Fighting Entropy with Informatics

an Agilent-GSK collaboration

Agilent Perspective

Support for the Allotrope Framework

Jerry Hall
Agilent Representative
Allotrope Foundation

Public

Executive Support
President and CEO, Mike McMullen

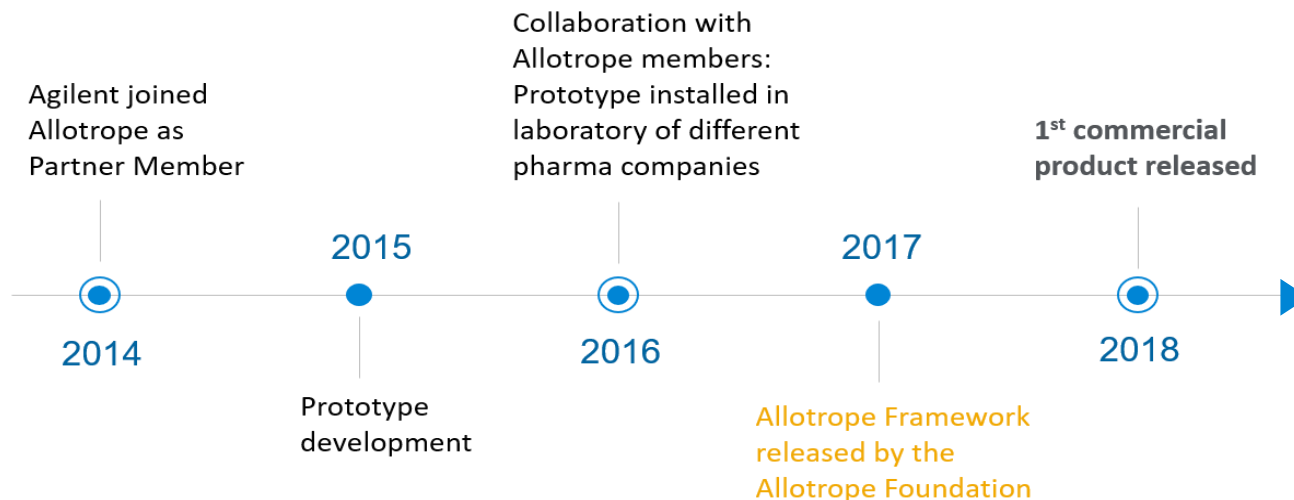"Customers are very focused on informatics as a way to create insight and drive lab efficiencies. We are determined to lead in lab informatics. For example, last week, Agilent released the first software supporting the new standardized data format called the Allotrope Data Format, or ADF for short. This format was created by a consortium of pharmaceutical companies for the pharmaceutical industry.

By standardizing the collection, exchange, and storage of analytical data captured in laboratory workflows, labs will be able to transfer and share data across platforms. We are proud to be the first company to develop and launch a commercial product to support this standard. We believe the adoption of standards like ADF will both shape the future of lab informatics and drive the adoption of our solutions."

Agilent Allotrope Engagement

Agilent joined Allotrope as Partner Member

Collaboration with Allotrope members: Prototype installed in laboratory of different pharma companies

1st commercial product released

2015

2017

2014

2016

2018

Prototype development

Allotrope Framework released by the Allotrope Foundation

Active Projects

Commercial	Prototypes	Allotrope Integration Projects	Allotrope Contributions
• Release ADFExport for **ChemStation C.01.09** • Development of ADFExport for **OpenLab CDS 2.4**	• More prototype functionality (CDS/ECM)	• MS metadata to ADF • Lab balance integration • Method export to	• Complete LC-UV model • GC data model • MS data model

Agilent

Allotrope ADFExport 1.0 for ChemStation C.01.09

Business Wire
A Berkshire Hathaway Company

Agilent First to Release Software Supporting Standardized Data Format for Pharmaceutical Industry

August 08, 2018 11:00 AM Eastern Daylight Time

SANTA CLARA, Calif.--(BUSINESS WIRE)--Agilent Technologies Inc. (NYSE: A) announced today the release of a new version of its chromatography data system that enables laboratories to export files in the Allotrope Data Format (ADF), an emerging standard developed by a consortium of pharmaceutical companies.

"It promises to increase data integrity, improve scientific reproducibility, boost efficiencies, enhance searchability, and fast-track the ability to use all the information collected from a given sample."

The Agilent data system, OpenLab CDS ChemStation Edition, is the first to support the new format, designed to standardize data from disparate sources.

The ADF was designed to standardize the collection, exchange, and storage of analytical data captured in laboratory workflows. ADF enables labs to transfer and share data across platforms. It is also expected to enable increased automation, reducing error-prone manual input.

"The development of ADF is an important step toward obtaining faster results and more insight from the data collected and produced within pharmaceutical organizations involved in research, development, and production of chemicals and biomolecules," said John Sadler, vice president and general manager of Agilent's Software and Informatics Division. "It promises to increase data integrity, improve scientific reproducibility, boost efficiencies, enhance searchability, and fast-track the ability to use all the

Complete press release (Aug 8th, 2018)
(you can find it also on LinkedIn or Twitter)
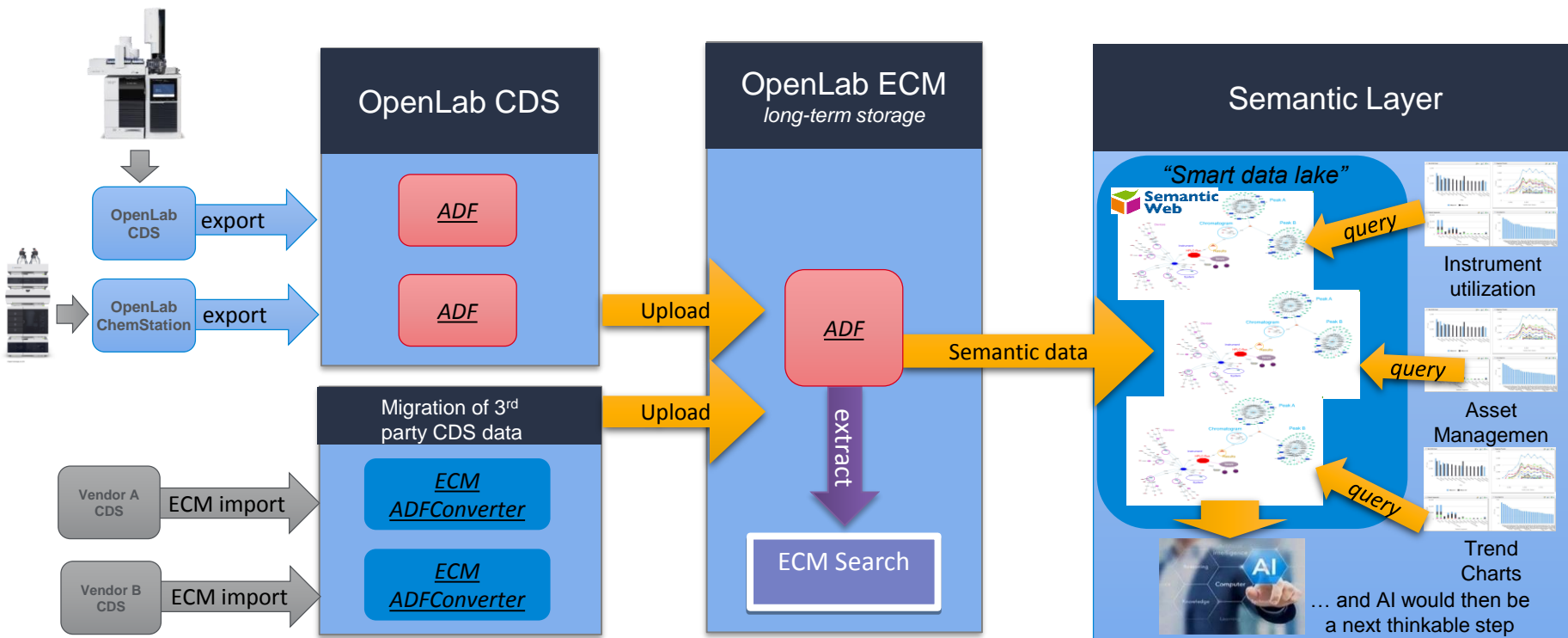
Existing prototypes

Chromatography Data Systems

- ADFExport for ChemStation → for LC, GC data (and MS-SQ rawdata)
- ADFExport for OpenLab CDS → for LC, GC data (and MS-SQ rawdata)

OpenLab ECM

- ECM ADF Filter: Upload, search ADF data and view using ADF Explorer
- ECM WebServices: ECM Server-side ADF export of ChemStation data

A vision for OpenLab….

GSK Perspective

Digital Transformation
Vern De Biasi

fighting entropy with informatics

entropy: a measure of disorder in a system

math
$$\ln(\Omega)$$

so what?   zero entropy when there is only one accessible state $\Omega = 1$

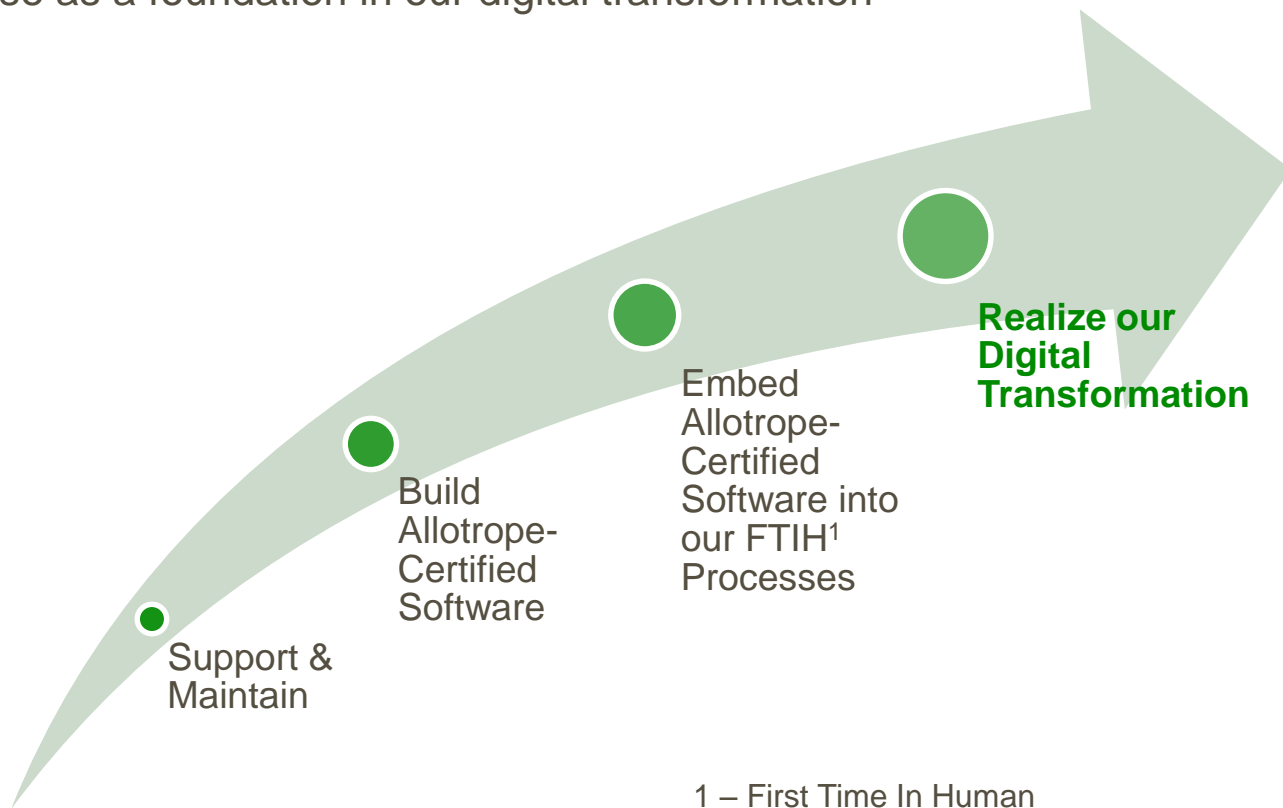**framework**   can drive entropy to zero across numerous processes

how?   ADM and AFO provide single-value terms and relationships ($\Omega = 1$)

in the lab…   remove the keyboard as a source of entropy

the Allotrope Framework

is ready to use as a foundation in our digital transformation

Realize our Digital Transformation

Embed Allotrope-Certified Software into our FTIH[1] Processes

Build Allotrope-Certified Software
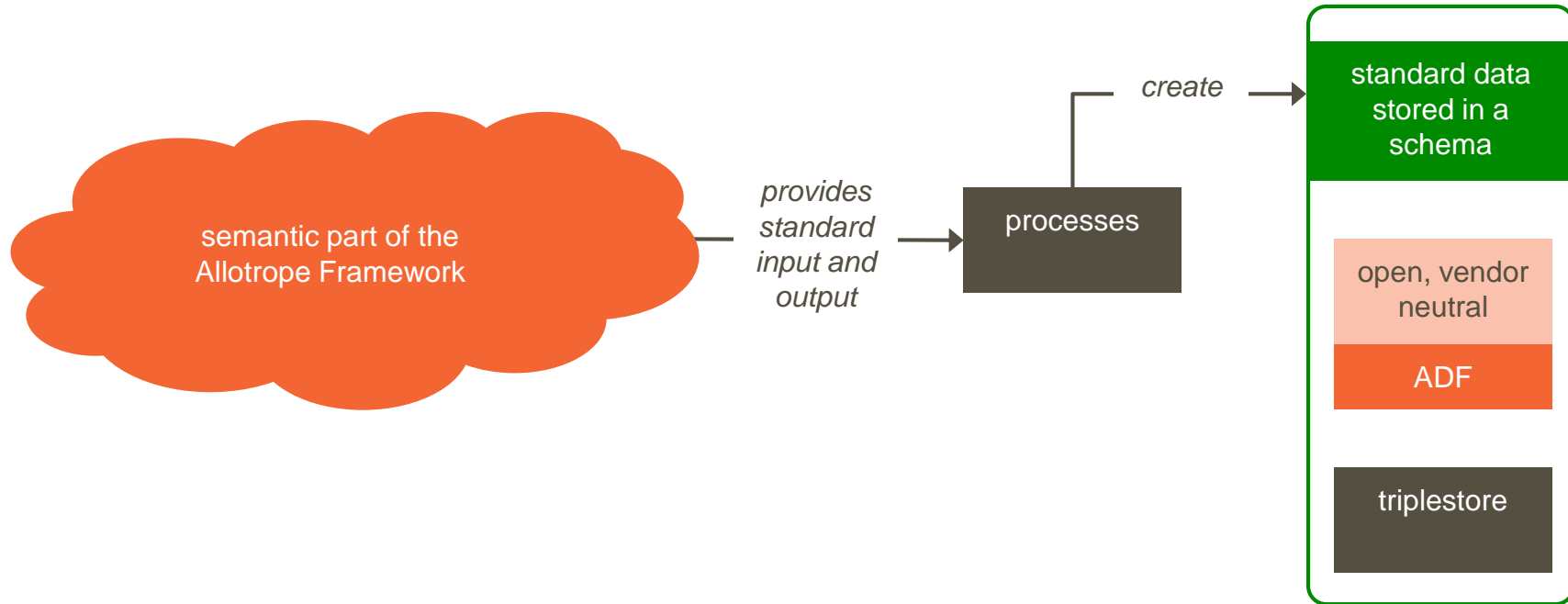
Support & Maintain
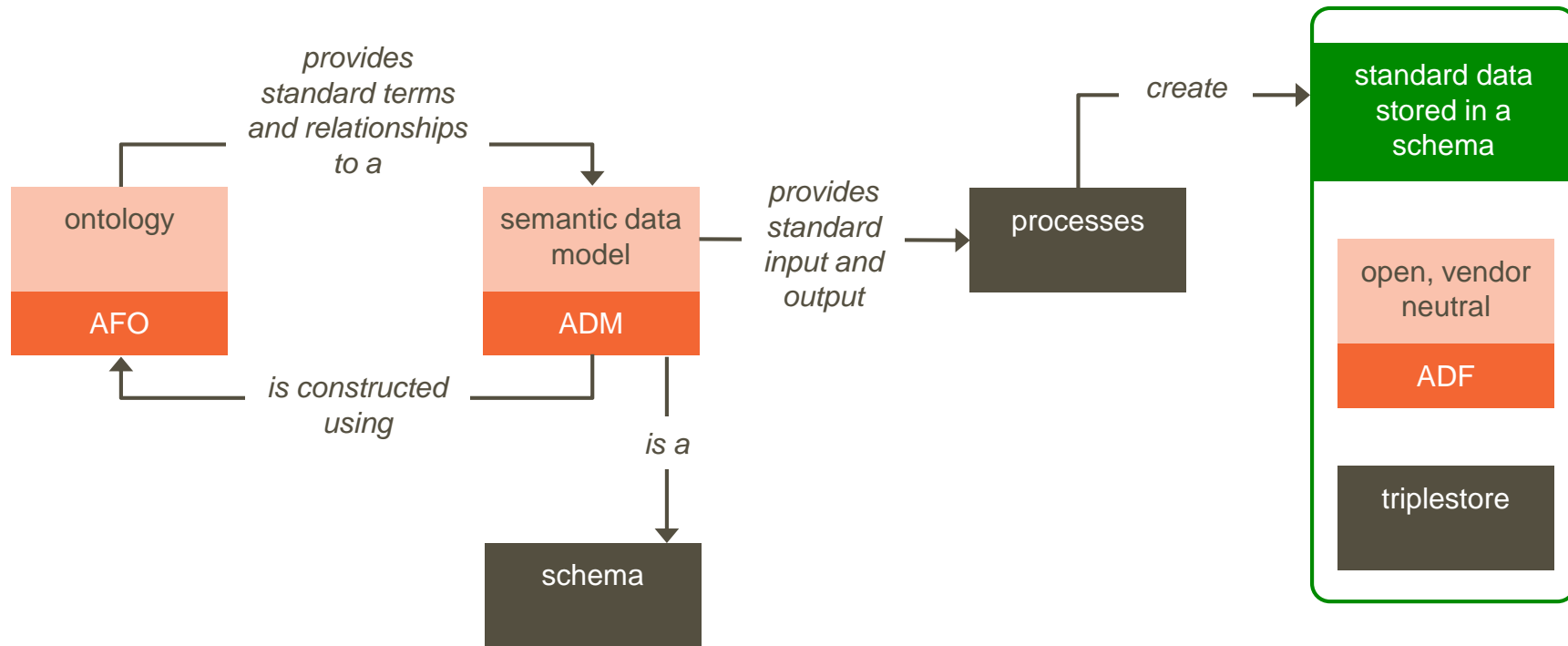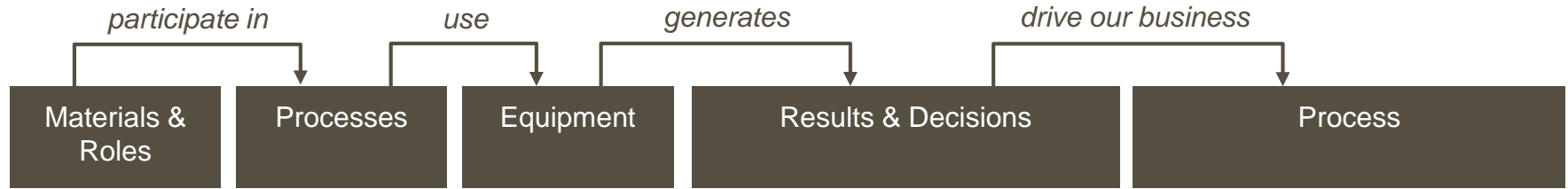
1 – First Time In Human

Allotrope @ GSK

James Roberts

FTIH Processes
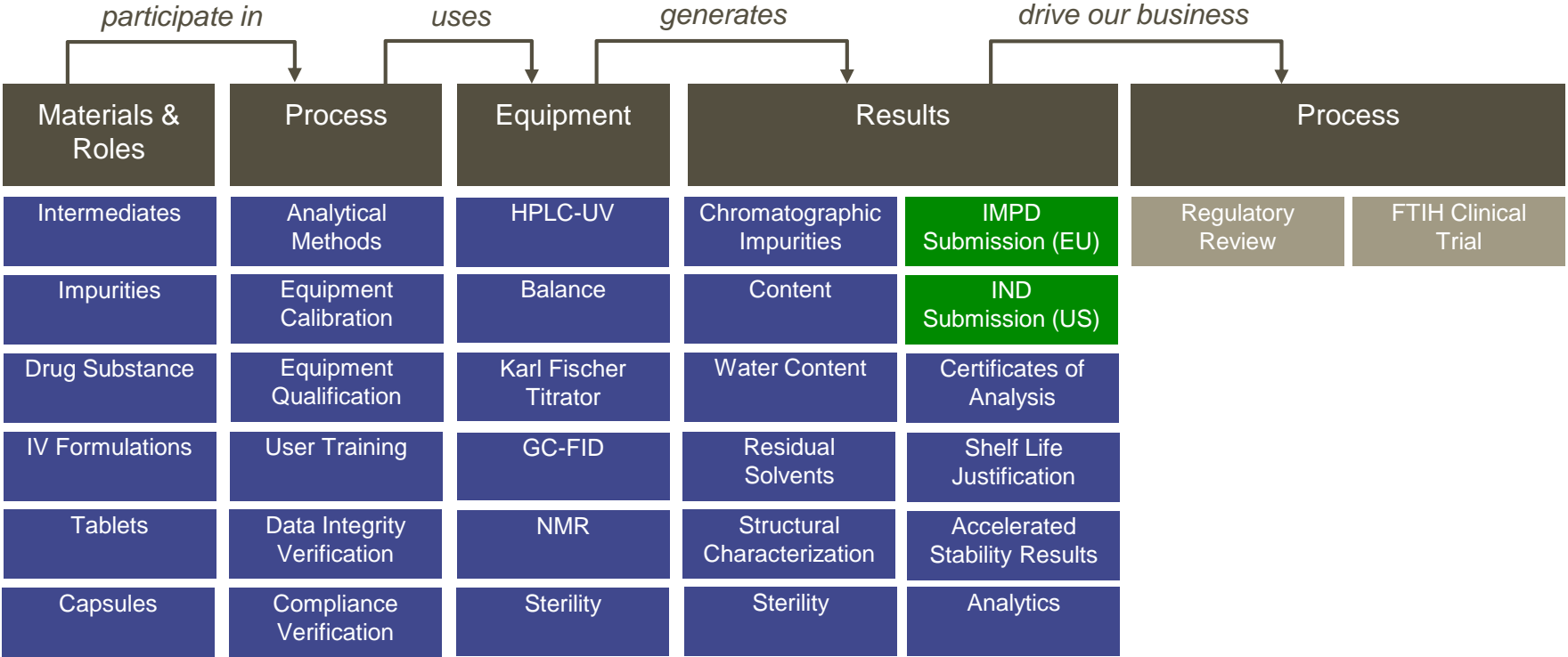
framework landscape: *value proposition*

framework landscape: *two semantic parts*

ontology landscape: *abstract*

| | participate in | | use | | generates | | drive our business | |

| Materials & Roles | Processes | Equipment | Results & Decisions | Process |

ontology landscape: *concretized for FTIH*

participate in		uses	generates		drive our business	
Materials & Roles	**Process**	**Equipment**	**Results**		**Process**	
Intermediates	Analytical Methods	HPLC-UV	Chromatographic Impurities	IMPD Submission (EU)	Regulatory Review	FTIH Clinical Trial
Impurities	Equipment Calibration	Balance	Content	IND Submission (US)		
Drug Substance	Equipment Qualification	Karl Fischer Titrator	Water Content	Certificates of Analysis		
IV Formulations	User Training	GC-FID	Residual Solvents	Shelf Life Justification		
Tablets	Data Integrity Verification	NMR	Structural Characterization	Accelerated Stability Results		
Capsules	Compliance Verification	Sterility	Sterility	Analytics		

use ADM and informatics to remove entropy from…

Allotrope Data Models + New Informatics Capabilities					
Materials & Roles	**Process**	**Equipment**	**Results**		
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Process	
Regulatory Review	FTIH Clinical Trial

target in 2019

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Process	
Regulatory Review	FTIH Clinical Trial

practical impact

winning the fight with entropy means we can

1. guarantee data integrity (ALCOA-CCEA) and FAIR principles
2. ensure quality and compliance into a process at the beginning of the data lifecycle
3. reduce number of quality investigations
4. eliminate manual transcription and data review
5. measure process performance to establish a baseline for continuous improvement
6. automate creation of numerous documents
7. lay the foundation for our digital transformation
8. accelerate delivery of medicines to patients

… saving time and money

GSK support for Allotrope

planned Allotrope activities in 2019

– GSK Contributions to Allotrope in 2019

  – AFO, ADM, ADF enhancements that support FTIH processes in a GMP environment in GSK

  – SVP support for a dedicated team to develop the above

  – co-funding Empower ADF converter Community Project

  – advocacy for Allotrope-enabled software development projects being executed by others in the community

– GSK Activities

  – hire semantic and software engineers

  – improve velocity to deliver software

  – deliver solutions incrementally in GSK to support FTIH activities

  – co-develop Allotrope-enabled solutions with Agilent (now) and other APN colleagues as appropriate

– Transition GSK roles in Allotrope

  – AFO Business Product Owner (James Roberts)

  – Engineering Lead: AFO, ADM, ADF, ADF Explorer, GitLab, testing, tutorials, tool development (Ben Woolford-Lim)

  – ADF Explorer (Joy Ginocchio)