



The Allotrope Framework 101

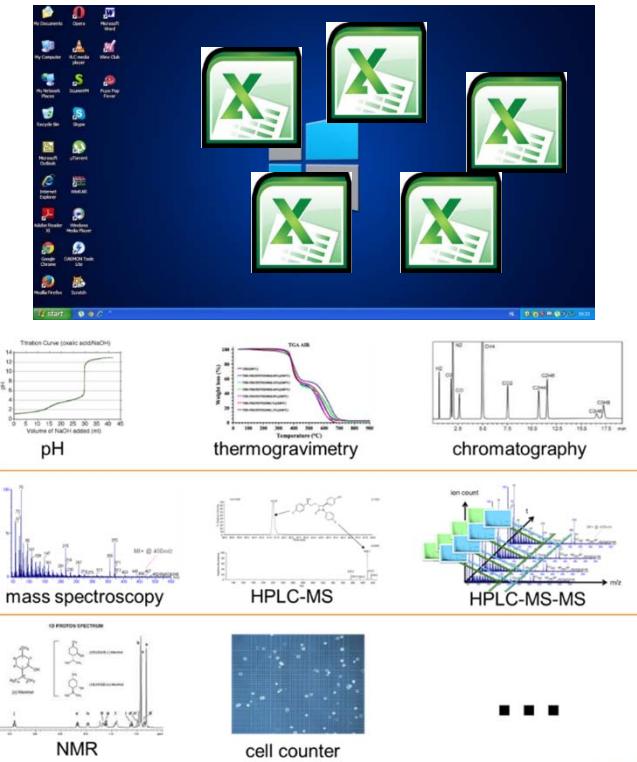
Allotrope Connect, April 25, 2018

Status quo in the laboratory

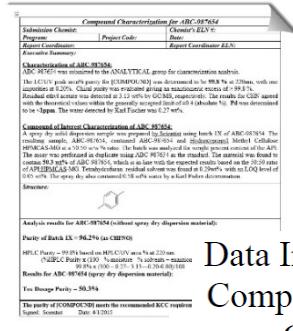
Many challenges for data capture, integration & sharing

- Manual transcription of methods
- Incompatible instruments & software systems
- Manual data handling that challenges data integrity
- Legacy architectures are brittle & rigid
- Knowledge & context resides in people's heads
- Silos of data, context and meaning

From Eric Little, OSTHUS



**Too much paper + manual tasks =
delayed medicine to patients & erosion of public confidence in data integrity**

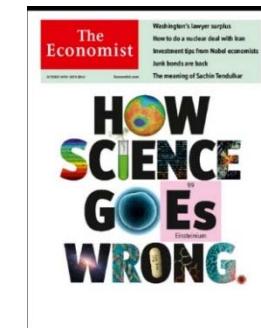
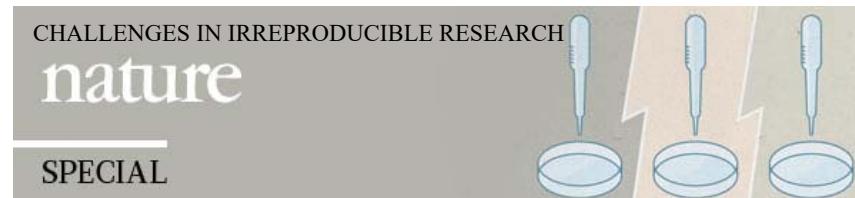


Data Integrity and Compliance With CGMP

Guidance for Industry



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Reduce Manual Effort & Paper



Better Scientific Reproducibility



Increase Data Integrity, Context, Quality



Simplified IT



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Streamlined Access,
Sharing, Integration



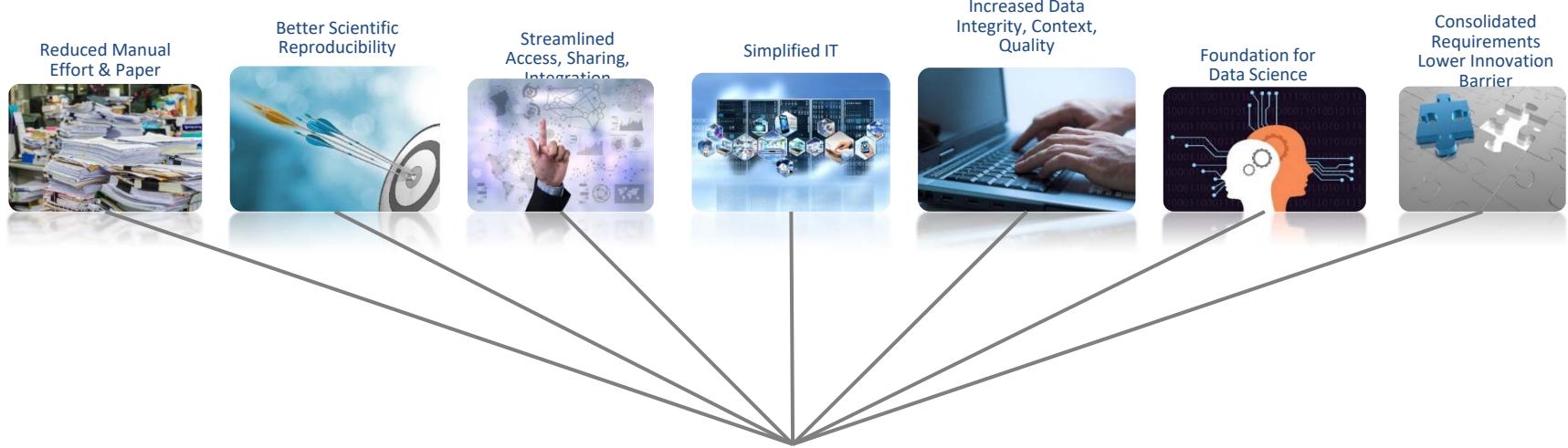
Foundation for
Data Science



Consolidate Requirements
Lower Innovation Barrier



The Benefits



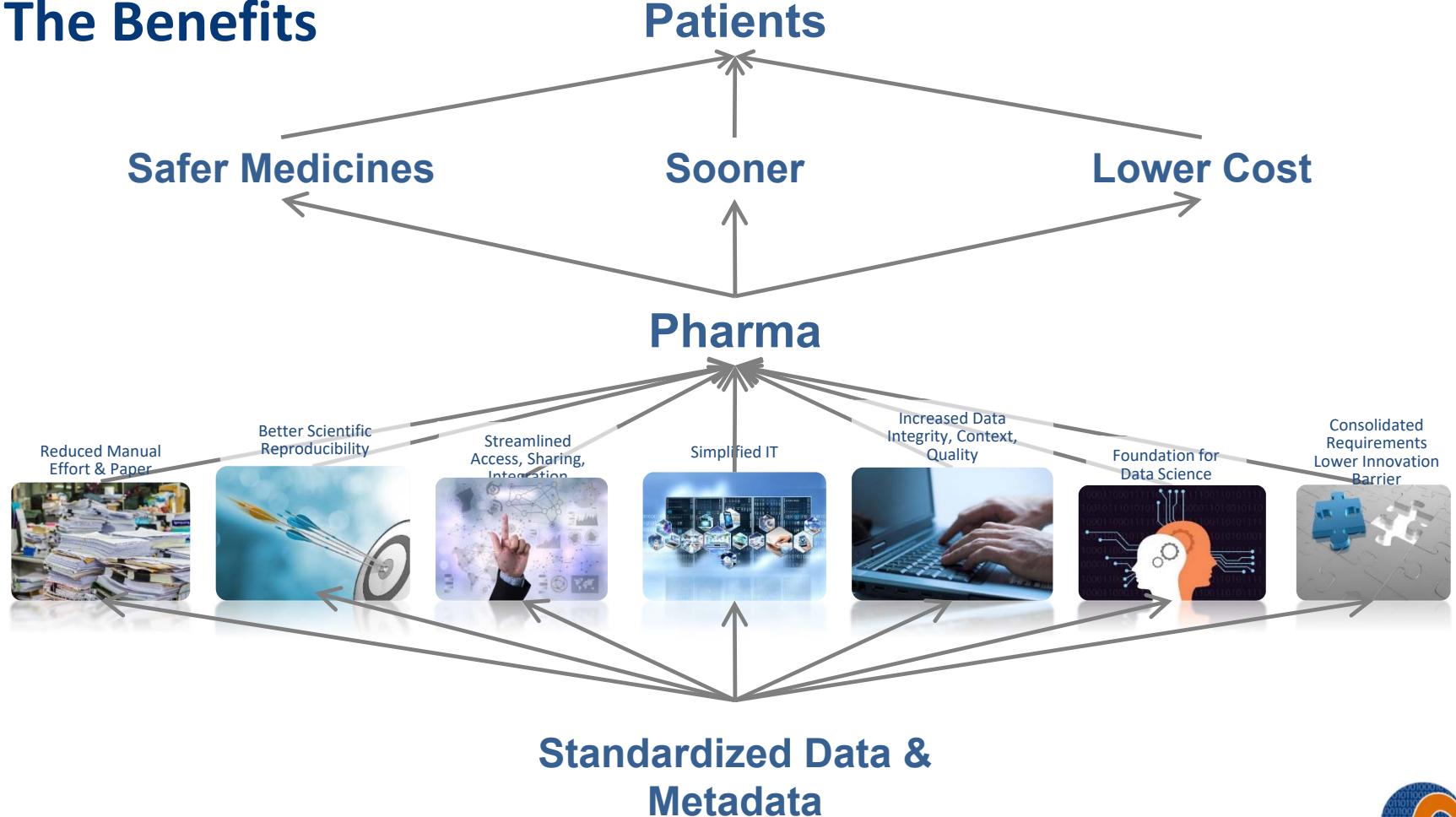
The Value Proposition



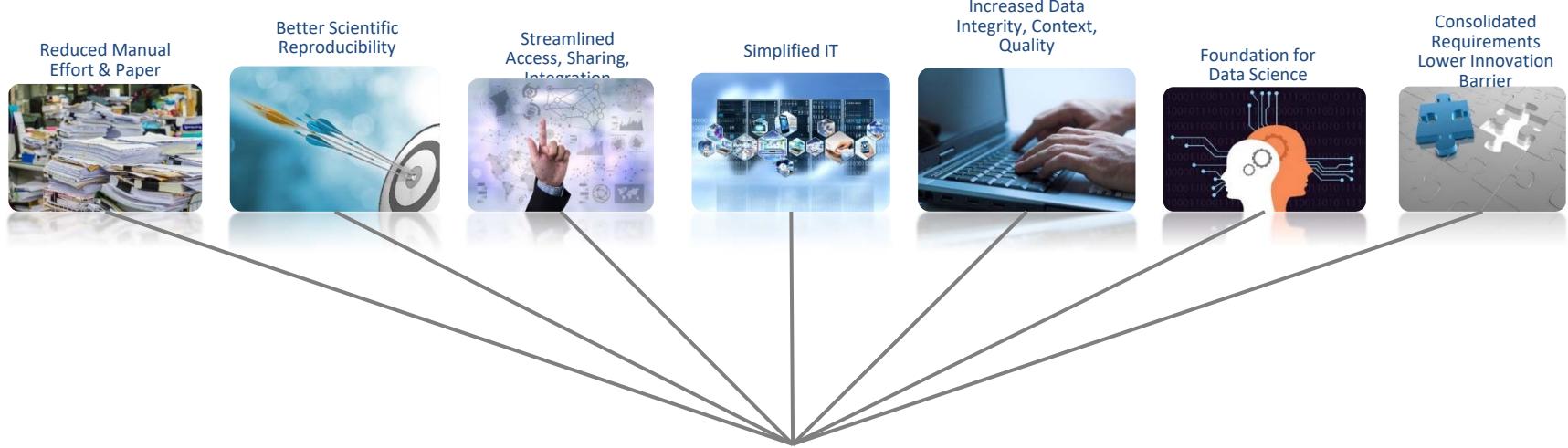
**The benefits of adoption help our customers serve their
customers better**



The Benefits



The Benefits



The Value Proposition

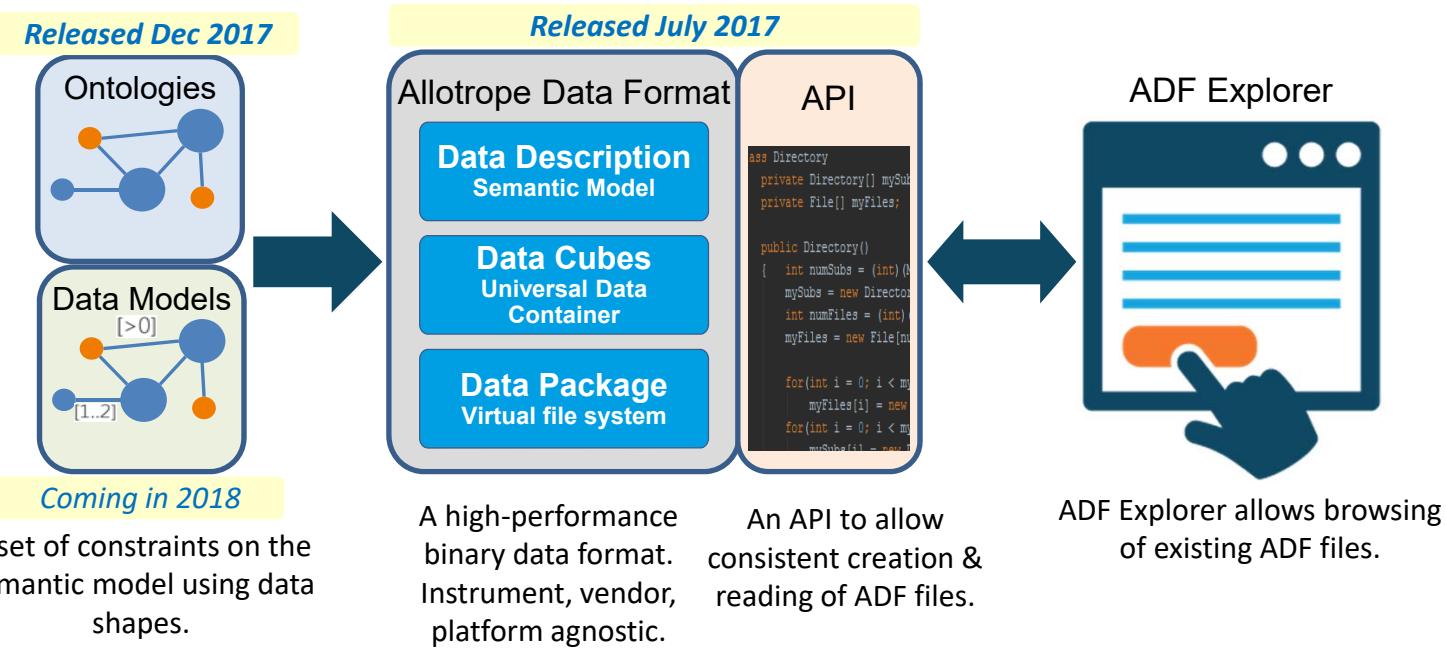
Standardized Data & Metadata

How do we deliver this?



The Allotrope Framework

A standardised semantic model for data & metadata.



Allotrope Data Format Example

Data Description

Request

```
<myAnalysisRequest> a adf:p-AnalyticRequest ;  
    adf:m-createdFrom <#0015-1> ;  
    adf:m-createdOn "2015-06-13T10:00:00Z" ;  
    adf:m-sample <#0015-1> ;  
    adf:m-sampleName "Aspirin" ;  
    adf:c-sampleCode "S0015" .
```

Sample

```
<#0015-1-2> a adf:m-Sample, adf:m-Solution ;  
    adf:m-createdFrom <#0015-1> ;  
    adf:m-createdOn "2015-06-13T10:00:00Z" ;  
    adf:m-sampleName "ACN/CHN" ;  
    adf:m-sampleType "Solid" ;  
    adf:m-stability adf:m-Absolute ;  
    adf:m-storageDuration "770" *adf:duration ;  
    adf:m-sampleConcentration "0.2" ;  
    adf:m-sampleVolume "0.01" ;  
    adf:c-volumetricFlask  
        adf:c-containment "In Autoplate" ;  
        gho:Picturegram gho:1, gho:3 ;  
        gho:ImageCode "1001231231" ;  
        adf:c-volumeUnit "mL" .  
<#0015-1-3> adf:m-consumed true .
```

Method

```
<#0007/HPLC> a adf:p-HighPerformanceLiquidChromatography ;  
    adf:p-instrumentSpecification <#0007/HPLCInstrument> ;  
    adf:p-instrumentTable <#0007/HPLCInstrumentTable> ;  
    adf:p-chromatogram <#0007/HPLCChromatogram> .  
  
<#0007/HPLCInstrument> a adf:c-InstrumentSpecification ;  
    adf:c-instrumentName "Agilent 1260 Infinity II" ;  
    adf:c-instrumentType "HPLC" ;  
    adf:c-manufacturer "Agilent Technologies" ;  
    adf:c-model "1260" ;  
    adf:c-software "Agilent ChemStation Rev B.04.01" .  
  
<#0007/HPLCInstrumentTable> a adf:p-EventTable ;  
    adf:p-instrumentTable <#0007/HPLCInstrumentTable> ;  
    adf:p-detection <#0007/HPLCInstrumentTableDetection> ;  
    adf:p-detectionWavelength "220 nm" ;  
    adf:p-detectionResolution "2.0 nm" .  
  
<#0007/HPLCInstrumentTableDetection> a adf:p-PhotodiodeArrayDetection ;  
    adf:p-detectionType "Photodiode Array" ;  
    adf:c-range "200-400 nm" ;  
    adf:c-minimum "100 nm" ;  
    adf:c-maximum "400 nm" .
```

Run

```
<#0007/HPLCRun> a adf:c-Run ;  
    adf:c-instrument <#0007/HPLCInstrument> ;  
    adf:c-instrumentTable <#0007/HPLCInstrumentTable> ;  
    adf:c-chromatogram <#0007/HPLCChromatogram> .  
  
<#0007/HPLCChromatogram> a adf:c-Chromatogram ;  
    adf:c-measurementDevice <#0007/HPLCInstrument> ;  
    adf:c-measurementTime "2015-06-24T14:05:51" ;  
    adf:c-measurementURL <#0007/HPLCChromatogram> ;  
    adf:c-structure <#0007/HPLCChromatogram> .
```

Data & Results

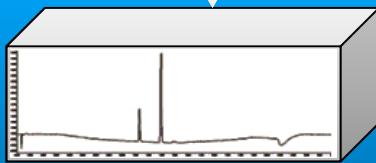
```
<#0007/HPLCRun> a Run ;  
    adf:c-result <#0007/HPLCChromatogram>, <#0007/HPLCChromatogram> .  
  
<#0007/HPLCChromatogram> a adf:c-Dataset, adf:c-Chromatogram ;  
    adf:c-measurementDevice <#0007/HPLCInstrument> ;  
    adf:c-measurementTime "2015-06-24T14:05:51" ;  
    adf:c-measurementURL <#0007/HPLCChromatogram> ;  
    adf:c-structure <#0007/HPLCChromatogram> .  
  
<#0007/HPLCChromatogram> a adf:c-Chromatogram ;  
    adf:c-measurementDevice <#0007/HPLCInstrument> ;  
    adf:c-measurementTime "2015-06-24T14:05:51" ;  
    adf:c-measurementURL <#0007/HPLCChromatogram> ;  
    adf:c-structure <#0007/HPLCChromatogram> .  
  
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    adf:c-measurementTime "2015-06-24T14:05:51" ;  
    adf:c-measurementURL <#0007/HPLCChromatogram> ;  
    adf:c-structure <#0007/HPLCChromatogram> .
```

Descriptive metadata about

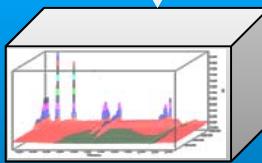
- Method, instrument, sample, process, result, etc.
- Data Cube, Data Package contents
- Provenance, audit trail, data models

Data Cubes

Chromatogram: 2D



Chromatogram: 3D



Analytical data represented by one- or multidimensional arrays of homogeneous data structures.

Data Package



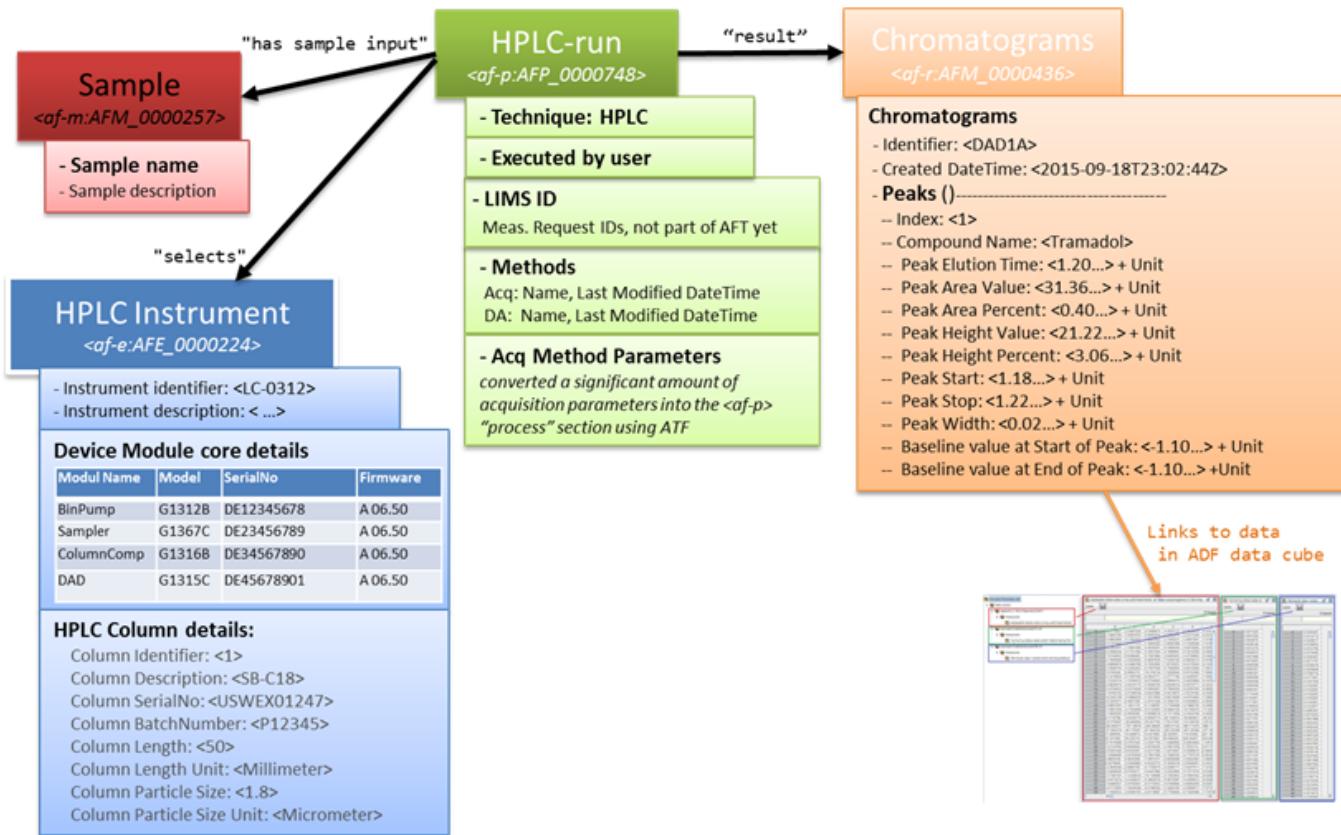
Platform Independent File Format

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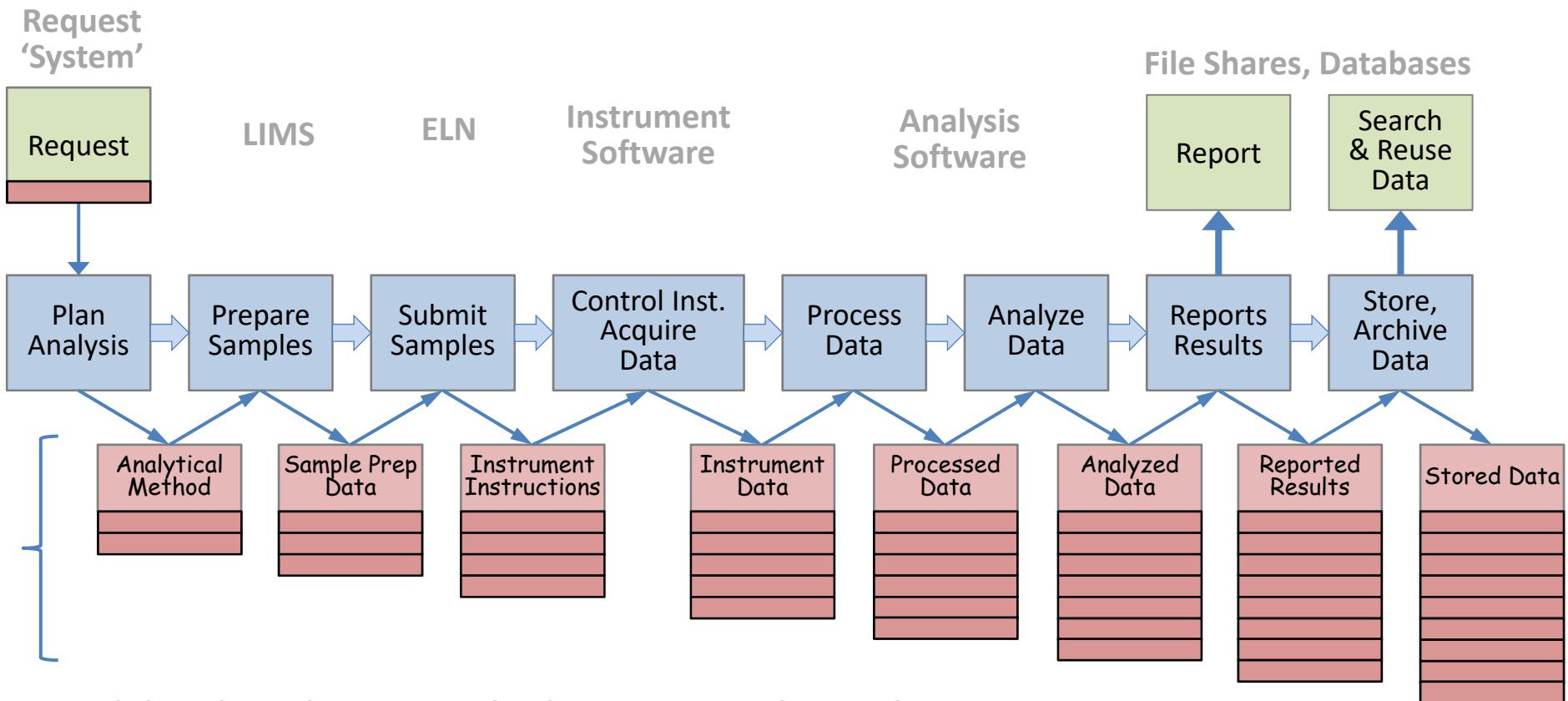
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Example: ChemStation Metadata Content

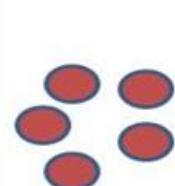


Contextual meta data accumulates along every step...



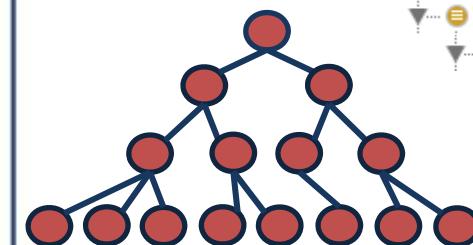
Ontologies

Terminology



chromatography
column chromatography
liquid chromatography
chromatogram
peak
spectrum
ultraviolet spectrum

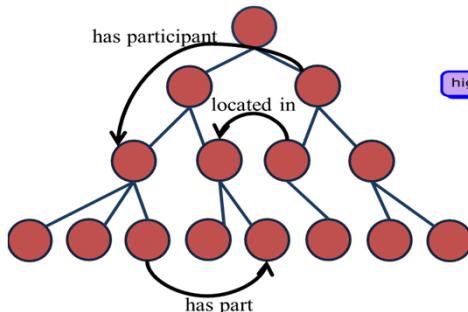
Taxonomy



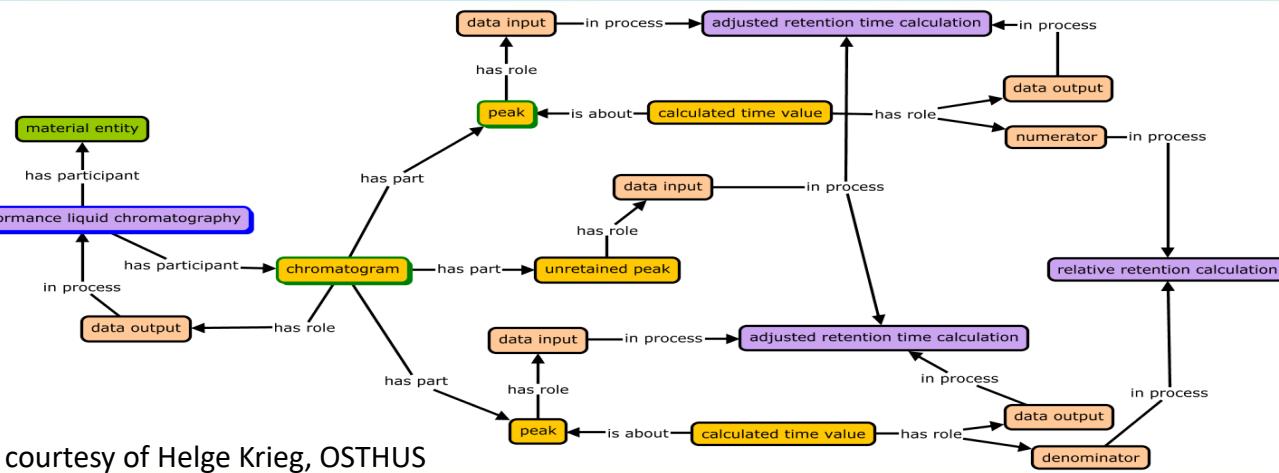
```

occurred ≡ TemporalEntity ≡ AFC_0000079
process ≡ AFP_0001617
  'planned process'
  'material processing' ≡ AFP_0003275
  'separation method'
  chromatography
    'column chromatography'
      'high-performance liquid chromatography'
      'liquid--solid chromatography'
      'high-performance liquid chromatography'
  
```

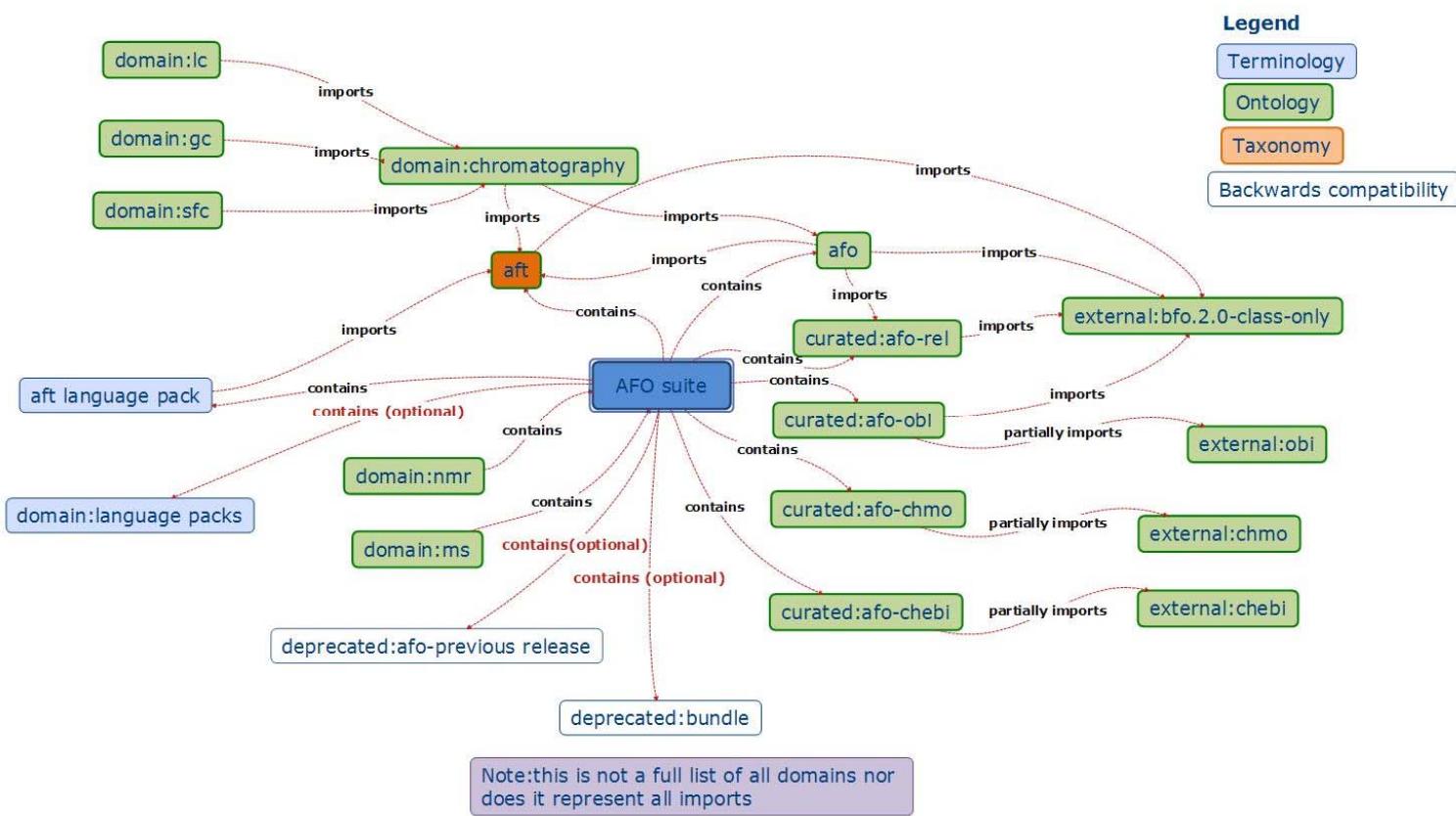
Ontology



Model courtesy of Helge Krieg, OSTHUS

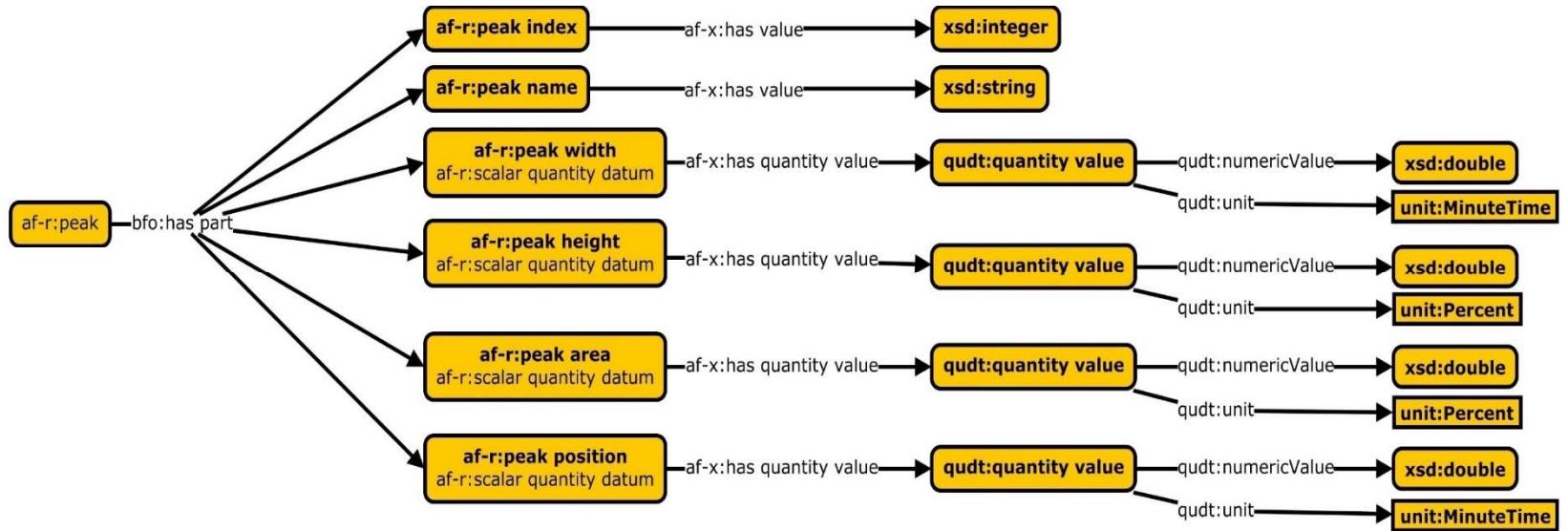


Allotrope Foundation Ontologies (AFO) Suite

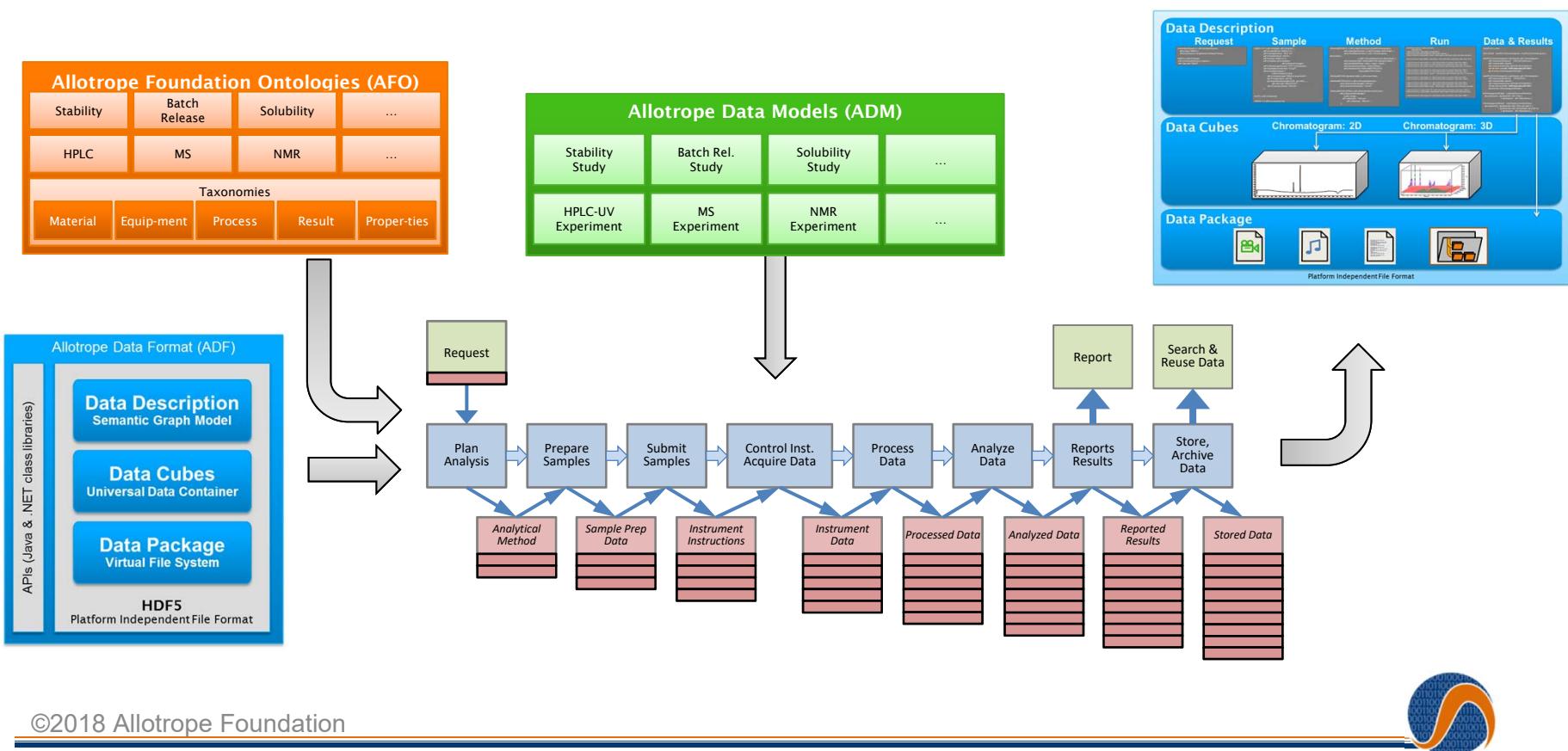


Data Models: Example- HPLC

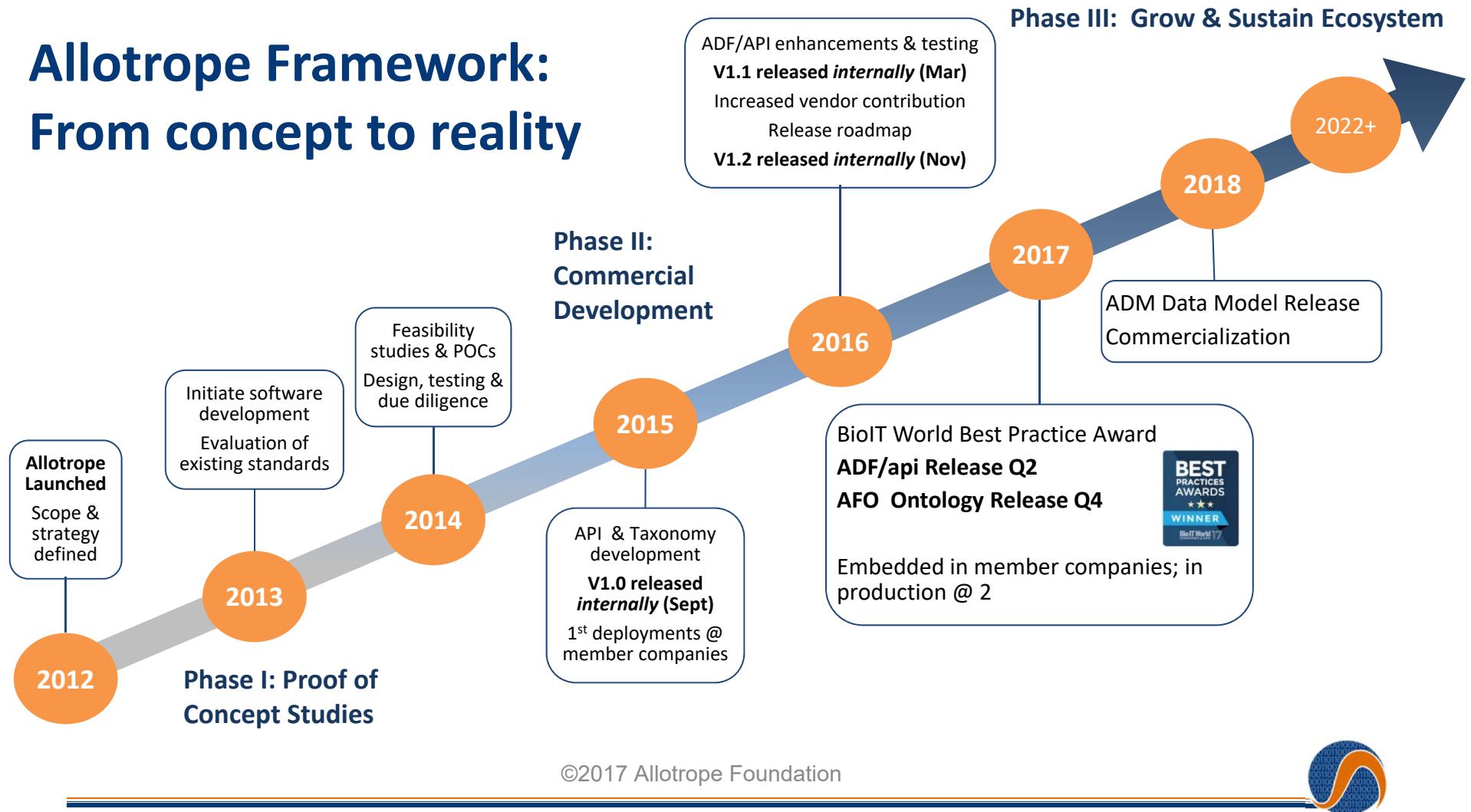
- Ontologies provide an unconstrained vocabulary we can use to describe things (instances) in our open world and give them a meaning (= **what** it is)
- Data structures (schemas, templates) describe **how** to use the ontologies for a given purpose in a standardized (reproducible, predictable, verifiable) way
- Shapes Constraint Language (SHACL, expressed as RDF) is a WC3 standard to do this, used for Allotrope ‘Data Models’



A Foundation for Interoperability & Next Generation Analytics



Allotrope Framework: From concept to reality



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2018

Framework

- Complete v1 Data Model (ADM)
- Operationalize ontology & model development

Drive adoption

- Community Projects- drive adoption & demonstrate value

Organization

- Create focus on support for commercial entities & developer community



Allotrope Developer Community and Governance

Open Source
Exchange

- Developers share their code with others (public or internal)
- No structured governance (some guidelines may apply)
- <https://gitlab.com/allotrope-open-source>

Community
Projects

- Multiple companies collaborate on a shared development
- Governed by the project leader (some guidelines may apply)
- <https://gitlab.com/allotrope-community>

Incubator

- Contributions accepted by the Foundation
- Alignment of contributions with the Allotrope Standards
- Governed by the Foundation
- <https://gitlab.com/allotrope-incubator>

Product

- Released Allotrope products
- Maintenance and sustainment
- Governed by the Foundation
- <https://gitlab.com/allotrope>



Join Allotrope Foundation!

Influence direction
of development



Be part of an expanding
community of experts



Receive support & training



Benefit from shared Investment



Align internal strategy with
the future of data



Ensure sustainability & adoption



The Allotrope Community Today



abbvie

Baxter

Genentech
A Member of the Roche Group



BIO-RAD

LEAP TECHNOLOGIES



Bristol-Myers Squibb



novo nordisk®

AMGEN®



Lilly

Biogen

Boehringer Ingelheim

MSD INVENTING FOR LIFE

MESTRELAB RESEARCH
Chemistry Software Solutions

ZONTAL... KNOWLEDGE CONNECTED

Science & Technology Facilities Council

LAMSADE UMR CNRS 7243

BRUKER

University of Strathclyde Glasgow

ACD/Labs

The HDF Group



OSTHUS®
success with R&D

Drinker Biddle®

Malvern Panalytical

DEXSTR

Cognizant

idbs Riffyn

paradigm4

Thermo Fisher SCIENTIFIC

The HDF Group

Astrix Technology Group • BSSN Software • Elemental Machines • Erasmus MC • Fraunhofer IPA • LabAnswer
Mettler Toledo • NIST • SciBite • Stanford University • University of Illinois at Chicago • University of Southampton