Moving forward the Allotrope Transformation
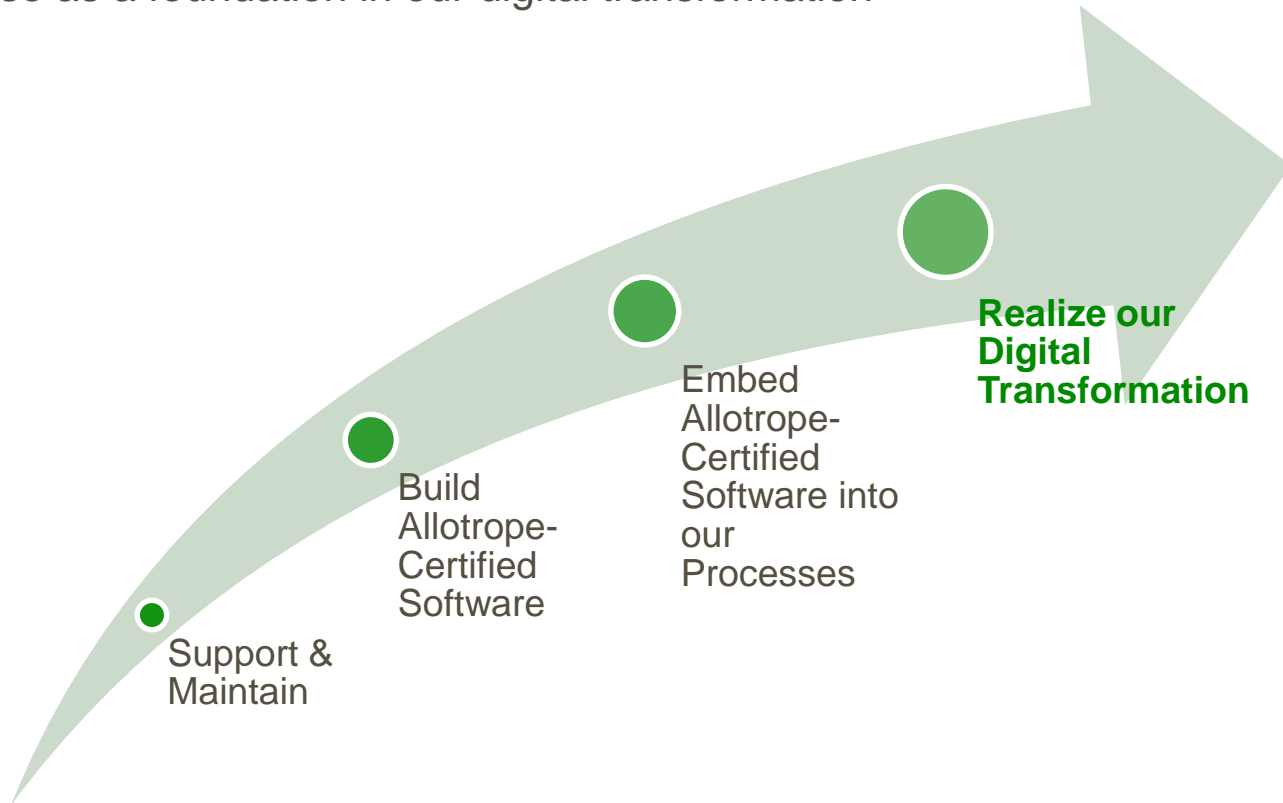
Verner de Biasi

Celebrate our successes

1. Stand back and think about it… you/we've done something amazing!
2. As a pre-competitive consortium we have
   - developed and delivered a foundational technology designed to address nearly every pain point in our data lifecycle
   - given our senior leaders across IT / Tech and "the business" a toolkit they can use to revolutionize their digital data and analytics
   - created a large community of competitors that is collaborating
   - created a better approach to how pharma will receive and use commercial off-the-shelf software

The Allotrope Framework

is ready to use as a foundation in our digital transformation

Support &
Maintain

Build
Allotrope-
Certified
Software

Embed
Allotrope-
Certified
Software into
our
Processes

**Realize our
Digital
Transformation**
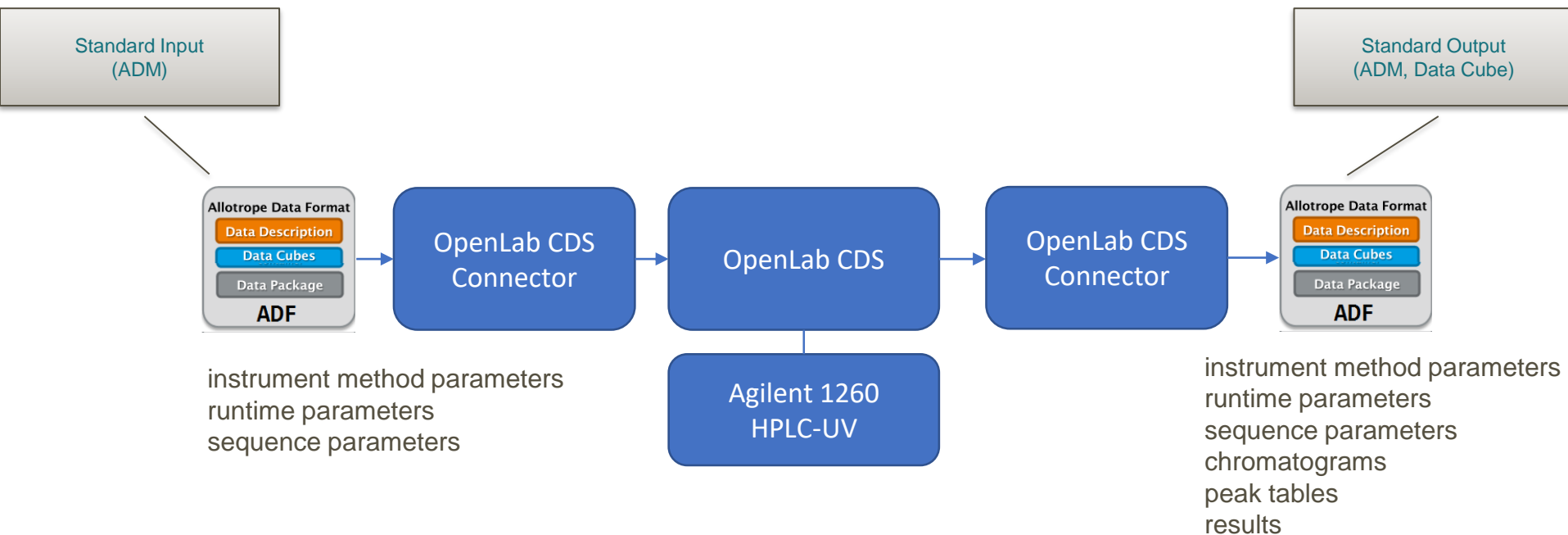
Success means commercial software in use in our companies

1. The Framework is now fit for purpose – new enhancements to it should be made primarily through the development of commercial solutions

2. Pharma companies should be helping the vendor community use the Framework (and enhance it where necessary) to develop software to meet industry needs

3. APN vendor companies should bring their own new innovative Framework-enabled solutions forward (and engage their own senior leadership and development teams to ensure this happens)

EXAMPLE: GSK and Agilent are collaborating to codevelop Framework-enabled solutions that target first-time-in-human (FIH) analytical activities. Senior leadership and development teams at both companies are engaged.

Our path toward Framework-enabled solutions

- Objective: one public "digital standard" for LC-UV

- Others in Allotrope are delivering an LC-UV 'output' data converter and data model

- Our work is focused on how to utilize an LC-UV 'input' data connector and data model for use with any CDS, any instrument – a "digital method"
  - we are supporting the collaboration with Pistoia and Allotrope
  - we are testing the data model through use with software, instruments and experiments being run in laboratories at GSK and Agilent

Our path toward Framework-enabled solutions

Standard Input
(ADM)

Standard Output
(ADM, Data Cube)

Allotrope Data Format
- Data Description
- Data Cubes
- Data Package

ADF

OpenLab CDS
Connector

OpenLab CDS

OpenLab CDS
Connector

Allotrope Data Format
- Data Description
- Data Cubes
- Data Package

ADF

Agilent 1260
HPLC-UV

instrument method parameters
runtime parameters
sequence parameters

instrument method parameters
runtime parameters
sequence parameters
chromatograms
peak tables
results

ADM = Allotrope Data Model, a standardized graph-based, semantic representation
of metadata that has been approved through the Allotrope governance process (*i.e.*,
a released, public digital standard)
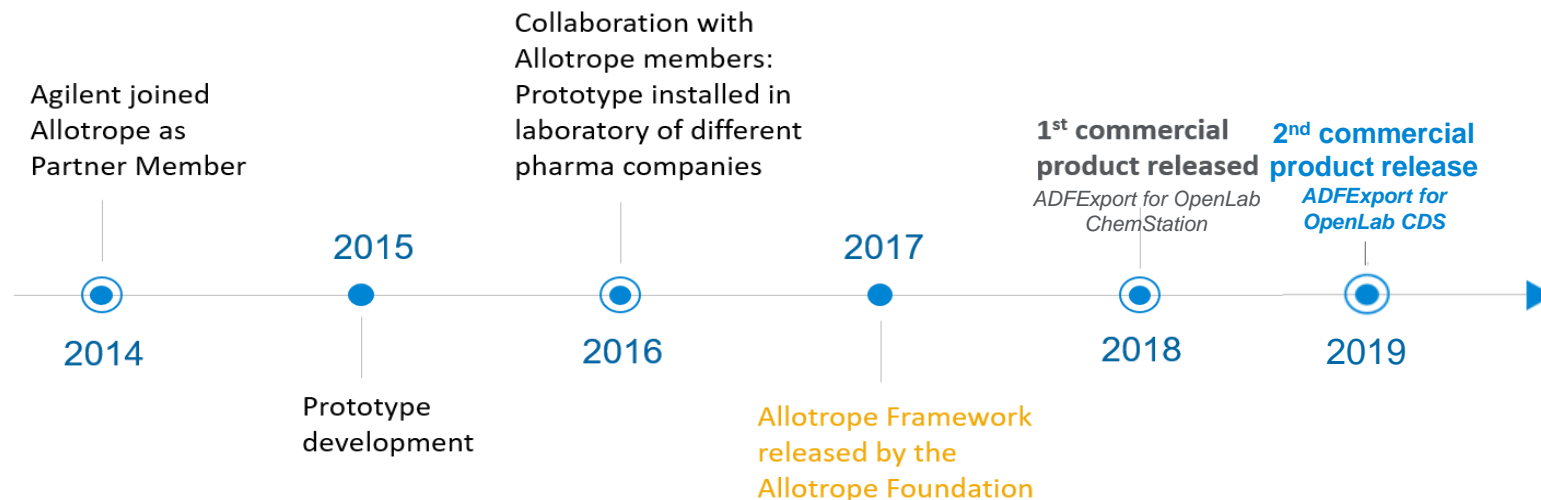
Agilent's Allotrope activities

Allotrope Connect Workshop
Vélizy-Villacoublay

Ralph Mueller
Product Marketing Manager

April 9th, 2019

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**
*ADFExport for OpenLab
ChemStation*

**2nd commercial
product release**
*ADFExport for
OpenLab CDS*

2015

2017

2014

2016

2018

2019

Prototype
development

Allotrope Framework
released by the
Allotrope Foundation

Active Projects

Commercial
- ADFExport for OpenLab CDS
  ChemStation Rev. C.01.09
- ADFExport for OpenLab
  CDS Rev. 2.4

Prototypes
- ADFExport for ChemStation → for
  LC, GC, MS-SQ rawdata
- ADFExport for OpenLab CDS → for
  LC, GC, MS-SQ rawdata
- ECM ADF Filter: Upload, search ADF
  data and view using ADF Explorer
- ECM WebServices: ECM Server-side
  ADF export of ChemStation data

Allotrope Integration Projects
- GSK Collaboration
- Merck ADFExport
- BMS MassHunter BioConfirm
- Pistoia Alliance MethodDB
- MS metadata to ADF
- Lab balance integration

Allotrope Contributions
- Complete LC-UV model
- GC data model
- MS data model
- Raman Spec DataCube model

Allotrope Integration Project_GSK collaboration: OpenLab CDS connector

Standard Input: Test client UI

Agilent commercial product: ADFExport for OpenLab CDS

Standard Output:

1. Export automatically via post-processing plugin
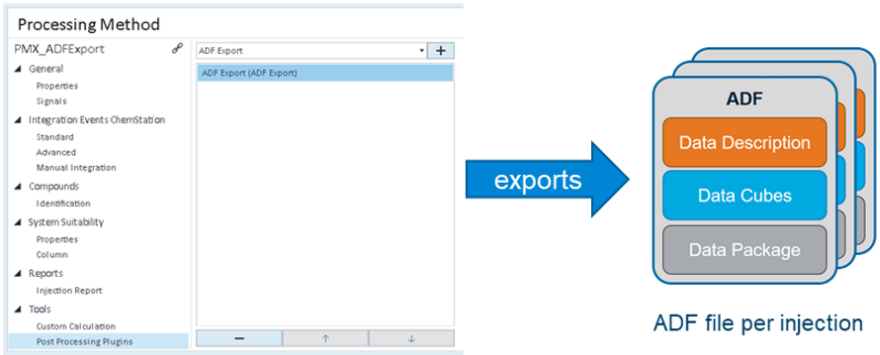
Automatically at the end of a run

ADF file per injection

2. Export manually via ribbon command
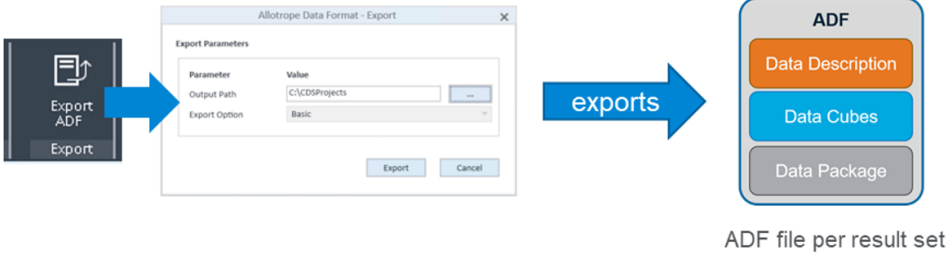
Interactively from DA UI

ADF file per result set

Allotrope end-to-end workflows

Selection of Pharma pain points

- Long-term archiving in a proprietary data format → not able to view data in 10-20 years
- Along the workflow no re-use of data because of data silos & different terminologies
- Not possible to efficiently exchange data with: external contract labs/ vendor proprietary formats

www.allotrope.org