

Simplifying Instrument Data Integration

Pathways to Digital Success in the Lab

Gene Tetreault

3DEXPERIENCE[®]



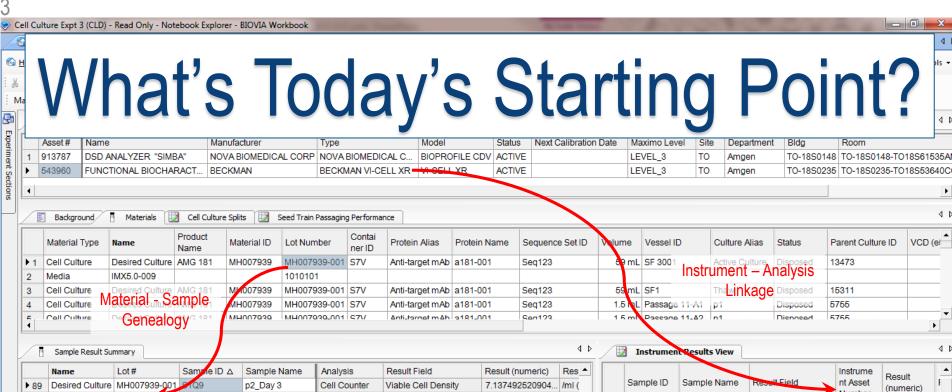


Where we are today

A Simplified Reference Data Configuration for Equipment Measurements

An Updated approach for Reading and Writing ADF





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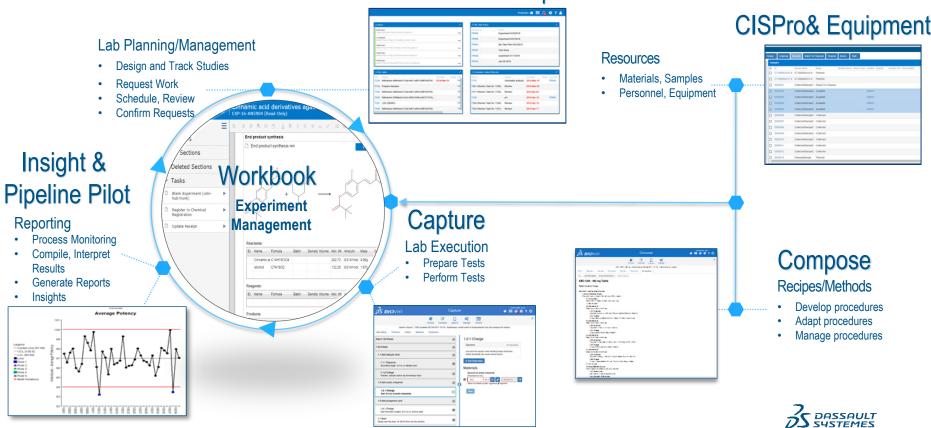
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BIOVIA ONE Lab

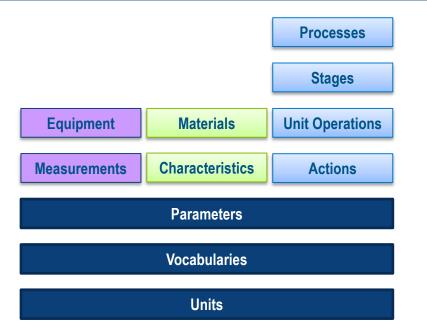
Task Planner & Samples

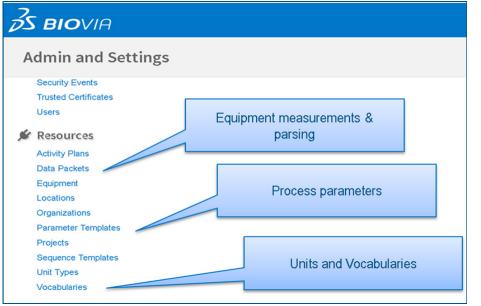


Reference Data & Ontologies

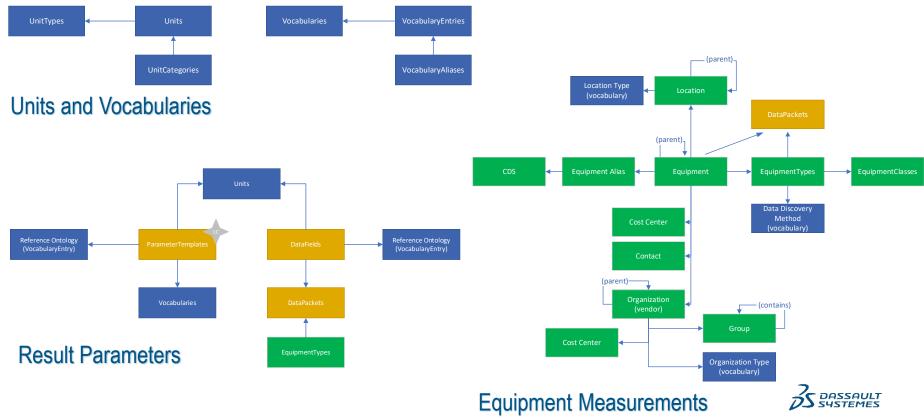
Common master data management & reference ontologies







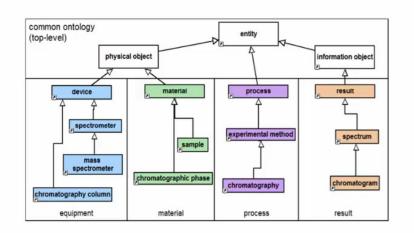
Reference Data Schematic



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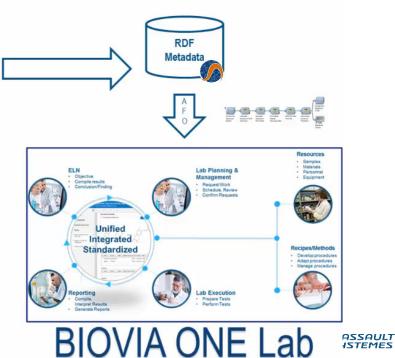
Taxonomy and Ontology Synchronization

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



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



Dassault Systèmes | 11/12/2019 | ref:: 3DS_Document_2019

Result Groups (AFR_) as Vocabularies

Allotope Result Group: nuclear magnetic resonance peak (AFR_0000451) Peak resulting from a NMR acquisition. OSTHUS Allotope Result Group: nuclear magnetic resonance spectrum (AFR_0000453) Any spectrum that shows the response of spin-active nuclei to radio frequency radiation in an applied magnetic field. CHMO Allotope Result Group: numeric term (AFR_0000622) An term in a series containing a numeric value. OSTHUS Allotope Result Group: numeric terms (AFR_0000622) An term in a series containing a numeric value. OSTHUS Allotope Result Group: numeric series (AFR_0000622) An term in a series containing a numeric value. OSTHUS Allotope Result Group: numeric series (AFR_0000623) A netric series is a series on numeric value. OSTHUS Allotope Result Group: parkit e sizing result (AFR_0000413) A particle sizing result is the outcome of a process of particle sizing. OSTHUS Allotope Result Group: parkit series (AFR_0000413) A peak describe a part of a spectrum/thromatogram/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 Image: Allotope Result Group: parkit series (AFR_000032) A peak describe a part of a spectrum/thromatogram/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 Image: Allotope Result Group: park is targe Group: park is targe Groups park is a pactic purpose OSTHUS Collection of p	ou ca	Let up the second secon	History
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Allotope Result Group: mass spectrum (AFR_0000439) Plot of the relative abundances of ions forming a beam or other collection as a function of their miz values. IUPAC MS REC Image: Allotope Result Group: Mathieu stability diagram (AFR_0000453) Graphical representation expressed in terms of dimensionless reduced coordinates that describes the stability or instability of narsped particle motion in a transmission quadrupole mass spectrum (AFR_0000453) Allotope Result Group: nuclear magnetic resonance peak (AFR_0000453) Peak resulting to ma NMR acquisition. OSTHUS Allotope Result Group: nuclear magnetic resonance spectrum (AFR_000022) Any spectrum that shows the response of spin-active nuclei to radio frequency radiation in an applied magnetic field. CHMO Image: Allotope Result Group: numeric term (AFR_000022) An uneric series is a series on tinumeric values. OSTHUS Image: Result Group: park (AFR_000022) A park (espring result sho outcome of a process of park (espring result sho outcome of a process of park (espring result sho outcome of a process of park (espring result (AFR_000022) Image: Result Group: park (AFR_000023) A park (espring result sho outcome of a process of park (espring result sho outcome of a process of park (espring result (ndependent variable) of the spectrum. This definition includes a single data point of the spectrum. OSTHUS Image: Result Group: park (Ist (AFR_0000423) A peak descritic purpose OSTHUS Image: Result Group: park (Ist (AFR_0000432) Collection of pask or pask groups for a specific purpose OSTHUS Image: Result Group: pa			Localized region of relatively intense detector resonse in a mass spectrum when ions of a specified miz are detected. If resolving power is insufficient two or more components of similar miz may contribute to one unresolved mass peak. IUPAC
Allotope Result Group: Mathieu stability diagram (AFR_000453) Graphical representation expressed in terms of dimensionless reduced coordinates that describes the stability or instability of naturality and particle motion in a transmission quadrupole mass spectrometer or Paul Ion trap, based on an appropriate Allotope Result Group: nuclear magnetic resonance peak (AFR_0000453) Peak resultation expressed in terms of dimensionless reduced coordinates that describes the stability or instability of naturality and particle motion in a transmission quadrupole mass spectrometer or Paul Ion trap, based on an appropriate Allotope Result Group: nuclear magnetic resonance peak (AFR_0000453) Any spectrum that shows the response of spin-active nuclei to radio frequency radiation in an applied magnetic field. CHIAO Allotope Result Group: numeric term (AFR_000022) An term in a series containing a numeric value. OSTHUS Allotope Result Group: pack (AFR_0000745) A particle sizing result is the outcome of a process of particle sizing. OSTHUS Allotope Result Group: pack (AFR_0000745) A particle sizing result (AFR_0000745) A particle sizing result is the outcome of a process of particle sizing. OSTHUS Allotope Result Group: pack (AFR_000012) A particle sizing ort a specific purpose OSTHUS Electrome of a process of particle sizing. OSTHUS Iolitope Result Group: pack (AFR_000032) A phanesument result is the outcome of a the process of pH measurement. OSTHUS Electrome of a pack orgen p			
Allotope Result Group: nuclear magnetic resonance peak (AFR_0000451) Peak results from a NMR acquisition. OSTHUS Allotope Result Group: nuclear magnetic resonance spectrum (AFR_000023) Any spectrum that shows the response of spin-active nuclei to radio frequency radiation in an applied magnetic field. CHMO Allotope Result Group: numeric term (AFR_000022) An term in a series containing a numeric value. OSTHUS Allotope Result Group: numeric steries (AFR_000023) An term in a series containing a numeric value. OSTHUS Allotope Result Group: pack (AFR_0000745) A netric series is a series on tunnet' value. OSTHUS Allotope Result Group: pack (AFR_0000745) A partice sizing oSTHUS Allotope Result Group: pack (AFR_0000745) A partice sizing oSTHUS Allotope Result Group: pack (AFR_0000745) A partice sizing oSTHUS Allotope Result Group: pack (AFR_0000745) A partice sizing oSTHUS Allotope Result Group: pack (AFR_0000745) Celection op packs or pack inclus proces of THUS Allotope Result Group: pack (AFR_0000025) A peak servent result is the outcome of a process of princess of THUS Allotope Result Group: proced dimage (AFR_0000351) A data set consisting of a 2D representation obtained from a sample. CHMO			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.
Allotope Result Group: nuclear magnetic resonance spectrum (AFR_000023) Any spectrum that shows the response of spin-active nuclei to radio frequency radiation in an applied magnetic field. CHMO Allotope Result Group: numeric tem (AFR_0000622) An item in a series containing a numeric value. OSTHUS Allotope Result Group: numeric series (AFR_0000623) A numeric series is a series of numeric value. OSTHUS Allotope Result Group: particle sizing result (AFR_0000745) A numeric series is a series of numeric value. OSTHUS Allotope Result Group: particle sizing result (AFR_0000745) A pack descrites a part of a spectrum/tromatogram/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 Allotope Result Group: pack (AFR_0000042) Collection of packs or pack groups for a specific purpose OSTHUS Allotope Result Group: pack (IAFR_000042) Collection of packs or pack groups for a specific purpose OSTHUS Allotope Result Group: precorded image (AFR_000025) A pheasument result is the outcome of a the process of pH measument. OSTHUS Intorpe Result Group: precorded image (AFR_0000391) A data set consisting of a 2D representation obtained from a sample. CHMO		Allotrope Result Group: nuclear magnetic resonance peak (AFR_0000451)	Peak resulting from a NMR acquisition. OSTHUS
Alordore Result Group: numeric series (AFR_0000623) A numeric series is a series of numeric values. OSTHUS Alordore Result Group: particle sizing result (AFR_0000745) A particle sizing result is the outcome of a process of particle sizing. OSTHUS Alordore Result Group: peak (AFR_000043) 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 Alordore Result Group: peak (Ist (AFR_0000432) Collection of peaks or peak groups for a specific purpose OSTHUS Alordore Result Group: peak (Ist (AFR_0000425) A phe masurement result is the outcome of a the process of ph measurement. OSTHUS Alordore Result Group: recorded image (AFR_0000391) A plata set consisting of a 2D representation obtained from a sample. CHMO		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
Allotope Result Group: particle sizing result (AFR_0000745) A particle sizing result is the outcome of a process of particle sizing. OSTHUS Allotope Result Group: peak (AFR_000043) 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 Allotope Result Group: peak list (AFR_0000432) Collection of peaks groups for a specific purpose OSTHUS Allotope Result Group: recorded image (AFR_000032) A peak accompany of a the process of ph measurement. OSTHUS Allotope Result Group: recorded image (AFR_000031) A plata set consisting of a 2D representation obtained from a sample. CHMO		Allotrope Result Group: numeric item (AFR_0000622)	An Item in a series containing a numeric value. OSTHUS
Allotope Result Group: peak (AFR_000043) A peak describes a part of a spectrum/chromatogram/piot at a definite range of the experimental parameter (independent variable) of the spectrum. This definition includes a single data point of the spectrum. OSTHUS Allotope Result Group: peak list (AFR_0000432) Collection of peaks groups for a specific purpose OSTHUS Allotope Result Group: per measurement result (AFR_0000325) A H measurement result is the outcome of a the process of pH measurement. OSTHUS Allotope Result Group: recorded image (AFR_0000391) A data set consisting of a 2D representation obtained from a sample. CHWO		Allotrope Result Group: numeric series (AFR_0000623)	A numeric series is a series of numeric values. OSTHUS
Allotrope Result Group: peak list (AFR_0000432) Collection of peaks groups for a specific purpose OSTHUS Allotrope Result Group: pH measurement result (AFR_000025) 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: particle sizing result (AFR_0000745)	A particle sizing result is the outcome of a process of particle sizing. OSTHUS
Image: Constraint of the constr		Allotrope Result Group: peak (AFR_0000413)	A peak describes a part of a spectrumic/tromatogram/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: recorded image (AFR_0000391) A data set consisting of a 2D representation obtained from a sample. CHMO		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
Allateres Desuit Crausy result (AFD, 000007)		Allotrope Result Group: recorded image (AFR_0000391)	A data set consisting of a 2D representation obtained from a sample. CHMO
Allourupe result (Arre_boulded)		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: spectrum (AFR_0000068)	A plot of a measured quantity against some experimental parameter. CHMO

8

Measurements (AFX_) as Vocabulary Entries

S BIOVIA

Vocabularies

You can define lists of terms that are available to applications that use BIOVIA Foundation. These lists are maintained in the vocabularies section.

Admin and Settings > Vocabularies

0 0 peak 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) 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 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) 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. 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 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) Allotrope Result Group; mass spectrometry peak (AFR_0000077) neak 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 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) Allotrope Result Group: peak (AFR 0000413) beak 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 neak 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) 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 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) 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 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 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 (AER: 0000413) 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 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) 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 Allotrope Result Group: peak (AFR 0000413) relative peak heigh 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 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) 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

Gene Tetreault

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MES



Existing Direct Connections

Accumet950	Julabo MD	Mettler MXS	Mettler XP204	Photovolt Aquatest-2010
AccumetAR15	Kraemer Elektronik HC 97	Mettler PB1502-S	Mettler XP205	Radiometer CDM230
AccumetAR20	Leica Auto ABBE	Mettler PB3001-S	Mettler XP20SDR	Radiometer PHM210
Advanced Instruments 3250	Metrohm 702SM Titrino	Mettler PB3002	Mettler XP26	Radiometer PHM220
Advanced Instruments 3300	Metrohm 712	Mettler PB3002-S	Mettler XP56	Radiometer PHM93
Advanced Instruments 3D3	Metrohm 737 KF Coulometer	Mettler PB302	Mettler XS1003-S	Sartorius A200
AND HR-200	Metrohm 756 KF Coulometer	Mettler PB403-S	MettlerXS104	Sartorius A200-S
Anton Paar DMA 4500	Metrohm 780	Mettler PB602-S	MettlerXS204	Sartorius AC210S
Anton Paar/Citizen DMA 5000	Metrohm 787 KF Titrino	Mettler PG1003-S	Mettler XS205	Sartorius AC211S
Beckman 360	Metrohm 795 Titrino	Mettler PG2002-S	MettlerXS205DU	Sartorius BP210D
Beckman 45 pH Meter	Metrohm 831 Coulometric	Mettler PG3001-S	Mettler XS3DU	Sartorius BP211D
Brinkmann 756 KF	Metrohm 841 KF Titrando	Mettler PG4002-S	Mettler XS603-S	Sartorius BP221S
Coulometer	Metrohm 841 Titrando	Mettler PG403-S	MettlerXS802-S	Sartorius BP3100S
Brinkmann Metrohm 713	MettlerAG104	Mettler PG6002-S	Millipore Miliflex PLUS	Sartorius BP4100S
Brookfield DVIII-LV	Mettler AG135	Mettler PM100	Mitsubishi CA-100	Sartorius CP124S
Brookfield DVIII-RV	Mettler AG204	Mettler PM1200	Mitsubishi CA-200	Sartorius CP2201
Buchi B-540	Mettler AG245	Mettler PM2000	Mitsubishi CAVA-100	Sartorius CP2202S
Corning350	Mettler AT200	Mettler PM2500	Ohaus EP-413C	Sartorius CP225D
Cornina540	Mettler AT201	Mettler PR2002	OHAUS EP612C	Sartorius CP2P-F
Cosa Instruments CAVA-100	Mettler AT250	Mettler PR2003	OHAUS Explorer	Sartorius ED6202S
Distek 2100B	MettlerAT261	Mettler PRS002	Ohaus V12140	Sartorius Genius
Dr. Schleuniger8M	Mettler AX105	Mettler PR503	Orion 150	Sartorius L 420 S
Fisher Scientific AR25	Mettler AX105DR	Mettler PR8002	Orion 150A	Sartorius LA2200S
Fiske 210	Mettler AX205	Mettler PR803	Orion 162A	Sartorius LA230S
Fluke 1523	Mettler AX26	Mettler RE40	Orion 250A	Sartorius LA310S
GTB Dissoprep MX8	Mettler AX304	Mettler SB16001	Orion 350	Sartorius LC12001S
Hach2100AN	Mettler DE40	Mettler SevenCompact	Orion 370	Sartorius LC2201
Hach Ultra Met One 3400	Mettler DL31	Mettler SevenEasy	Orion 420A	Sartorius LC220S
Hanson Research SR8 Plus	Mettler DL36	Mettler SevenMulti	Orion 720A	Sartorius LC4200S
Holland C50	Mettler DL38	Mettler SR16001	Orion 920A	Sartorius LE2202S
Jerway 3020	Mettler HB43	Mettler UMX2	Paar DMA48	Sartorius LE225D
Jerway 3320	Mettler MPC227	Mettler WXSS205DU	Perkin Elmer 341	Sartorius LE26P
Julabo F26MV	Mettler MT5	Mettler XP1203-S	Photovolt Aquatest - 10	Sartorius LE4202S

)	Sartorius LP1200	Thermo Orion 420A+
	Sartorius LP2200S	Thermo Orion 520A+
	Sartorius LP3200D	Thermo Orion 720A Plus
	Sartorius LP4200S	TSI4043
	Sartorius LP5200P	Turner Quantech FM109535
	Sartorius LP620S	VanKel 25-1000
	Sartorius M-power	Vankel VK 200
	Sartorius MSP	Vankel VK7000
	Sartorius MA40	WWR sympHony SB70P
	Sartorius M451	WVR sympHony SB80PC
	Sartorius MC210P	WVR sympHony SP21
	Sartorius MC210S	WVR sympHony SP70P
	Sartorius MC5	WVR sympHony SR301
	Sartorius ME215P	WVR sympHony SR301
	Sartorius ME215S	WWR sympHony SR40C
	Sartorius ME235	Wescor5520
	Sartorius ME235P	YSI 3200
	Sartorius ME235S	Zeiss MCS311
	Sartorius ME36S	266510/04011
	Sartorius ME5	
	Sartorius MSA6.6S	
	Sartorius R160P	
	Sartorius R200-D	
	Sartorius RC210S	
	Sartorius SE2	
	Sartorius TE612	
	Shimadzu AUW1200	
	Sotax HT1	
	Stanford Research OptiMelt	
	Thermo Orion 150 A+	
	Thermo Orion 3 Star	
	Thermo Orion 370	
	Thermo Orion 4 Star	

Existing Parsers

ABI 7900 HT ABI QuantStudio7 Agilent 2100 Expert Bioanalyzer Agilent Cary 60 AKTA Crossflow AKTA Explorer Analytical ultracentrifuge Barcode Labeling Biacore 3000 **BioRad ChemiDoc MP BioRad ChemiDoc ProteinGel** Bruker B-ACS120 NMR Bruker Vertex 70 FTIR CARY 50 Cedex Cedex HR Circular Dichroism Compression Tester **Digital Coordinate Measuring Machine Dynamic Vapor Sorption** Force Tester Fortebio

GUAVA EASTCYTE Headspace Analyzer FMS-1400 Headspace Analyzer FMS-760 iCDataCenter ICP-MS Korsch XM12 Leak Detector 325 Leak Detector 455 Leak Detector 655 Lyophilizer Lyostar II Lyophilizer Lyostar III Malvern Particle Sizer (Mastersizer 2000 and 3000) Micro Flow Imaging (MFI) Multi-Angle static Light Scattering Nano Drop 1000 Nova Biomedical Flex Nova CDV **Optical Comparator** Particle Counter (Single) HIAC Particle Counter Auto Particle Vision System Pendotech

Plate Reader (Envision) Plunger Inspection Device Polarimeter (Autopol V Plus) PVM Raman Rigaku Firstguard Robotic Drop Tester TA DSC TecanMagellan Tecan-gPCR Tenney Environmental Chamber Tensiometer Thermogravimetric Analyzer GA Q500 Tiamo KF Transportation Lab Environmental Chamber Tristar Surface Area Varian Cary SoloVPE Varian Spec 4000 ViCell Viscometer (Rheometer) VMAX X-Ray (Xpert Data Viewer) 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

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Ea	uipment						
	in and Settings > Equipm	nent					History
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	ments and other equipm				d Items:		
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Regist	ering a piece of equipm	ent involves sel	ecting its type (see	• Eq	uipment Types		
Equipr	ment Types) and may in						
with it	to retrieve readings.						
	Filter Equipment						
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		T Barcode BAL1	Nickname PRP-BAL-1	Equipmen Mettler AG245	Serial Number US9849878	Location Prep Lab	Primary
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	Display Name BAL1 (PRP-BAL-1)	BAL1	PRP-BAL-1	Mettler AG245	US9849878	Prep Lab	Primary
	Display Name BAL1 (PRP-BAL-1) BAL2 (PRP-BAL-2)	BAL1 BAL2	PRP-BAL-1 PRP-BAL-2	Mettler AG245 Mettler AG245	US9849878 US8978787	Prep Lab Prep Lab	Primary
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	Display Name BAL1 (PRP-BAL-1) BAL2 (PRP-BAL-2) BAL3 (CHM-BAL-1) BAL4 (MCR-BAL-1)	BAL1 BAL2 BAL3 BAL4	PRP-BAL-1 PRP-BAL-2 CHM-BAL-1 MCR-BAL-1	Mettler AG245 Mettler AG245 Mettler AG245 Mettler AG245	US9849878 US8978787 US8798798 US88789798	Prep Lab Prep Lab Chemistry Lab Micro Lab	Primary
	Display Name BAL1 (PRP-BAL-1) BAL2 (PRP-BAL-2) BAL3 (CHM-BAL-1) BAL4 (MCR-BAL-1) BAL5 (MCR-BAL-2)	BAL1 BAL2 BAL3 BAL4 BAL5	PRP-BAL-1 PRP-BAL-2 CHM-BAL-1 MCR-BAL-1 MCR-BAL-2	Mettler AG245 Mettler AG245 Mettler AG245 Mettler AG245 Mettler AG245	US9849878 US8978787 US8798798 US88789798 US88789798	Prep Lab Prep Lab Chemistry Lab Micro Lab Micro Lab	Primary
	Display Name BAL1 (PRP-BAL-1) BAL2 (PRP-BAL-2) BAL3 (CHM-BAL-1) BAL4 (MCR-BAL-1) BAL5 (MCR-BAL-2)	BAL1 BAL2 BAL3 BAL4 BAL5	PRP-BAL-1 PRP-BAL-2 CHM-BAL-1 MCR-BAL-1 MCR-BAL-2	Mettler AG245 Mettler AG245 Mettler AG245 Mettler AG245 Mettler AG245	US9849878 US8978787 US8798798 US88789798 US88789798	Prep Lab Prep Lab Chemistry Lab Micro Lab Micro Lab	Primary
	Display Name BAL1 (PRP-BAL-1) BAL2 (PRP-BAL-2) BAL3 (CHM-BAL-1) BAL4 (MCR-BAL-1) BAL5 (MCR-BAL-2)	BAL1 BAL2 BAL3 BAL4 BAL5	PRP-BAL-1 PRP-BAL-2 CHM-BAL-1 MCR-BAL-1 MCR-BAL-2	Mettler AG245 Mettler AG245 Mettler AG245 Mettler AG245 Mettler AG245	US9849878 US8978787 US8798798 US88789798 US88789798	Prep Lab Prep Lab Chemistry Lab Micro Lab Micro Lab	Primary
	Display Name BAL1 (PRP-BAL-1) BAL2 (PRP-BAL-2) BAL3 (CHM-BAL-1) BAL4 (MCR-BAL-1) BAL5 (MCR-BAL-2)	BAL1 BAL2 BAL3 BAL4 BAL5	PRP-BAL-1 PRP-BAL-2 CHM-BAL-1 MCR-BAL-1 MCR-BAL-2	Mettler AG245 Mettler AG245 Mettler AG245 Mettler AG245 Mettler AG245	US9849878 US8978787 US8798798 US88789798 US88789798	Prep Lab Prep Lab Chemistry Lab Micro Lab Micro Lab	Primary
	Display Name BAL1 (PRP-BAL-1) BAL2 (PRP-BAL-2) BAL3 (CHM-BAL-1) BAL4 (MCR-BAL-1) BAL5 (MCR-BAL-2)	BAL1 BAL2 BAL3 BAL4 BAL5	PRP-BAL-1 PRP-BAL-2 CHM-BAL-1 MCR-BAL-1 MCR-BAL-2	Mettler AG245 Mettler AG245 Mettler AG245 Mettler AG245 Mettler AG245	US9849878 US8978787 US8798798 US88789798 US88789798	Prep Lab Prep Lab Chemistry Lab Micro Lab Micro Lab	Primary
	Display Name BAL1 (PRP-BAL-1) BAL2 (PRP-BAL-2) BAL3 (CHM-BAL-1) BAL4 (MCR-BAL-1) BAL5 (MCR-BAL-2)	BAL1 BAL2 BAL3 BAL4 BAL5	PRP-BAL-1 PRP-BAL-2 CHM-BAL-1 MCR-BAL-1 MCR-BAL-2	Mettler AG245 Mettler AG245 Mettler AG245 Mettler AG245 Mettler AG245	US9849878 US8978787 US8798798 US88789798 US88789798	Prep Lab Prep Lab Chemistry Lab Micro Lab Micro Lab	Primary
	Display Name BAL1 (PRP-BAL-1) BAL2 (PRP-BAL-2) BAL3 (CHM-BAL-1) BAL4 (MCR-BAL-1) BAL5 (MCR-BAL-2)	BAL1 BAL2 BAL3 BAL4 BAL5	PRP-BAL-1 PRP-BAL-2 CHM-BAL-1 MCR-BAL-1 MCR-BAL-2	Mettler AG245 Mettler AG245 Mettler AG245 Mettler AG245 Mettler AG245	US9849878 US8978787 US8798798 US88789798 US88789798	Prep Lab Prep Lab Chemistry Lab Micro Lab Micro Lab	Primary
	Display Name BAL1 (PRP-BAL-1) BAL2 (PRP-BAL-2) BAL3 (CHM-BAL-1) BAL4 (MCR-BAL-1) BAL5 (MCR-BAL-2)	BAL1 BAL2 BAL3 BAL4 BAL5	PRP-BAL-1 PRP-BAL-2 CHM-BAL-1 MCR-BAL-1 MCR-BAL-2	Mettler AG245 Mettler AG245 Mettler AG245 Mettler AG245 Mettler AG245	US9849878 US8978787 US8798798 US88789798 US88789798	Prep Lab Prep Lab Chemistry Lab Micro Lab Micro Lab	Primary





Equipment Model Overview

Equipment Class



Equipment

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 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.

> 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



Equipment Classes

Admin and Settings > Equipment > Equipment Classes

Classifications make it easier for users to find equipment by grouping simil classes include balances, pH meters, and HPLCs.

Equipment class is a required field when defining an equipment type.

0 0 2	Filter Equipment Classes
	Name
	Analytical Balance
	Analyzer
	Balance
	Bioreactor
	Calorimeter
	Conductivity Meter
	Conductometer
	Coulometer
	Densitometer
	Density Meter
	Dissolution Bath
	DissoPrep
	Flow Meter
	Flaorometer
	Gas Chromatograph
	DO SYSTEMES

Equipment Example

Equipment Class

Gas Chromatograph

Equipment Type Agilent 6890

S BIOVIA

Agilent 6890 Gas Chromatograph

Admin and Settings > Equipment > Equipment Types > Agilent 6890 Gas Chromatograph

General Inventory	Name: Agilent 6890 Gas Chromatograph	Manufacturer: Agilent
Commands	Data Packet:	Equipment Class
	GC Data	Gas Chromatograph

Equipment Instance CHM-GC-1





Equipment Example

Equipment Class

Gas Chromatograph

Equipment Type Agilent 6890 35 BIOVIA

Agilent 6890 Gas Chromatograph

Equipment:

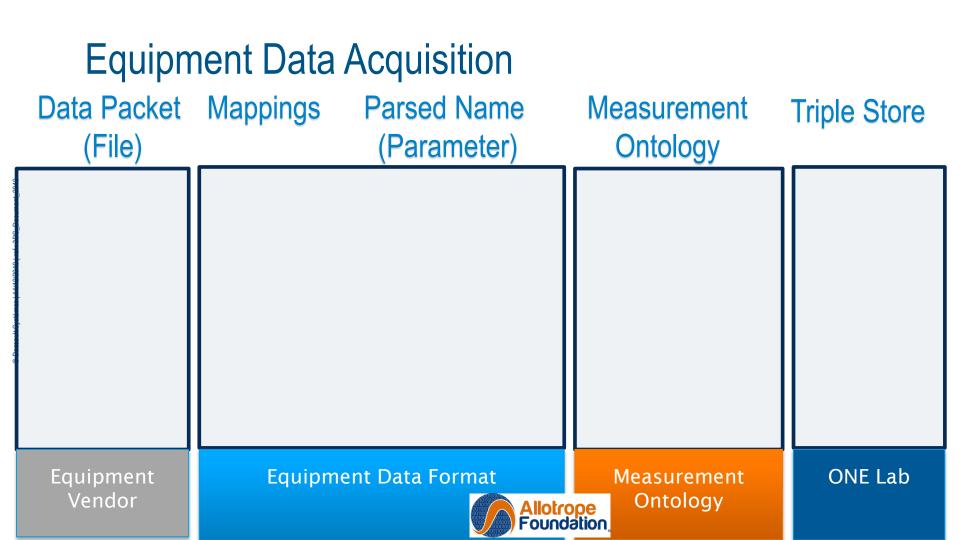
Admin and Settings > Equipment > Equipment Types > Agilent 6890 Gas Chromatograph

General Inventory Commands

GC-1 (CHM-GC-1) Milford Aqilent 6890 Gas Chromatograph (Gas Chromatograph)

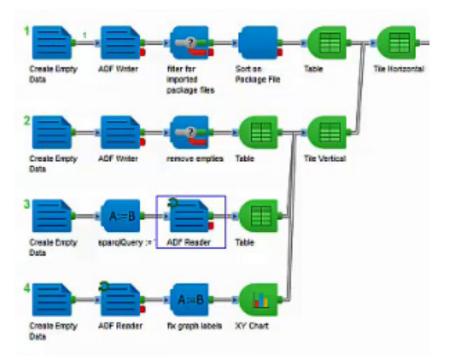
Equipment Instance CHM-GC-1





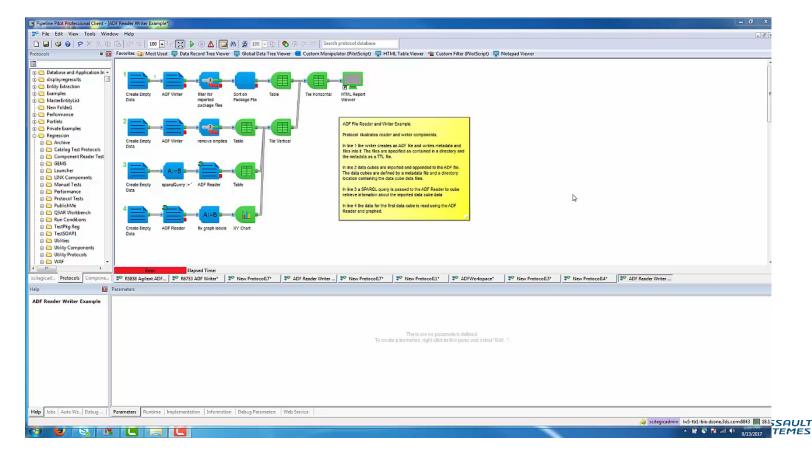
BIOVIA – Allotrope ADF Support in ONELab

- 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





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

	Weight Admin and Settings > Data Packets > Data Fields >	Weight
	Data Packet:	
	Balance	
	Is Sample Id:	
	Is Group By:	
	Display Order:	
BGA D	ata	
Admin and S	ettings > Data Packets > BGA Data	
Description:		▼
This is a data p	acket for BGA	
		▼
Data Fields:		
mPO2		v
mpH		
mPCO2		
mBP		
iFIO2		
« «	Page 1 of 2	
Last Updated	d:	





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



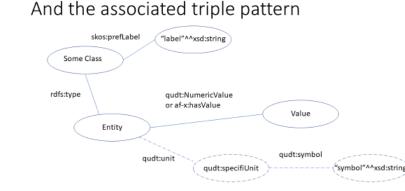
BIOVIA – Allotrope Ontology Support

- 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 <u>name:value</u> pairs

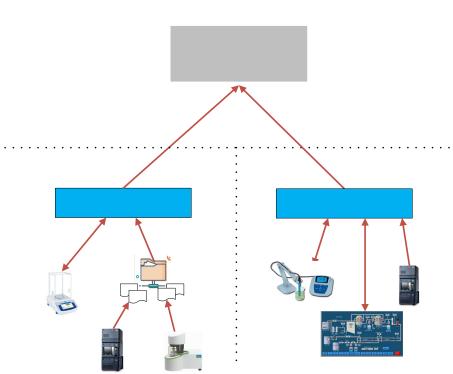
Vi-CELL XR 2.04

Beckman Coulter, Inc.

Sample ID	Dilution	Sample date	Viability	Total cells	Viable cells	Avg. diam.
	factor		(%)	/ml (x10^6)	/ml (x10^6)	(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

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)
 - \triangleright 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 Labconnected equipment
 - Reading Allotrope ADF files from Allotropeenabled instruments





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).



