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
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

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**
- **2015**
  - Prototype development
- **2016**
  - Allotrope Framework released by the Allotrope Foundation
- **2017**
- **2018**
- **2019**

**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

1. Login OpenLab Shared Services
2. Select
   - CDS-Instrument
   - CDS-Project
3. Select
   - CDS-Acquisition base method
   - CDS-DataProcessing method
4. Select Allotrope acquisition method (.ttl)
5. Enter Injection location and Sample Name
6. Submit Single Sample Run or Sequence
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