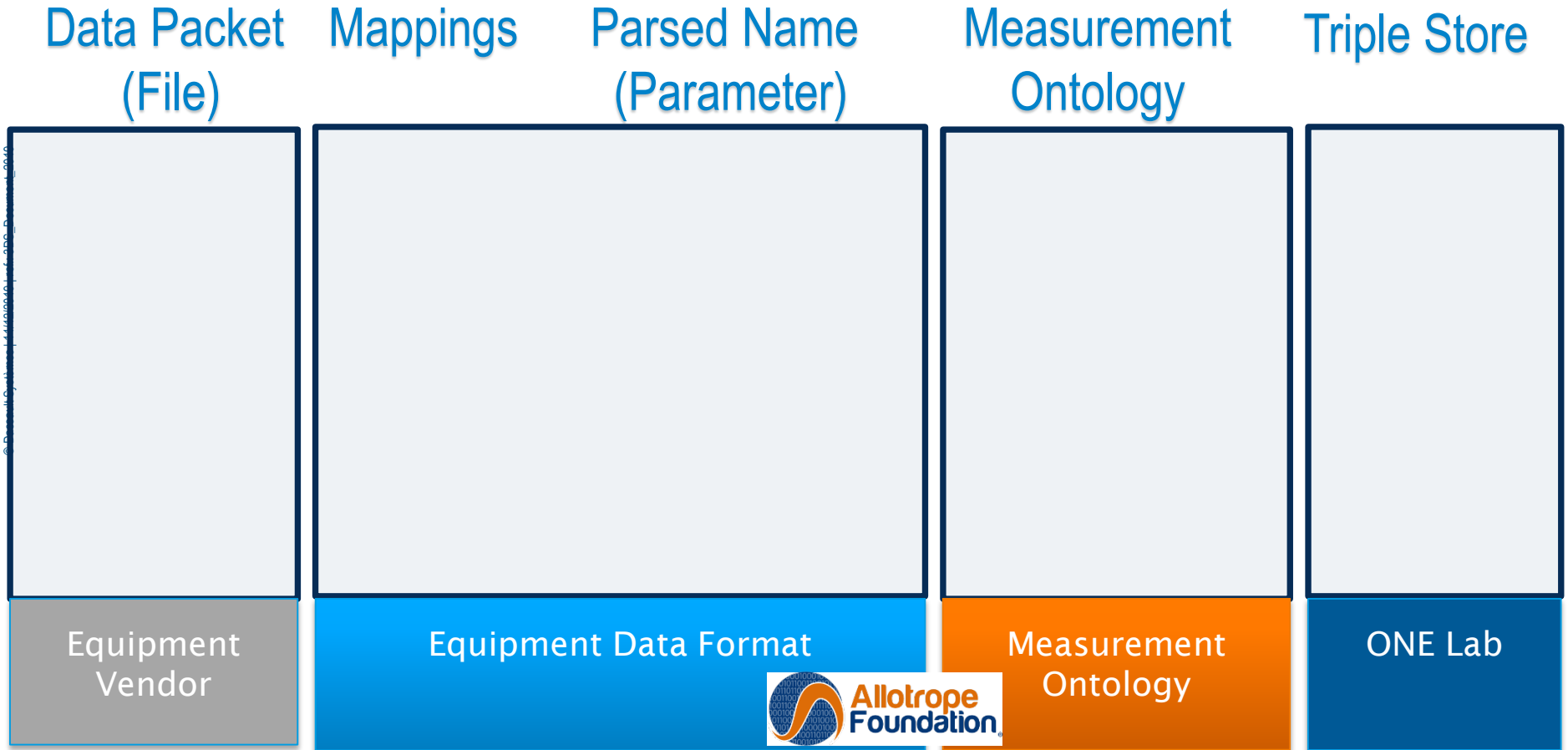
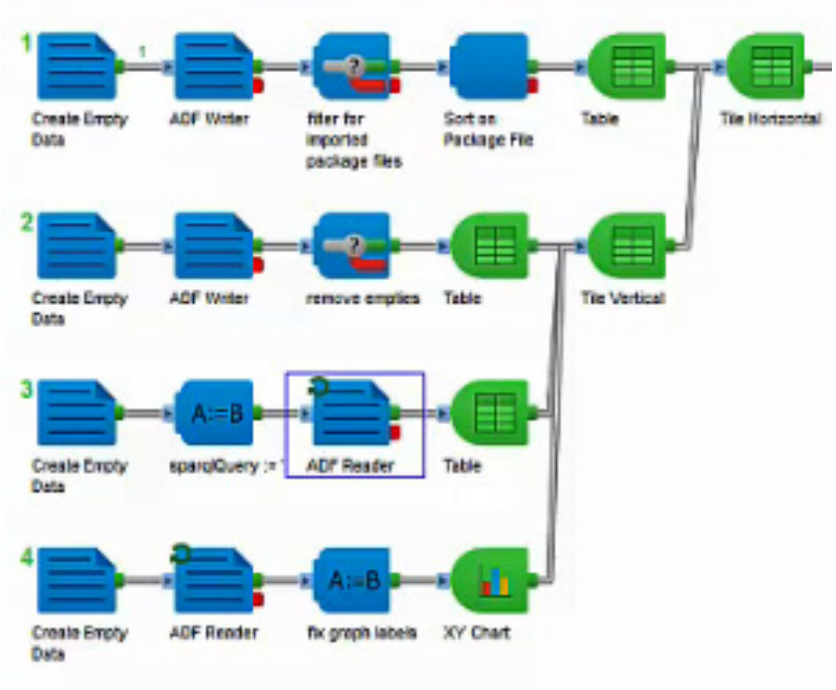


Equipment Data Acquisition



BIOVIA –Allotrope ADF Support in ONELab

- Pipeline Pilot Components for Allotrope ADF manipulation
  - Read and write ADF version 1.3 since Fall 2017
- Designed to support custom ADF read or write capabilities



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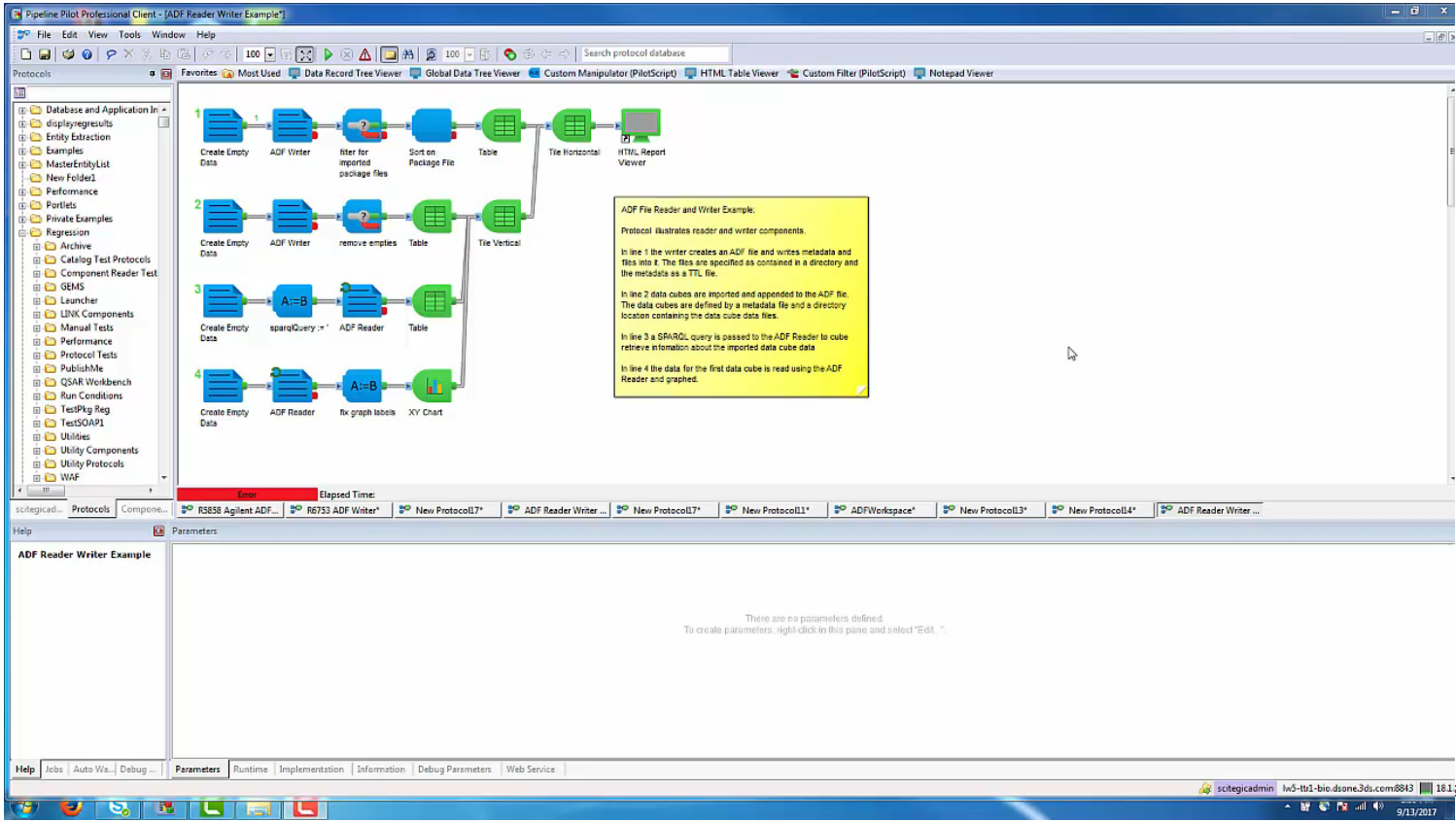
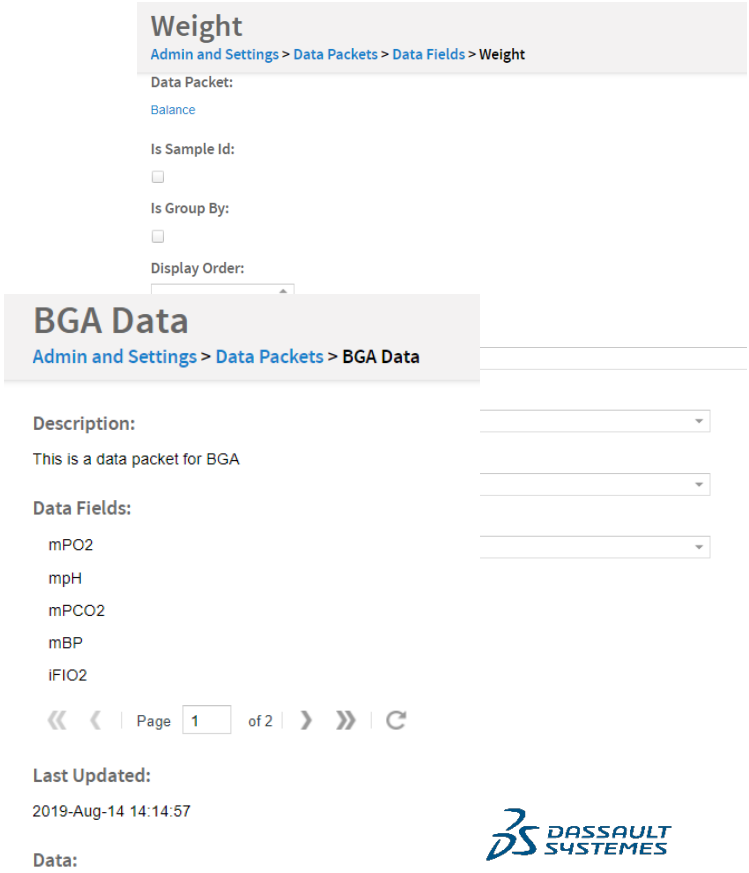
ADF Parsing (Click to play video)



Going Forward: Simplified Equipment Configuration

- Why is this needed?
  - Configuring readings for equipment can be complex
  - Requires creation and configuration of Parameter Templates, Data Packets, Parsers, Data Fields for every Equipment Type
  - Need simpler way to add equipment from any known class



Going Forward: Simplified Equipment Configuration

- Re-align the Equipment Class-Equipment/Data Field relationships
- Support association of the Allotrope Result Group ontology (AFR) with the Equipment Class (AFX- AFO)
  - Provides higher level of re-use of configuration defined by Allotrope and simplification of the definition of Measurement results
  - Allows pre-definition of readings for Equipment Classes, requiring an Admin only to map vendor readings to AFO readings
  - When parsing vendor-supplied ADF files, readings would not require user definition other than mapping to parameter and setting context

BIOVIA – Allotrope Ontology Support

- Currently ULM supports the association of results with the Allotrope Measurement ontology (AFX) through Data Field reference vocabularies and Parameter Template external Ids
- Roadmap for ONE Lab ULM Equipment
  - Re-align the Equipment Class-Equipment/Data Field relationships to support association of the Allotrope Result Group ontology (AFR) with the Equipment Class
  - Provides higher level of re-use of configuration defined by Allotrope and simplification of the definition of Measurement results

Positive Allotrope Direction – Simplification

- Leaf Node Model
- Fundamentally more practical for broader array of implementations
- More facile engineering with broader array of tools
- Much more generalizable to the Equipment Class Level
- More comprehensible to a broader array of users

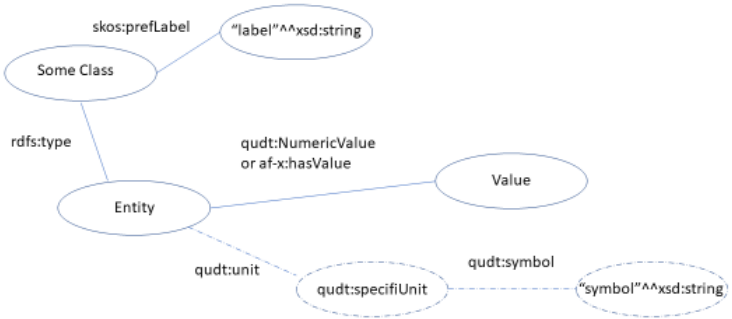
Example: Cell Counter Data
This is essentially name:value pairs

Vi-CELL XR 2.04

Beckman Coulter, Inc.

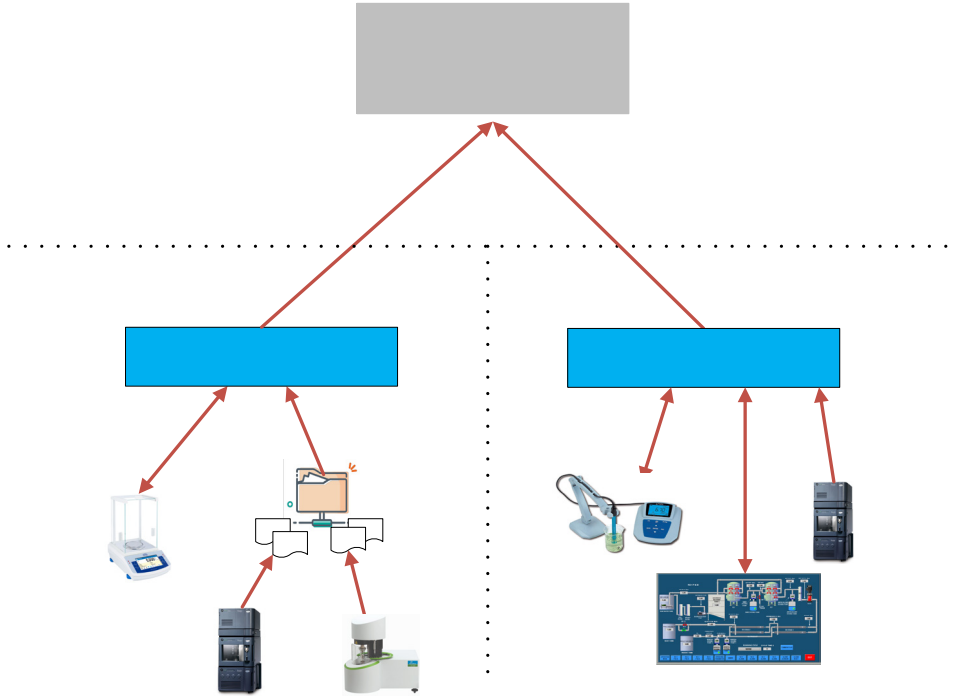
Sample ID	Dilution factor	Sample date	Viability (%)	Total cells /ml (x10^6)	Viable cells /ml (x10^6)	Avg. diam. (microns)
water check 03 Aug 2017	1.0	3 Aug 2017 10:55:55 AM	30.8	0.013	0.004	9.39
water check 080317 2	1.0	3 Aug 2017 11:09:19 AM	33.3	0.003	0.001	6.05
wil2s 080317 pre tf	1.0	3 Aug 2017 11:47:19 AM	97.4	1.61	1.57	13.59
wil2s 080317 post tf	1.0	3 Aug 2017 11:56:43 AM	97.0	0.71	0.68	13.68
U2OS IL23R P2 CF 03Aug17	1.0	3 Aug 2017 1:19:02 PM	94.4	0.16	0.15	15.37
U2OS IL12R P3 CF 03Aug17	1.0	3 Aug 2017 1:31:15 PM	85.3	0.15	0.13	16.21
NK92 P30 CF 04Aug17	1.0	4 Aug 2017 1:11:06 PM	94.2	2.85	2.68	15.57

And the associated triple pattern



ONE Lab Integration Appliance

- The Integration Appliance provides a bridge between any number of site laboratories and the central installation of ONE Lab
- The Integration Appliance will support
  - Discovering data files from laboratory instruments for results parsing (e.g. TGA)
  - Reading data from network-connected port devices (e.g. balances)
  - Local label printing
  - Reading data from OPC-enabled equipment (e.g. protein purification equipment)
  - Providing data to OPC-enabled software (e.g. MES)
  - **Writing Allotrope ADF files from ONE Lab-connected equipment**
  - **Reading Allotrope ADF files from Allotrope-enabled instruments**



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Conclusion

- The new Equipment Class mode in ONE Lab will permit the **alignment** of **Equipment Class** and **Allotrope Result (AFR) ontology**.
- Configure an Equipment Class once, align it with the AFR and for each new manufacturer, you only need to alias the field names to the Equipment Class/AFR. Much **easier to maintain and scale Equipment** definitions.
- The **leaf-node approach** lets us create a more general solution to support **ADF** read/write enhancing **scalability**.
- The **Pipeline Pilot** components available for use in any application that require more **specific/deeper use of the ADF** file (e.g. data cubes writing or reading).