The Empower CDS Allotrope Community Project

Community Presentation
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Background
Empower Community Project

• Since the beginning of Allotrope...
  • Top Priority: Chromatography Data...
• Empower Working Group
  • Formed in July 2016
  • Released RFP Q4 2017
• What’s a Community Project?
• APN Selection / Interview / Paperwork
  • Funding: Initially 4 Companies… then 5… 6… ← Tipping point funding/resources
• Today – 7 AF Member companies + TetraScience!
Potential Use Cases Beyond Today…

• Why do we want a CDS ADF?
  • Downstream analytics/integration: Spotfire, ACD, etc...
  • Long-term archiving: No software/version dependences
  • CDS mix match… Empower to Chromelon to Empower…
  • Method development: Use/reuse the data from 100+ runs

• Many things we haven’t even imagined yet will be possible once we able to access data freely

• Out of scope of this project
Business Case for a Chromatography ADF

• Use case brainstorming at an Allotrope F2F
• As a scientist I need to be able to…
  - Identify user entered input parameters
  - Identify how the experiment was set up
  - Identify system captured metadata
  - Identify parameters (system and user entered)
  - Provide results
  - Identify what system parameters were used to run instrument
Use Cases from 50K Feet

• **2 Broad Categories:** Routine Activities / Long Term Archive
  - **Routine:** Use cases from previous slide… the details
    - Business as usual how do I make my data available for further downstream activities
    - Support regulatory filing - Today
  - **Archive:**
    - Automation of legacy data conversion
    - Support regulatory filing – Tomorrow, emerging markets
TetraScience
The ADF Lifecycle for CDS’s
Empower
Chemstation
Chromeleon
Etc.

Connect

Import & Use
(Pre-ADF, JSON)

Spotfire
Other CDSs
Search Tools
AI/ML
Allotrope Tools

Convert & Export
(Pre-ADF, JSON)

Storage & Retrieval
(TS Data Lake)
The Pre-ADF

PRE-ADF FILE

- Modeled via JSON in the data package
- Data Description
- Data Cube
- Data Package

ADF FILE

- Data Description
- Data Cube
- Data Package
Special Thanks to the Merck Team for making this happen

Michael Fernando (IT Team Lead)
Chintan Patel (Lab SME)
Antonio Oliveira (Lab SME)
Dong Min Shen (Spotfire lead)
Zdenek Hribal (Empower team)
Michael McClellan (Empower team)
Jeff Feist (Cloud computing)
Project Plan (Design Process)
Empower/ADF Converter App Design Process

November 2018
Kickoff design workshop

December 2018
Develop design prototype individually with GSK, Pfizer, BI, Baxter, Bayer, Genentech, Merck

January 2019
Present design prototype to all parties

February 2019
Develop working prototype

March 2019
Present working prototype to all parties
Thank You/Questions?
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