AstraZeneca - Feedback from Trial Membership of Allotrope

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AZ Lab Blueprint

Collaboration across IT and Science

Transforming Data to Knowledge

Seamless Lab

Trial Objectives

Evaluate the Technology

- Small scale evaluation to address a specific business problem.
- Pragmatic investigation into the use of the Allotrope Data Format and tools.
- Investigate the effectiveness of converters from vendor format to Allotrope Data Format.
- Gain Practical experience of the Allotrope Data Format, converters, API Tools.

Gain Understanding of Allotrope

- Understand:
  - Working processes.
  - Maturity of standard and tools.
  - Pharma and vendor engagement.
- Collaborate with existing members.
- Understand FTE, skill sets required.

Value to AZ

- Understand how Allotrope will support AZ strategy on:
  - Transforming data to knowledge.
  - Data Integrity.
  - Data storage, archiving.
  - Data integration.
- Evaluate current capability v's future potential.
- Understand working model across scientific groups in AZ.
- Create business case.

Business Problem

ThermoFisher SCIENTIFIC CDS

Agilent HPLC

Waters THE SCIENCE OF WHAT'S POSSIBLE. CDS and HPLC

? Can we view data from Thermo Fisher CDS and Agilent HPLC without maintaining a suite of instrumentation and software?

? Can we compare data from historical and new CDS software and HPLC instruments?

? Will it be possible to re-process raw data from the legacy systems?

Managing Data Across Vendor Platforms

Evaluation of ADF as possible solution

- Is it possible to convert data from Thermo Fisher CDS to ADF?
- Is it possible to convert data from Waters CDS to ADF?
- Is it possible to convert data from Agilent HPLC to ADF?
- How do we view and compare data using the ADF explorer?
- Can we convert data from ADF back to vendor formats to view, compare and re-process data?

Evaluate the technology

Allotrope hands-on tech evaluation

Constrained trial

- Work with our own data
- On 1 existing HPLC process
- Limited, flexible, scope

Connect with internal stakeholders

- Spread word
- Identify use cases
- Support for membership

Connect with Allotrope community

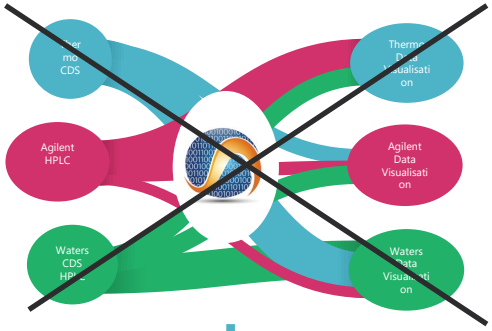
- Training, tutorials
- Connect with vendors
- Connect with pharma members & board

Evaluate the technology

Allotrope hands-on evaluation in AZ
Starting off the trial

How do we get data into ADF?

- Use software with inbuilt Allotrope compatibility
- Convert data to ADF Ourselves
- **Use vendor converters**



ADF Converter ChemStation

Agilent

How do we work with ADF?

- Allotrope tools
- Linked data tools

MedImmune
Bioprocess Dev

AstraZeneca
Pham Tech Dev

Evaluate the technology

Pharmaceutical Technology & Development

Working with HPLC data in ADF

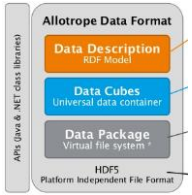
1) Integrate data from multiple Agilent HPLC runs

2) Used Agilent converters to turn data into Allotrope format

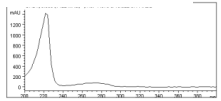
Agilent ChemStation

Batch process for convertors

3) Used standard Allotrope & linked data tools to manage & query across HPLC datasets



ADFexplorer



TURTLE

Jena

AllegroGraph
Franz Inc.

Chromatography data workflow in BPD
Can we use Allotrope to improve current process?

Consistent format across diff. software

Agilent OpenLab *ECM CDS*

Empower®

Mass Link

Export

X / Y Raw data

Formatting
- Normalising
- Scaling (MS)
- Shifting (MS)

ELN
- XY table & changes
- Other processed data

ADF for better data linkage

Easier to manage access to the data

PRISM

Formatting for BLA, IND and internal reports

Document stores

Reports

Allotrope audit trail to track changes

Figures, reports, sop stored in single location/format.

Chromatography data workflow in BPD

Consolidate all data & files in a single ADF?

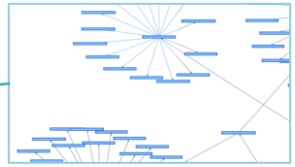
Allotrope Data Format

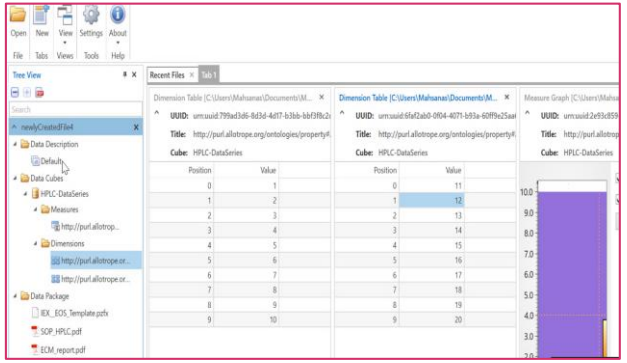
Data Description
Semantic Model

Data Cubes
Universal Data Container

Data Package
Virtual file system

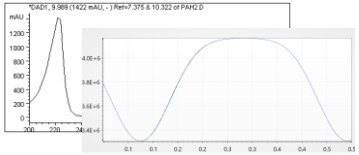
API





X/Y

Reports/SOPs

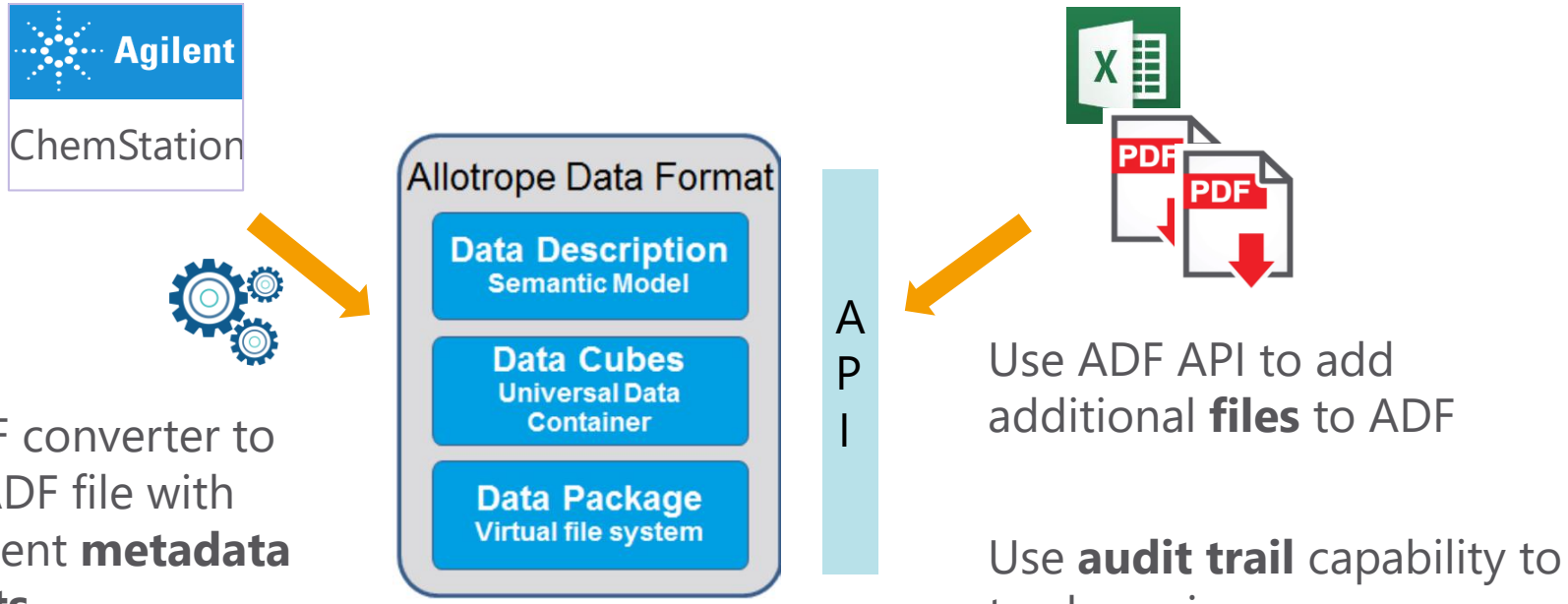


Figures

Prism files

Chromatography data workflow in BPD

Bringing it all together



Use ADF converter to create ADF file with experiment **metadata** & **results**

Use ADF API to add additional **files** to ADF

Use **audit trail** capability to track versions

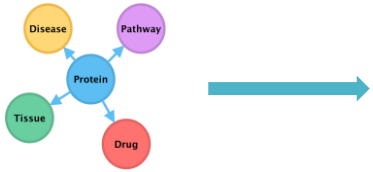
Evaluate the technology

Tech Evaluation Learnings

- Excellent work on Ontologies & ADF for HPLC
- Great training, tutorials, portal
- Meets needs for data: linkage, validation, access
- Useful audit trail capabilities
- Good vendor engagement
- Dependent on vendors for ADF converters
- ADF Explorer graph difficult to interpret
- No out of the box tools for scientists
- Need linked data skills – *difficult to search ontologies*

Tech Evaluation Conclusions

Some Open questions	How fast will vendors develop Allotrope compatibility & tools?
	Resources needed & potential risks for AZ
Huge potential value	Lab data access, integration, validation
	Right tech and organizational approach
	Need to power AI/ML – priority for AZ



Knowledge Graph

AI ML

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