



**Allotrope**  
**Foundation**  
Building an Open Framework for Laboratory Data

# Allotrope Framework implementation in the Bioanalytical Lab

**Dr. Gerhard Noelken**

Allotrope BoD member, Pfizer Allotrope Liaison

EBF 8<sup>th</sup> Open Meeting

19 November 2015



# Allotrope Foundation

## Member Companies

AbbVie  
Amgen  
Baxter  
Bayer

Biogen  
Boehringer Ingelheim  
Bristol-Myers Squibb  
Eli Lilly

Genentech/Roche  
GlaxoSmithKline  
Merck & Co.  
Pfizer

## Secretariat

DrinkerBiddle

- Project Management
- Legal & Logistical Support

## Professional Software Firm

  
success with R&D

- Framework Development
- Technical Leadership

## Partner Network



ACD/Labs

Agilent

Biovia

BSSN

IDBS

Mestrelab Research

Mettler Toledo

Persistent

Riffyn

Sartorius

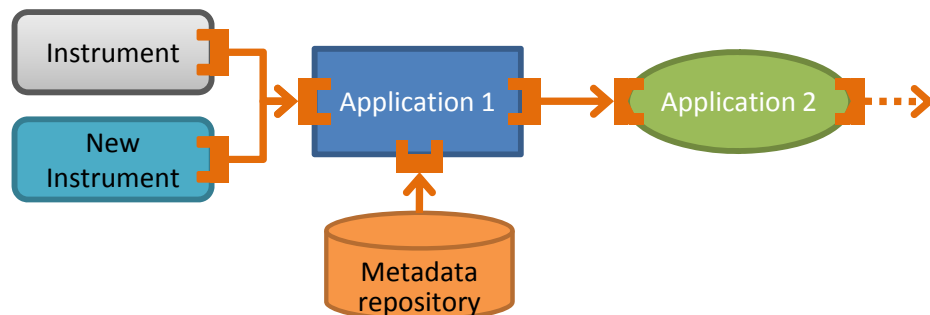
Shimadzu

Thermo Scientific

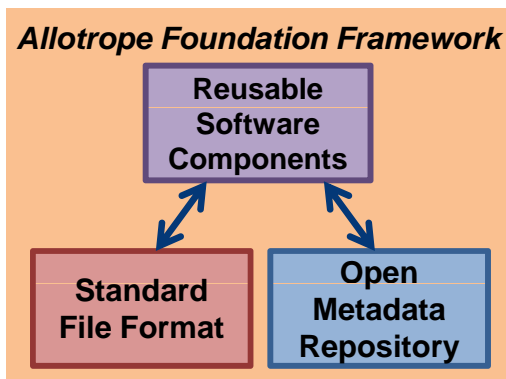
Waters

Erasmus Univ.  
Med Center  
University of  
Southampton

# What is Allotrope Creating?

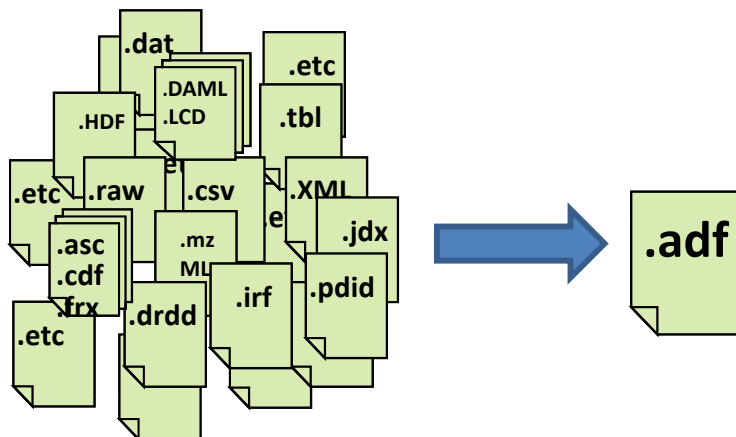


A **toolkit** that enables use of the standards & metadata in software development



File format for any technique or instrument

Standard vocabulary & structure for metadata

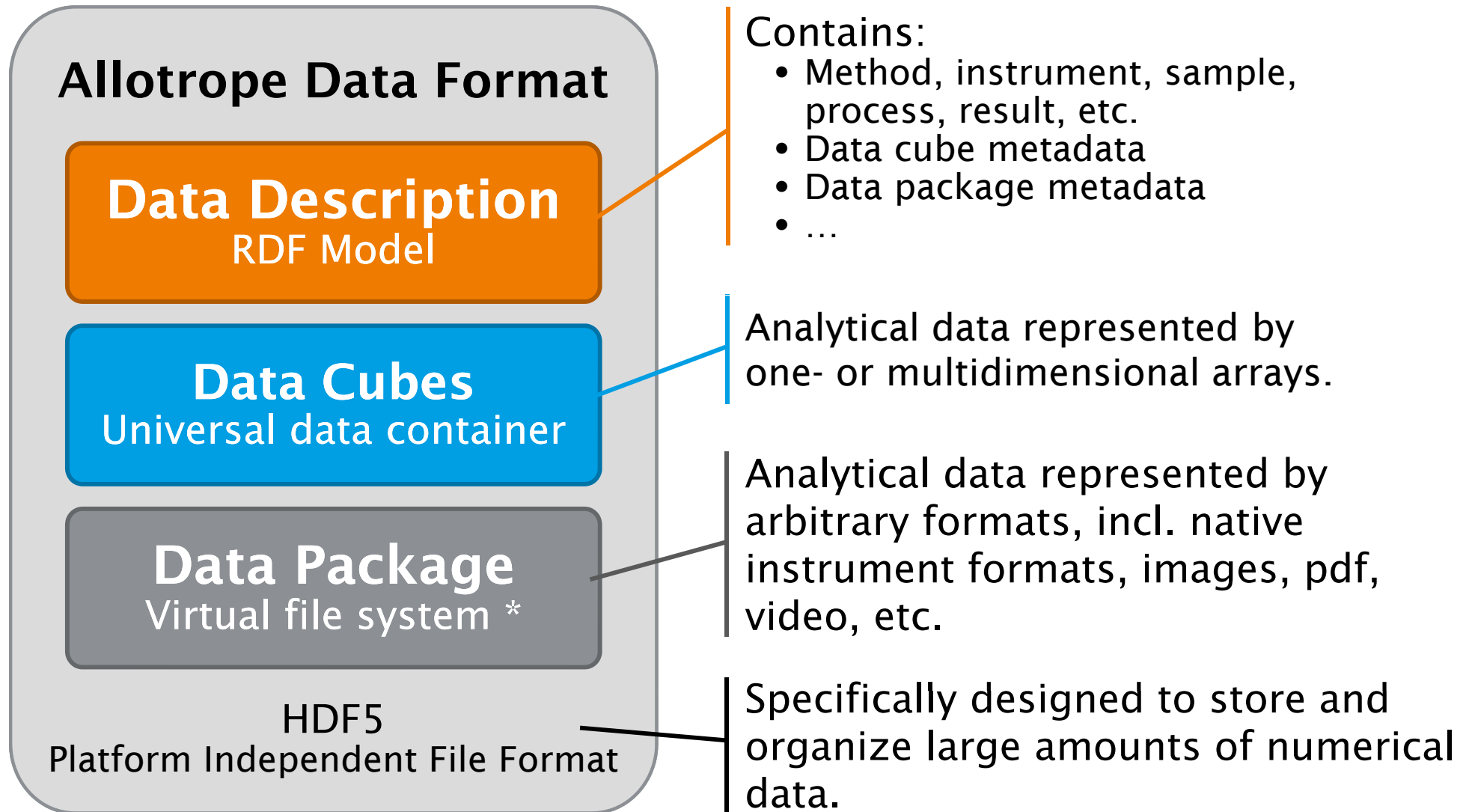


Project	Test	Instrument
AF 0012354	IR Fingerprinting	QC Lab #33B 380 FT-IR
AE0012764	Bulk & Tapped Density	ASTM Standard Seive #6
AF 12989	NMR Characterization	AM500
	Tapped & Bulk Density	Sieve XXX
AF0045674	Caractérisation RMN	Nouvelle DRX600
AF-0034558	IR	iS10 FT-IR

With the Metadata Repository

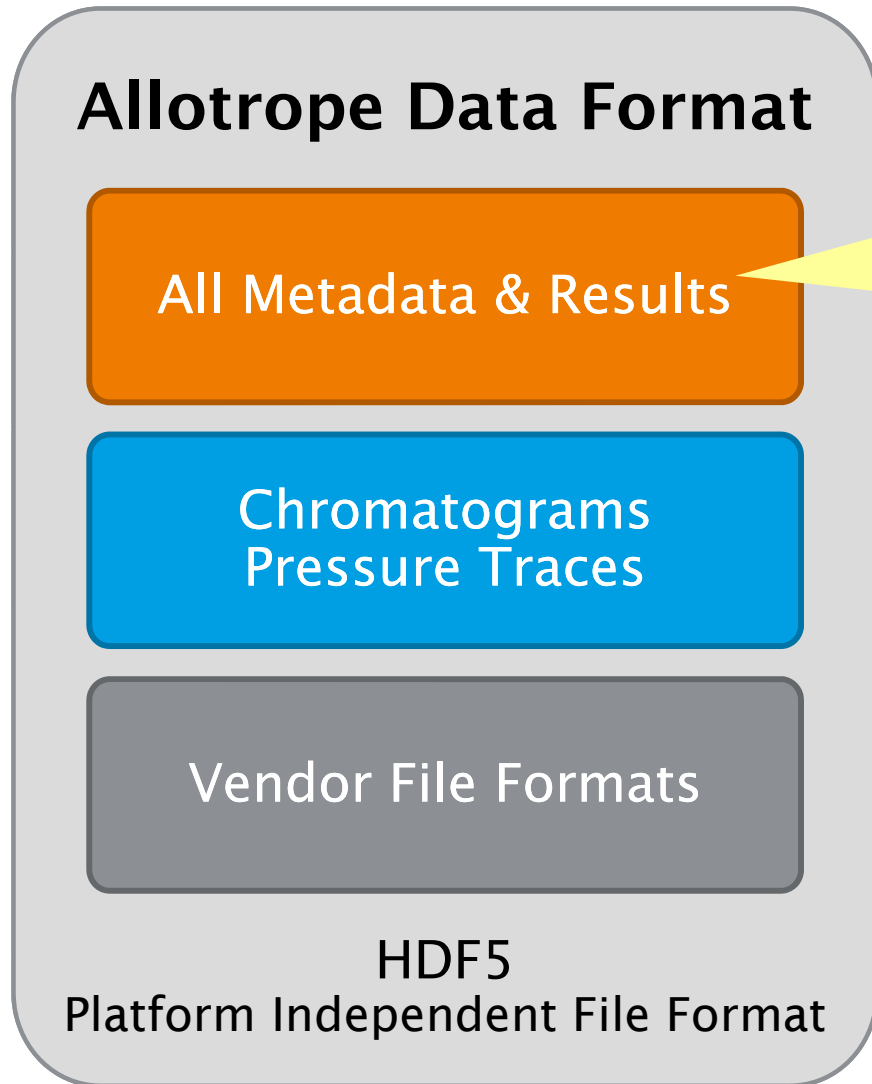
Project	Test	Instrument
AF0012354	IR Fingerprinting	380 FTIR/-SN/145453
AF0012764	Bulk and Tapped Density	ASTM Sieve-SN/3452
AF0012989	NMR Characterization	AM500-SN/0034578
AF0013142	Bulk and Tapped Density	ASTM Sieve-SN/09783
AF0045674	NMR Characterization	DRX600-SN/10234567
AF0034558	IR Fingerprinting	iS10 FTIR/-SN/341980

# Allotrope Data Format (ADF)



\* Use is optional

# Example: 36-Month Stability Protocol



Method, Impurities, Peaks, Decisions, Stability Time Point, Packaging Configuration, Storage Conditions, Sample Preparation Events, Weights, Concentrations, Specifications, Integration Events, Scientist, Time Stamps, Audit Trail, Measurement System, Real-Time SOP & Compliance Checks

Enterprise Analytics  
Long-Term Preservation  
Stability Reports  
Regulatory Submissions  
Inspections, Audits  
Data Exchange  
Confidence in Data



# Allotrope Taxonomies: An Extensible Metadata Model

- **A library of extensible taxonomies**
  - Uses W3C standards
  - Easy to understand and maintain by SMEs and Vendors
- **Start by harvesting existing available concepts**
  - PSI-MS; IUPAC; RSC Chemical Methods Ontology; Dictionary of weighing terms; AnIML, etc
- **Reproducible & efficient collaboration model**
  - Leverages knowledge engineers & member company scientists
  - 2-3 weeks to develop initial version of a new taxonomy
- **Initial versions of 12 analytical techniques already implemented:**
  - gas chromatography
  - Karl Fischer
  - liquid chromatography
  - mass spectrometry
  - nuclear magnetic resonance spectroscopy
  - thermogravimetric analysis
  - ultra violet spectrometry
  - cell counter
  - cell culture analyzer
  - blood gas analysis
  - balance
  - pH

# More Taxonomies Available in 1Q 2016

- **Instrument Taxonomies**

- Protein Characterization
- Microplate Reader
- Flow Cytometer
- Protein Purification
- Millipore Filtration System
- Differential Scanning Calorimetry (DSC)
- X-Ray Power Diffraction (XRPD)
- Particle Sizer
- Roller Press
- Tablet Pressing
- Tablet Coating
- Dynamic Vapor Sorption (DVS)
- solid-state NMR (ssNMR)
- Infrared Spectroscopy (IR)

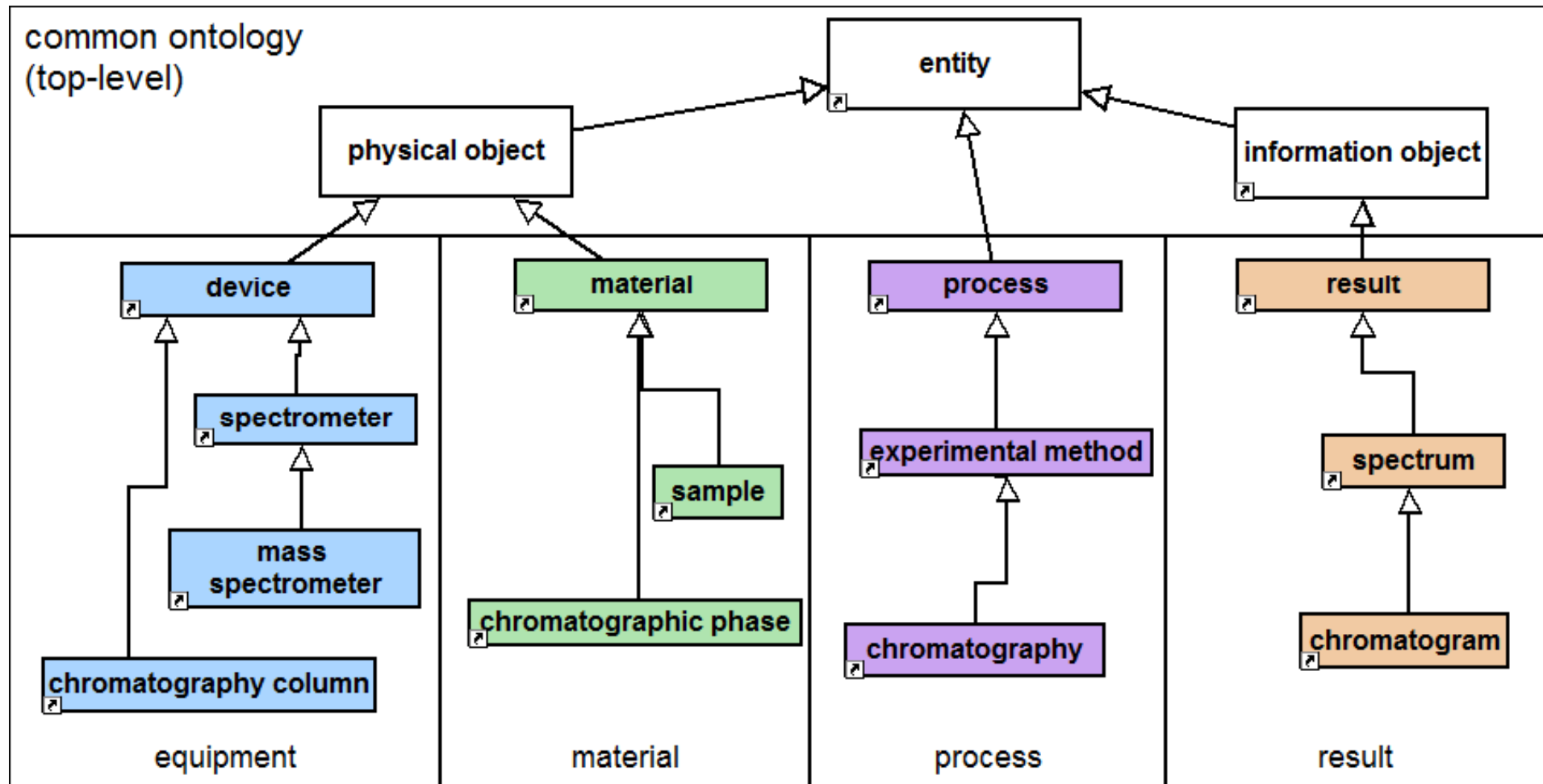
- **Other Taxonomies**

- IDMP-Identification of Medicinal Products
- Extend Process (S88)
- Extend Materials
- Extend Equipment
- Investigation/Study/Analysis
- Phase of Development
- Route of Administration
- Product Quality Attributes
- Container Categories
- Chemical Reactions

**Funded by Individual Allotrope  
Member**

**Shared with Allotrope Foundation**

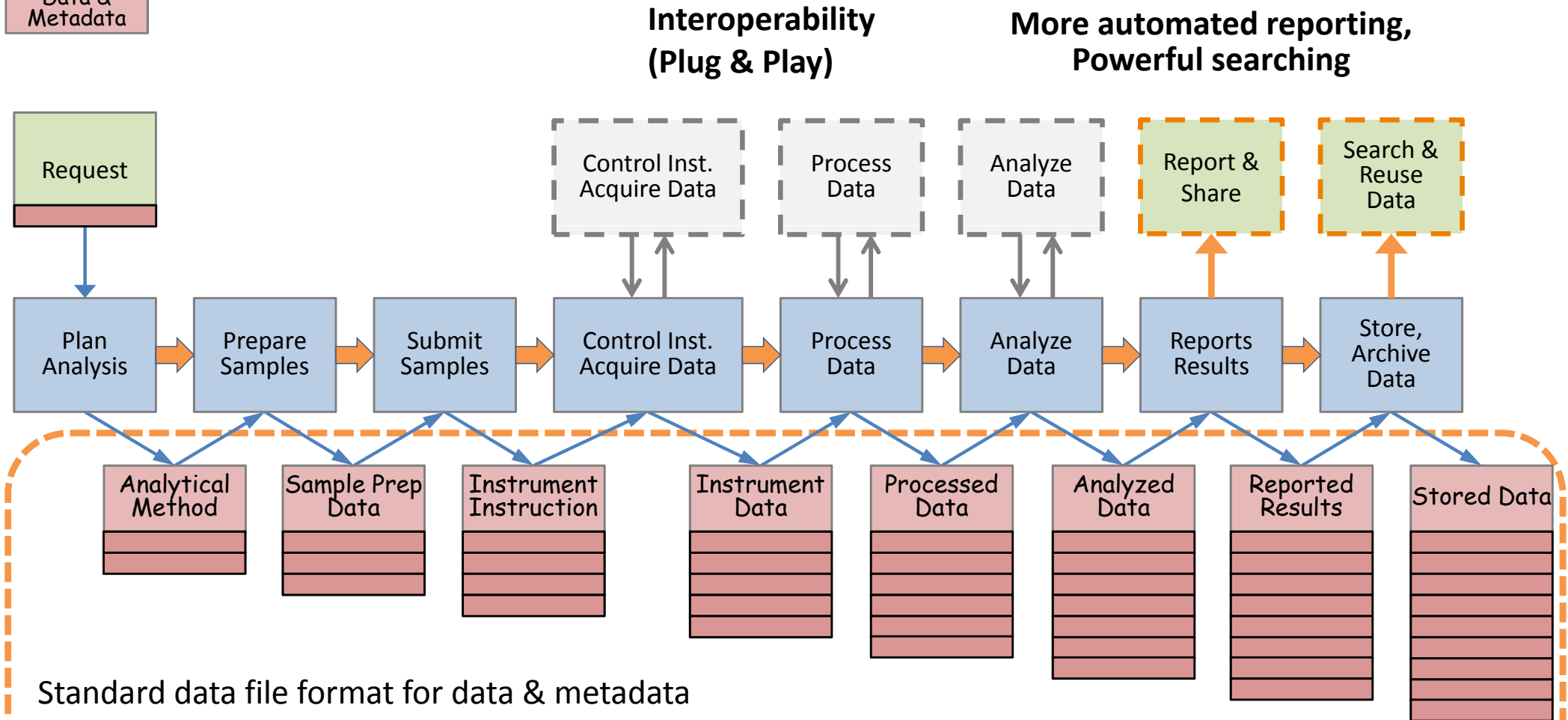
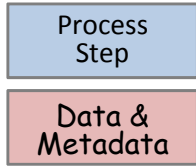
# Allotrope Foundation Taxonomies





# The ADF enables a self-contained documentation of the data & metadata

Legend



Standard data file format for data & metadata

Output from one system becomes the input to the next

The APIs enable the use of one vendor agnostic file format

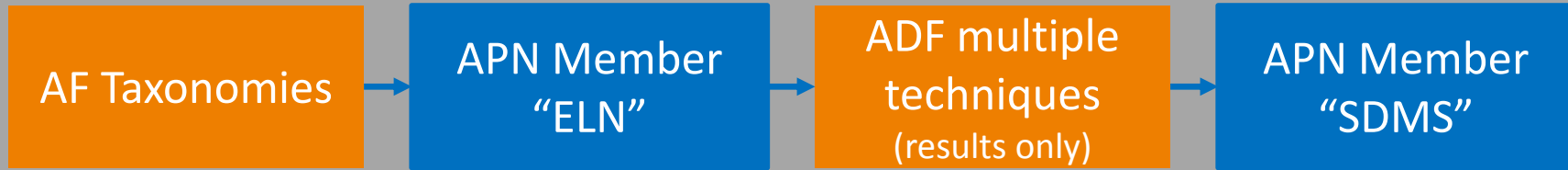
# Integration Projects Reduce it to Practice

- Divide and conquer: members share the costs and benefits
- Early adoption and acceleration of AF Framework development through delivery of Framework components.
- Accelerate vendor adoption via collaboration on delivering specific capabilities through the integration projects
- Ensure the validity of the Framework through real-world requirements and implementation.
- Benefit the sponsoring companies in terms of shared development of new functionality & shared experience
- Drive integration of the Framework into the IT/IS Roadmap

# Integration Projects

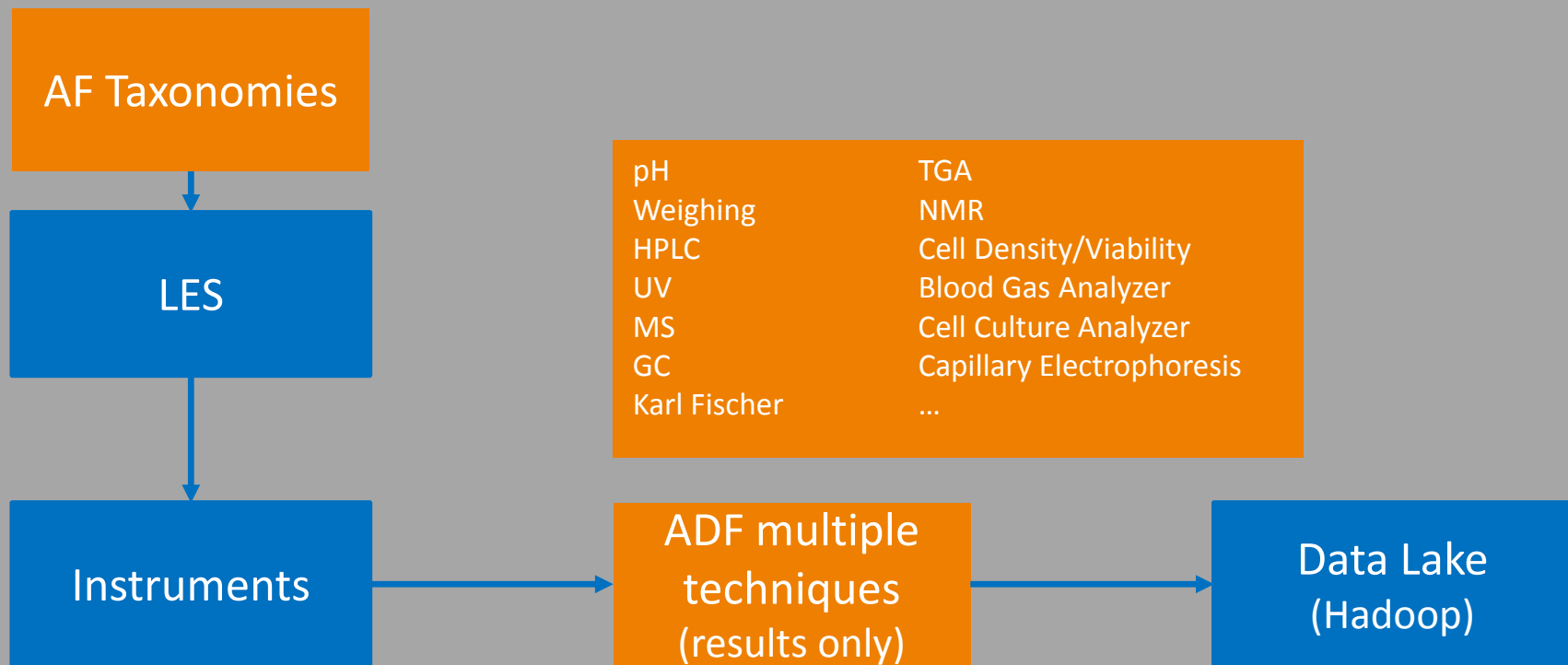
	Research	Development	Commercial	
A	pH, Weighing, GC, Karl Fischer, TGA, NMR, Cell Density/Viability, Blood Gas Analyzer, Cell Culture Analyzer, Capillary Electrophoresis ...	Multiple types	Small and Large Molecule CMC	
B		ICP-MS	Elemental Impurities	
C		Bioanalyzer	Fermentation Process Control	
D		HPLC-UV	CRO Integration	
E		HPLC-MS	Structure ID	
F	HPLC-UV/MS	Structure ID, Purification, In vitro Bioanalysis		
G	HPLC-UV	Assay, Purity		
H		HPLC-UV Balance	Drug Substance Release & Stability	
I	HPLC-UV/MS	Method Screening		
J	HPLC-UV	LC Data to ADF Converter/Adapter		
	Member	Instrument	non-GMP	GMP

## APN Member PoCs



# Integration Project A

## GMP Development



# Summary

2012

Allotrope Foundation



INTERNATIONAL  
INNOVATION  
PHARMACEUTICALS

2013

- Initiated software development and evaluations

2014

- Established feasibility through PoCs
- ADF design &

2015

- Framework Development
- Integration at Members

2016

- Framework used in production
- First Public release



**FOR IMMEDIATE RELEASE:** September 30, 2015

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## Allotrope Foundation Releases Allotrope Framework 1.0

Washington, DC – Allotrope Foundation today announces a major milestone: release of the first production version of its flagship Allotrope Framework to Allotrope Foundation and Allotrope Partner Network Members. The September internal release package includes version 1.0 of the Allotrope Data Format (ADF), the Application Programming Interfaces, (APIs), and the Allotrope Foundation Taxonomies (AFTs), marking the successful completion of the early phases of development. Designed for Allotrope Foundation by OSTHUS, a leading information management and technology services firm, the Allotrope Framework is an advanced data architecture that facilitates the creation, use and exchange of laboratory data by standardizing data representation across proprietary equipment and software.



# The Framework will provide Business benefit

## Less Manual Document Preparation

- Find data quickly/logically
- Eliminate Copy/paste
- No more Transcription/conversion
- Source agnostic

## Improved Data Integrity

- Eliminate error due to manual text entry or transcription
- Complete, consistent, accurate metadata

## Seamless data exchange & with partners & CROs

- One data file format
- One consistent vocabulary
- Reduced cost & complexity to CROs, CMOs, partnerships

## Lower Data Management Costs

- Interoperability
- Future-proof against future data migrations
- Reduced technical debt: no more maintenance of legacy systems
- Improved archiving

## Facilitate Regulatory Compliance

- Improved instrument & software validation tracking
- Reduced complexity in system documentation
- Simpler to support questions/investigations

## Extracting Knowledge & Value from Data

- Greatly enhance speed to answer/decision
- Remove data silos
- Create an ecosystem for innovation
- Facilitates data mining & analytics

***What are your priorities?***

# Thank you!

To join or get additional information, contact:

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