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.
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

Evaluate the Technology

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?
### Allotrope hands-on tech evaluation

<table>
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<tr>
<th>Constrained trial</th>
<th>Connect with internal stakeholders</th>
<th>Connect with Allotrope community</th>
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<tbody>
<tr>
<td>• Work with our own data</td>
<td>• Spread word</td>
<td>• Training, tutorials</td>
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<tr>
<td>• On 1 existing HPLC process</td>
<td>• Identify use cases</td>
<td>• Connect with vendors</td>
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<tr>
<td>• Limited, flexible, scope</td>
<td>• Support for membership</td>
<td>• Connect with pharma members &amp; board</td>
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How do we get data into ADF?

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

How do we work with ADF?

- Allotrope tools
- Linked data tools
1) Integrate data from multiple Agilent HPLC runs
2) Used Agilent converters to turn data into Allotrope format
3) Used standard Allotrope & linked data tools to manage & query across HPLC datasets

Pharmaceutical Technology & Development
Working with HPLC data in ADF
Chromatography data workflow in BPD
Can we use Allotrope to improve current process?

Consistent format across diff. software

**ADF for better data linkage**

Easier to manage access to the data

**Consistent format across diff. software**

**Mass Link**

**ECM**

**CDS**

**Empower**

**OpenLab**

Export

X / Y Raw data

**Formatting**

• Normalising
• Scaling (MS)
• Shifting (MS)

PRISM

Formatting for BLA, IND and internal reports

**Document stores**

Reports

**ELN**

• XY table & changes
• Other processed data

**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?

Evaluate the technology
Chromatography data workflow in BPD

Bring 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
**Tech Evaluation Learnings**

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

Tech Evaluation Conclusions

Evaluate the technology

Knowledge Graph
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