



The Allotrope Framework:

An innovative approach to improve data integrity, reduce waste, & realize the full value of your data

European Bioanalysis Forum e-data workshop

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Agenda

- Introduction to Allotrope Foundation (Gerhard Noelken, Pfizer)
- The elements of the Allotrope Framework (Wolfgang Colzman, Osthus)
 - Allotrope Data Format
 - Standard Vocabulary
 - Application Programming Interface

Current Allotrope Foundation Members

- AbbVie
- Amgen
- Baxter
- Biogen Idec
- Boehringer Ingelheim
- Bristol-Myers Squibb
- Eisai
- Genentech/Roche
- GlaxoSmithKline
- Merck
- Pfizer

* underlined are also EBF members

Allotrope Foundation

Pharmaceutical &
Biotechnology
Companies

- Subject Matter Experts
- Project Funding

Secretariat

DrinkerBiddle

- Project Management
- Legal & Logistical Support

Professional
Software Firm

 OSTHUS
success with R&D

- Software Development
- Technical Leadership

Partner Network

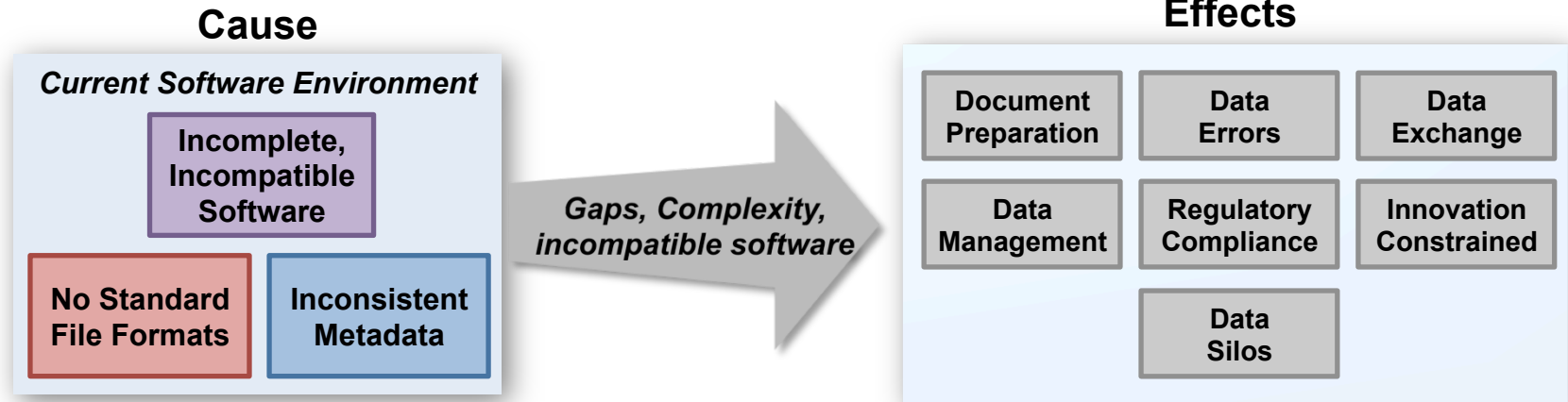


- Requirements & Specifications
- Contributions, PoC Applications

What problems are we trying to solve?

- It's hard to find data based on [study, project, analyst, technique, etc]
- It's hard to share, compare or integrate data from different labs or instruments because the file format is different
- It's hard to analyze or mine a collection or archive of data because the details of the experiment and the context is stored somewhere else (metadata)
- Can't understand /interpret data because the context is incomplete, inconsistent, often free text
- Other efficiency opportunities, e.g. Instruments and software are not interoperable
- **Common Costs & Limitations in Data Lifecycle with downstream effects well beyond the 'analytical lab'**

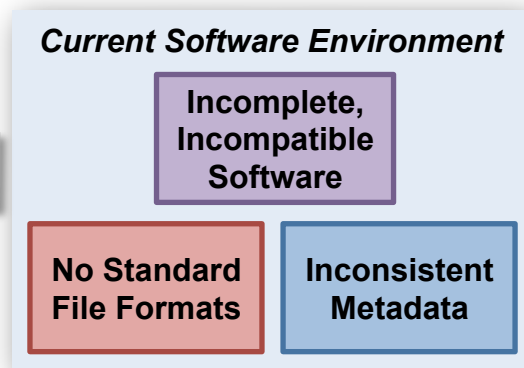
The Root of the Problem



The Framework Components

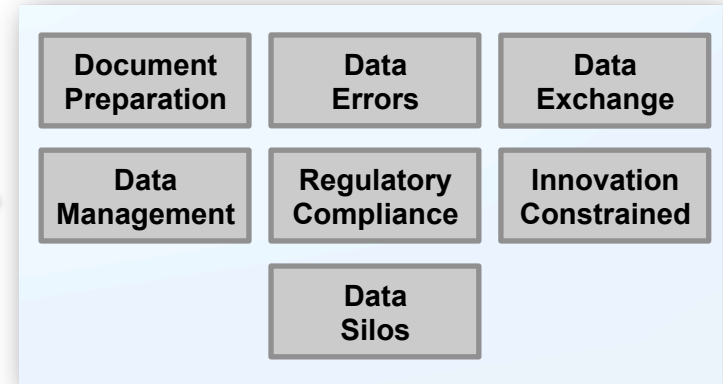
Fix the Root Cause

Cause

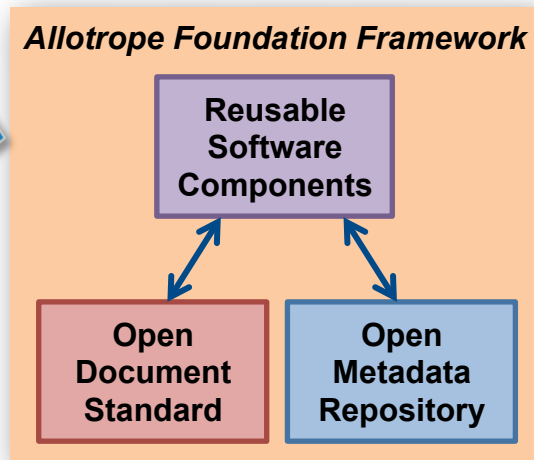


Gaps, Complexity, incompatible software

Effects

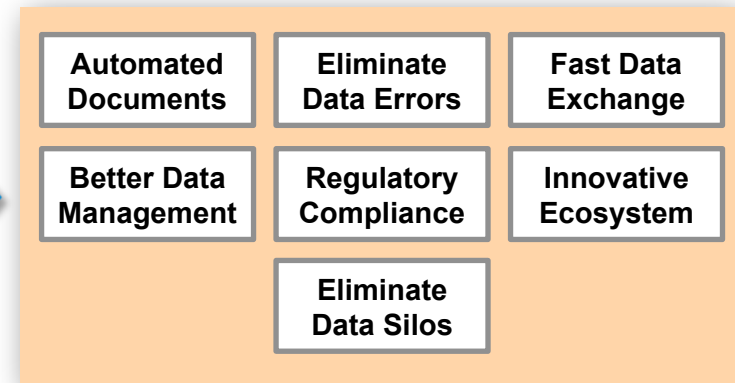


Fix the root cause



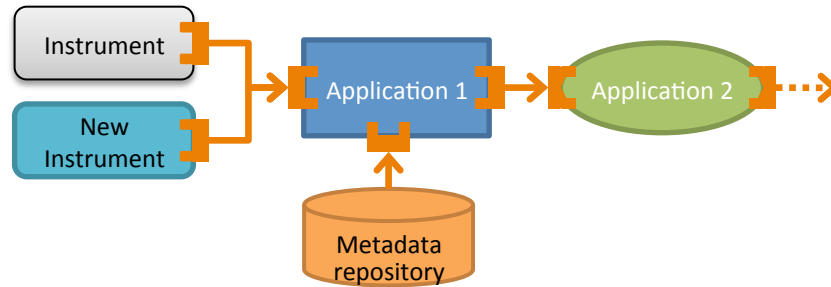
Efficient, Innovative, Powerful Software

Reap the benefits

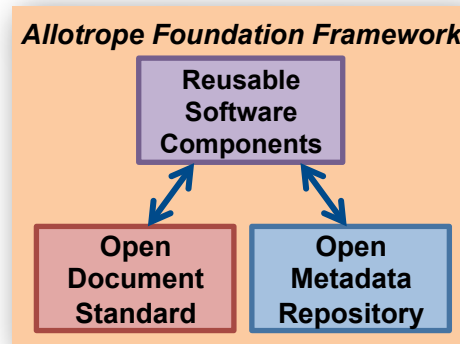


Scientists focus on science

What is Allotrope Creating?

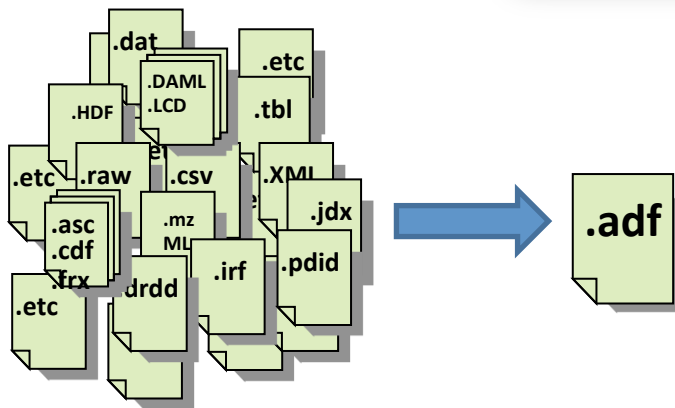


A **toolkit** that enables use of the standards and metadata in software development



The set of standards used based on our requirements

The core of the controlled vocabulary



Project	Test	Instrument
AF 0012354	IR Fingerprinting	QC Lab #33B 380 FT-IR
AE0012764	Bulk & Tapped Density	ASTM Standard Sieve #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

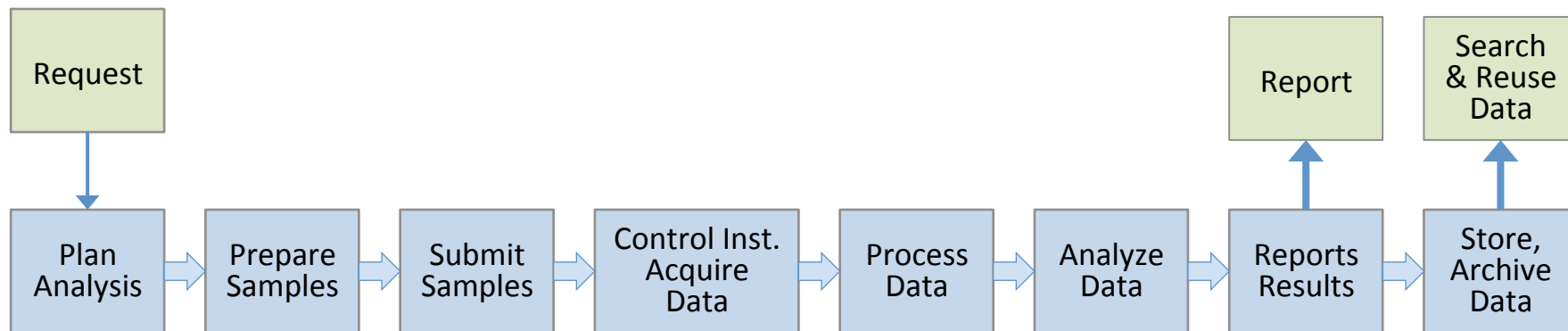
Project	Test	Instrument
AF0012354	IR Fingerprinting	380 FTIR/-SN/145453
AF0012764	Bulk and Tapped Density	ASTM Sieve-SN/3452
AF0012989	NMR Characterization	AM500-SN/0034578
AF0013142	Bulk and Tapped Density	ASTM Sieve-SN/09783
AF0045674	NMR Characterization	DRX600-SN/10234567
AF0034558	IR Fingerprinting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

The basic analytical workflow and data flow standardized

Legend

Process Step

Data & Metadata

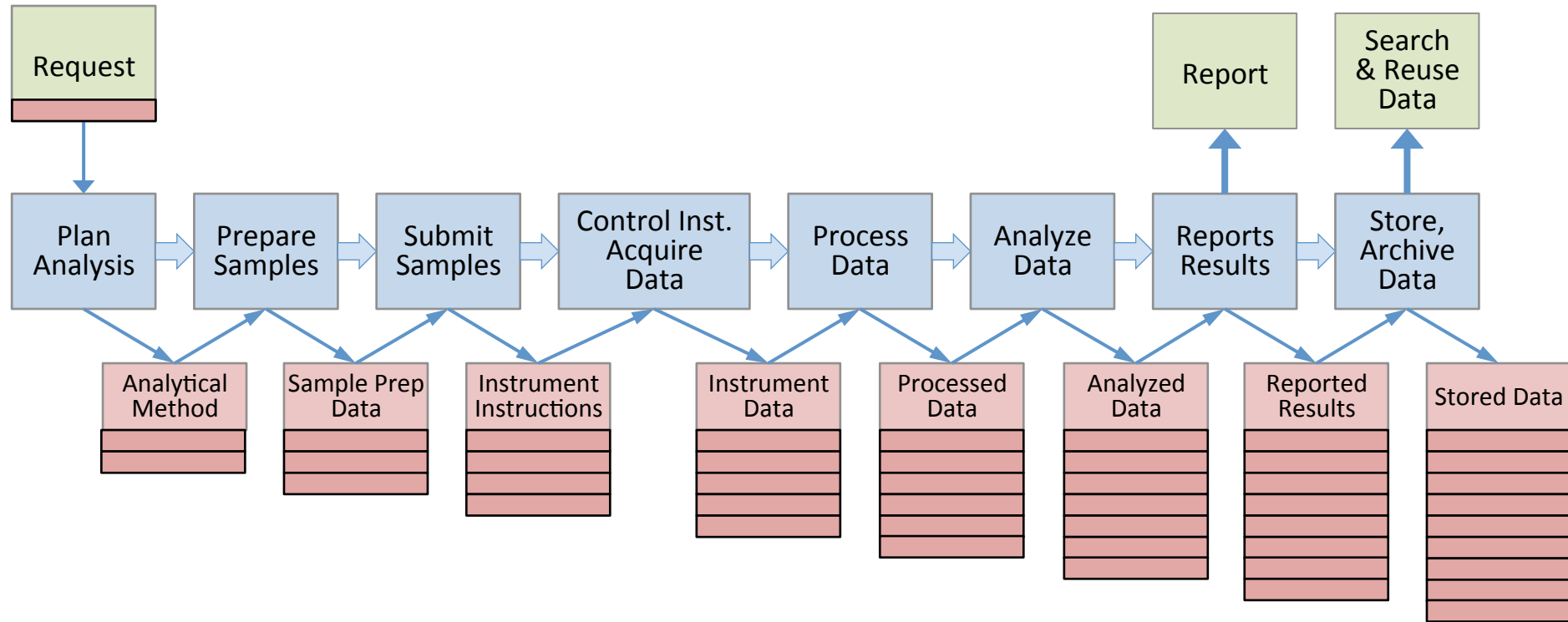


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Process Step

Data & Metadata

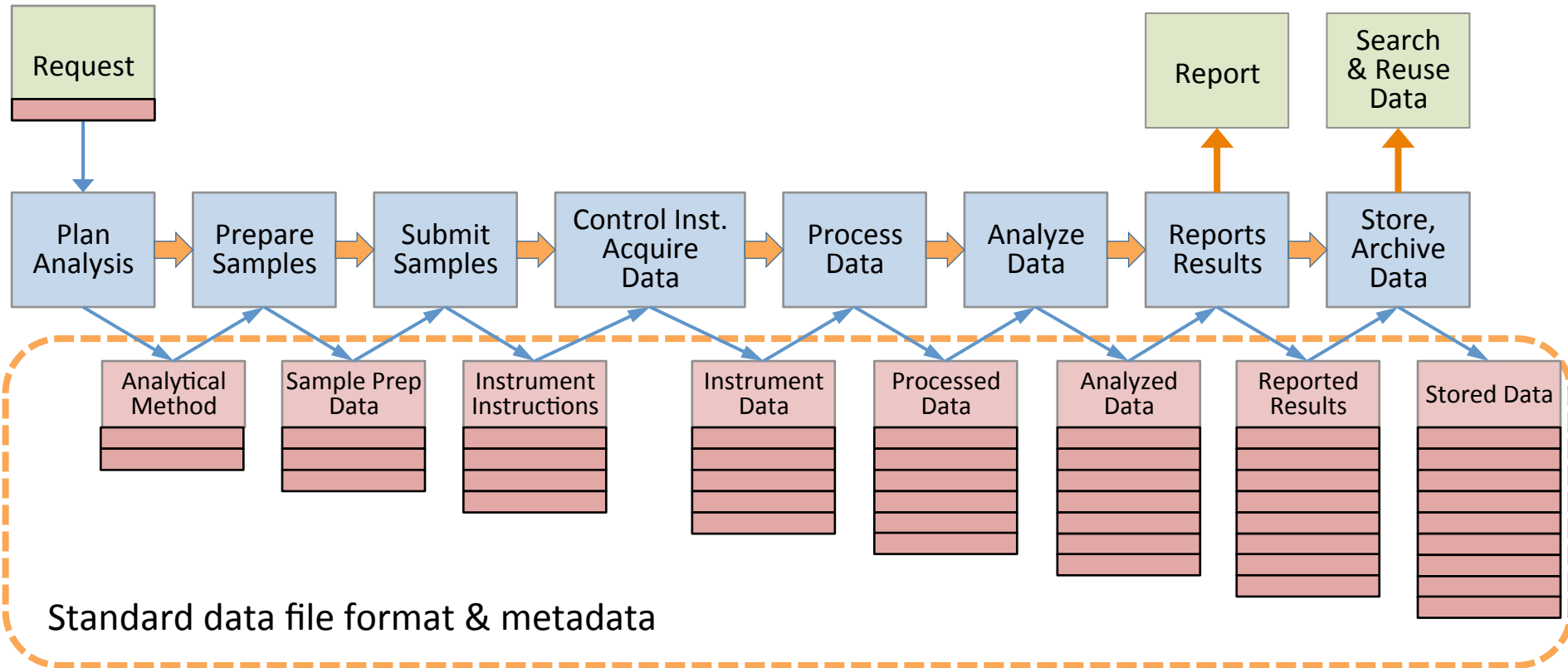


The basic analytical workflow and data flow standardized

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Process Step

Data & Metadata

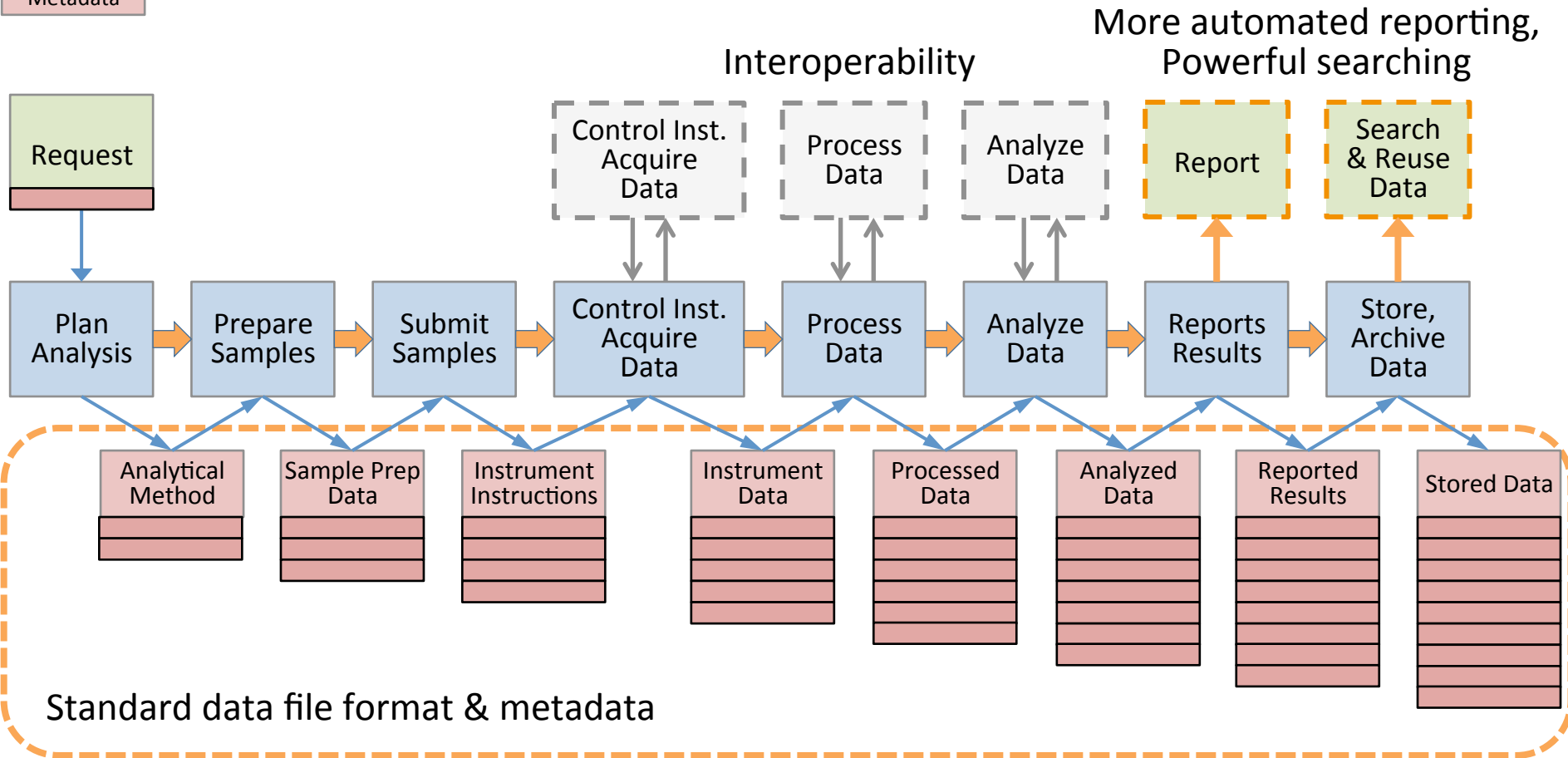


The basic analytical workflow and data flow standardized

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Process Step

Data & Metadata

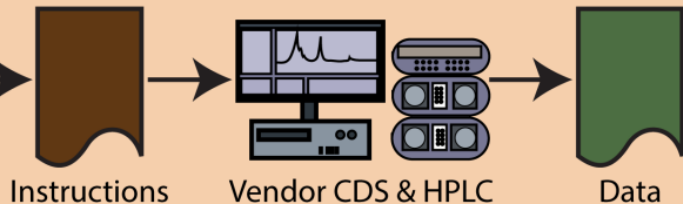


Proof of Concept (PoC) Applications (2014) to drive framework development and demonstrate capabilities

Instrument Software Integration PoC

Archive PoC

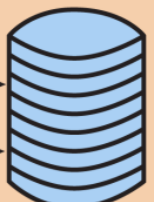
Web-based Method Form



- Same file for instructions & data
- Vendor agnostic: Waters/Agilent
- First API for open standard

Parameters	Instrument Name	Instrument Date	Method	Operator	Creation Date	Channel	Equity	Retention Period (years)
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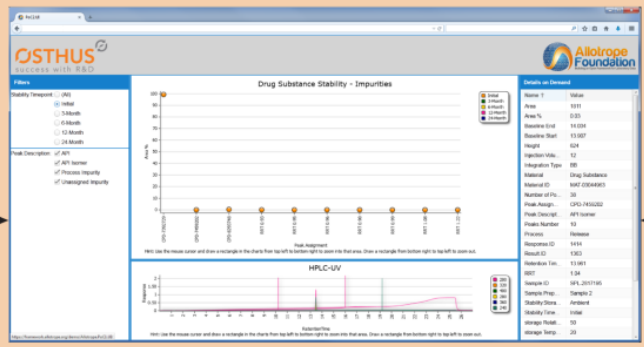
Web-based Archive Browser



Data Storage



Metadata Repository



Web-based Data Viewer

- First example of archive based on open standards
- Metadata extracted from file, and added in deposition,
- Automatic assignment of retention

- First example of mechanism to serve controlled vocabulary for context
- Feeds context throughout workflow, captured in data file

Capture of Contextual Workflow Metadata PoC