

EBF – Allotrope Collaboration

Towards a common standard on LCMS/MS
e-data

David Van Bedaf, on behalf of EBF e-data Topic Team
EBF 8th Open Symposium, Barcelona

Overview

- History
- EBF – Allotrope collaboration
- Workflow and Taxonomy
- Next steps
- Summary

History – 2 independent minds meet

- Milan, September 2012
 - 11th Annual ELNs & LIMS Meeting (iqpc)
 - Announcement of formation Allotrope Foundation
 - Presentation on AnIML format
- EBF Brussels, June 2013
 - EBF Workshop: managing e-data in the regulated BA lab
- EBF Barcelona, November 2014 – see next slide
 - Spotlight on e-data
 - Presentations from vendor, business and Allotrope
 - Good interactive discussions

Outcome EBF Spotlight on e-data

- An enormous interest in this topic was seen during the session (about 120 participants).
- Mutual interest both from vendor, business and regulations in working towards a common standard for analytical data.
- Participants are looking for solutions, which preferably are out-of-the-box.
- Not much interest in actively participate to work on the solution. General feeling is to let the vendors work together with Allotrope and wait and see what the outcome is.
- Allotrope on the other hand is looking for business input to work on a Mass Spectrometer use case. But at the same time cannot share solutions with non-members.

Needs and Solutions

- Exchange data (sponsor – CRO)
- Long Term Readability
- EBF: prep work on e-data challenges
 - Identified issues
- Allotrope: open framework
 - Looking for PoC's

Join hands to
build on a MS
use case

How to collaborate without being an Allotrope member?

EBF – Allotrope Collaboration

Three phases can be identified in the EBF-Allotrope collaboration:

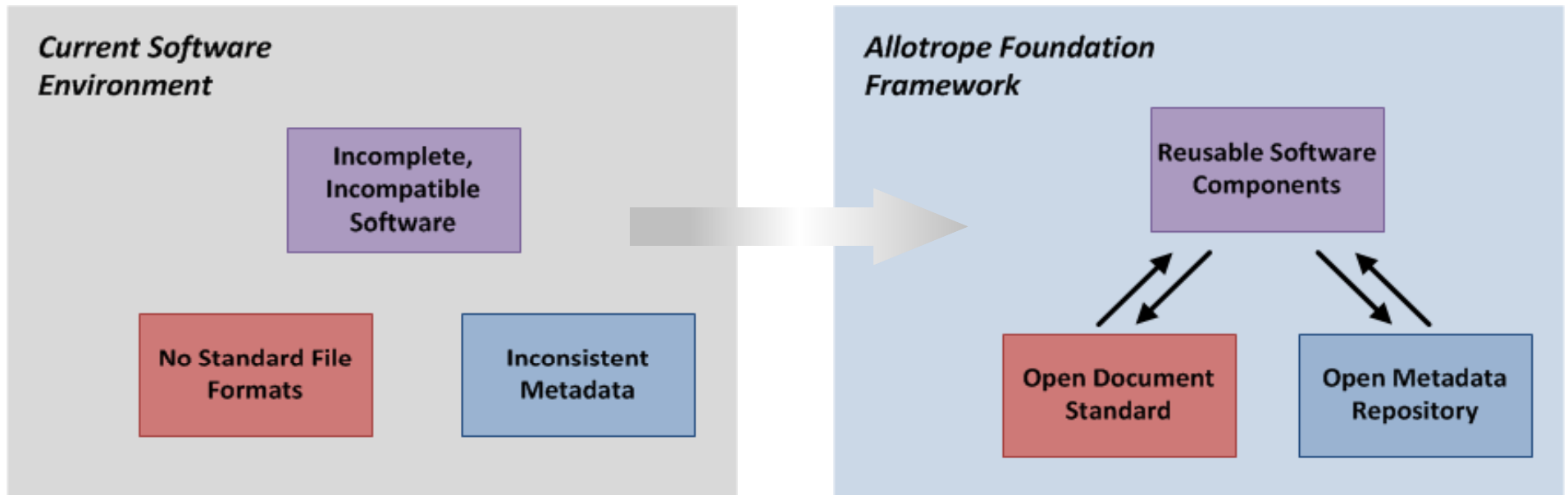
Today's topic

- Form a **Work Group** under the EBF umbrella:
 - Team existing out of Allotrope members (I.e. Abbvie and Boehringer-Ingelheim +Allotrope itself) extended with contributions of a larger group (= EBF)
 - Review the existing Allotrope Vocabulary (version 0.4) and possibly add specific LCMS/MS terms
 - Describe a typical Bioanalytical workflow (start to finish), including data exchange between sponsor- CRO

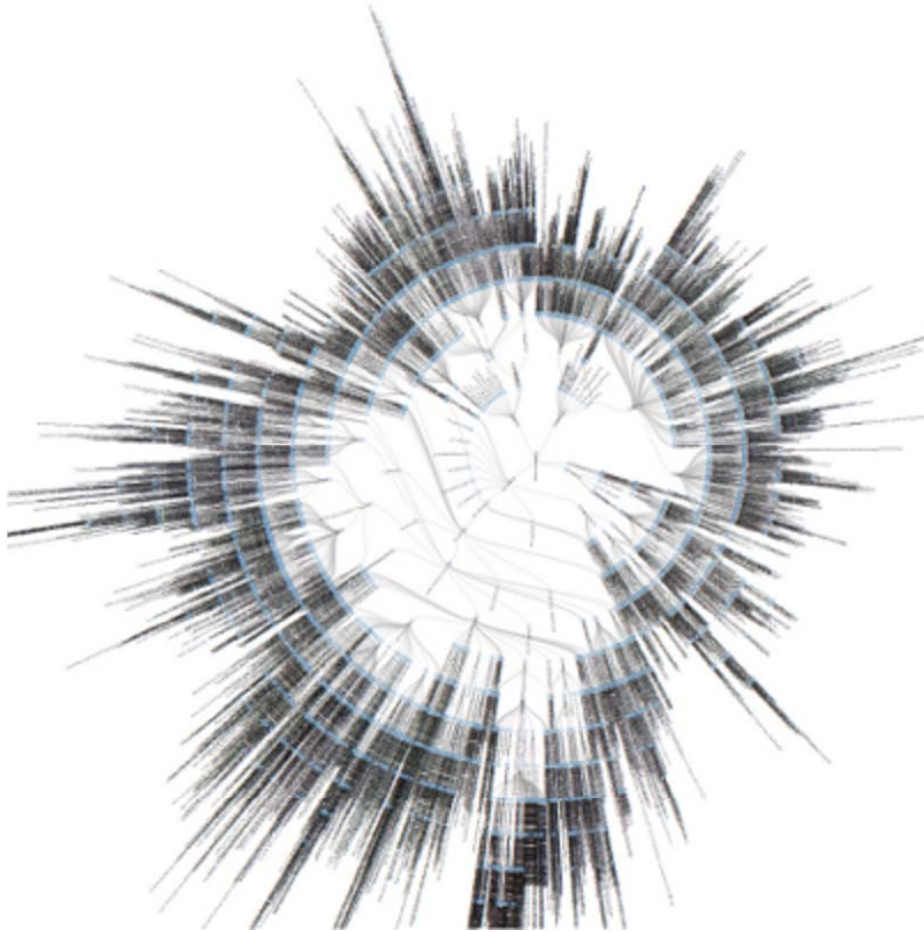
To be decided

- Organize a **Focus Workshop** in Allotrope
 - Bring experts in the Bioanalysis area together: member and non-member companies
 - Discuss the base layer
- Evaluate within Allotrope whether enough support can be found to start an **Integration Project**
 - Bring in Osthus to do the scoping and development
 - This step requires budget coming from Founding Members and others

Allotrope Framework

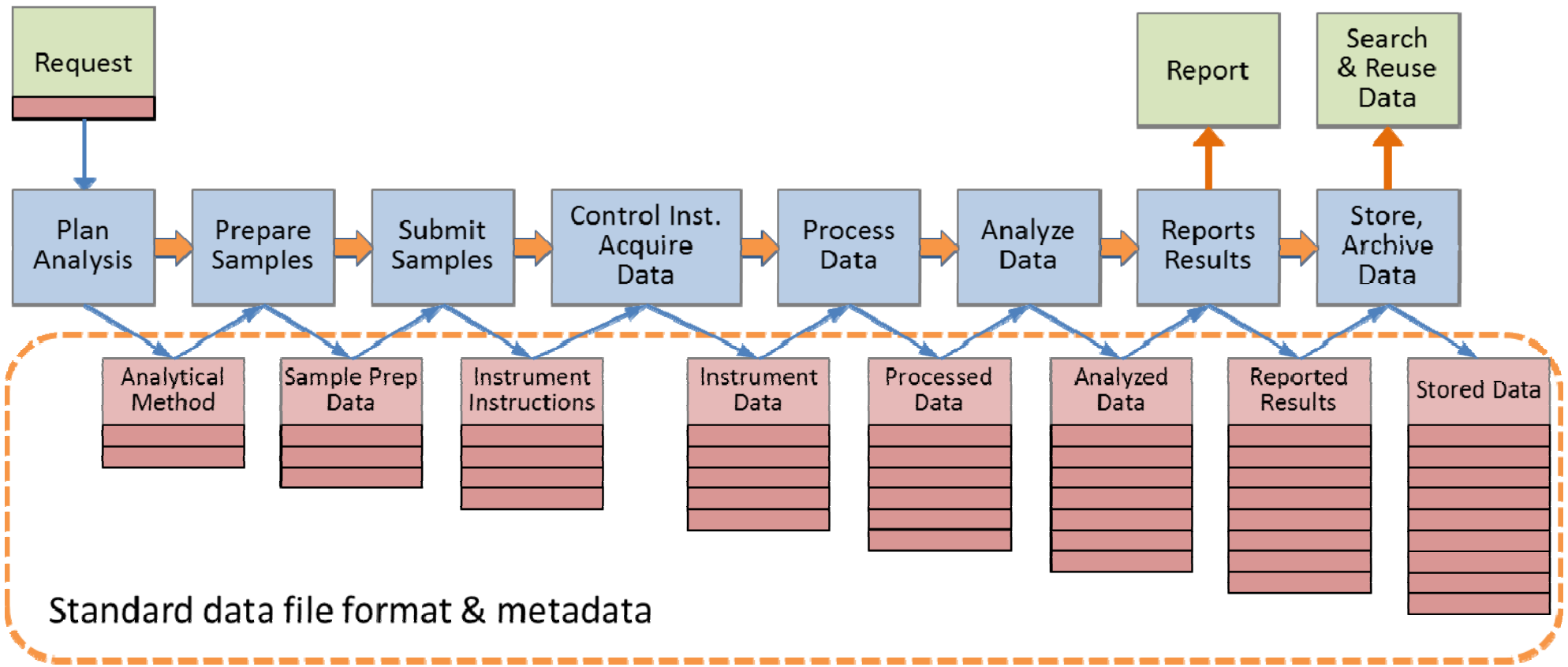


Allotrope Taxonomy



- Already very comprehensive and detailed
- Different views available
- Common – Equipment – Material – Process – Result
- Difficult to verify what details on Mass Spectrometry need to be added
- Contribution from vendors would be welcomed
- Some review feedback was given
 - Equipment, material, result
- Include CDISC and SEND glossary

Typical Analytical Workflow



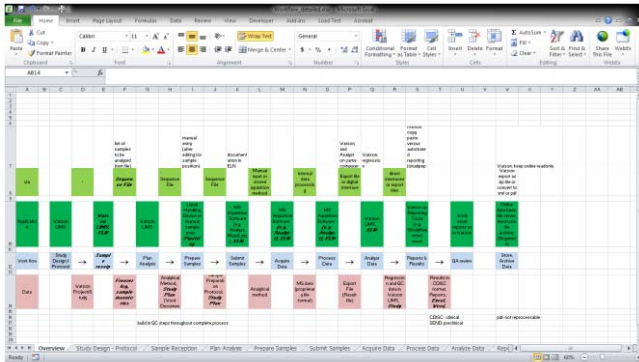
Typical BA Workflow

The screenshot shows a Microsoft Excel spreadsheet titled "Workflow_detailed.xlsx". The spreadsheet is organized into a grid with columns labeled A through AB and rows numbered 1 through 21. The data is organized into several rows:

- Row 7:** Contains text notes such as "list of samples to be analyzed (text file)", "manual entry (after editing for sample position)", "documentation in ELN", "Watson and Analyst on same computer", "manual copy paste versus automated reporting (Istudyrep)", and "Watson: keep online readonly".
- Row 8:** Contains terms like "via", "Sequence File", "Manual input or stored acquisition method", "internal data processing", "Export file or digital interface", "direct interfaces or export files", and "Watson: export as zip file or convert to xml or pdf".
- Row 9:** Contains "Application", "Watson LIMS", "Watson LIMS, ELN", "Watson LIMS", "Liquid Handling Device or manual sample prep, Pipetting", "MS Acquisition Software (e.g. Analyst, Masslynx), ELN", "MS Acquisition Software (e.g. Analyst ()), ELN", "MS Acquisition Software (e.g. Analyst ()), ELN", "Watson LIMS, ELN", "Watson or Reporting Tools (e.g. IStudyReporter) excel", "Word, excel reports or in Watson", and "Online data base, file server, electronic file archive, (Nugenisis)".
- Row 10:** Contains a flow diagram: "Workflow → Study Design / Protocol → Sample receipt → Plan Analysis → Prepare Samples → Submit Samples → Acquire Data → Process Data → Analyze Data → Reports & Results → QA review → Store, Archive Data".
- Row 11:** Contains "Data", "Watson Project/Study", "Freezer log, sample inventories", "Analytical Method, Study Plan (Word Document)", "Sample Preparation Protocol, Study Plan", "Analytical method", "MS data (proprietary file format)", "Export File (Result file)", "Regression and QC data in Watson LIMS, Study", and "Results in CDISC format, Reports, Excel, Word".
- Row 12:** Contains "build in QC steps throughout complete process" and "CDISC : clinical SEND: preclinical".
- Row 13:** Contains "pdf: not reproducible".

The spreadsheet also features a ribbon at the top with tabs for File, Home, Insert, Page Layout, Formulas, Data, Review, View, Developer, Add-Ins, Load Test, and Acrobat. The status bar at the bottom shows "Ready" and "60%" zoom.

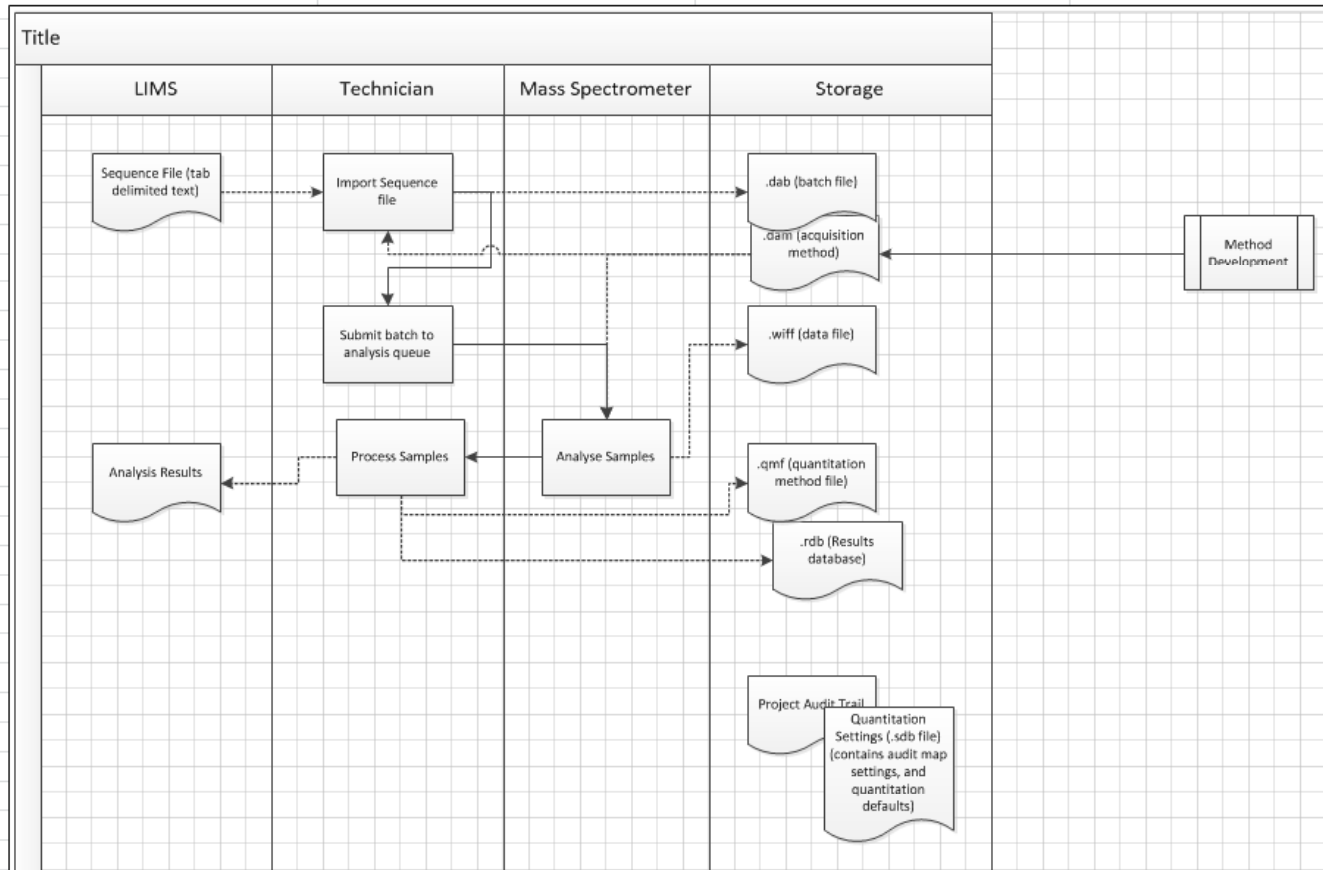
Typical BA Workflow



- Detailed workflow in excel with sections per step
- Looked at data generated by multiple software packages: Analyst, Masslynx and LCQuan
- Multiple iterations within the team
- Also added some Visio charts for more information
- Ready for peer review

Typical BA Workflow – submit samples

A	B	C	D
Input	Process	Output	Remarks
sequence file (.txt)	Analyst: build acquisition batch	acquisition batch file (.dab)	import seq file, batch file in Analyst
sample list (.spl)	Masslynx: build use method	HPLC method (.szu) Autosampler method (.pmx) Mass transition (.exp) Tuning info (.ipr)	Development of Masslynx-to-ADF adapter will start
sequence file (.csv)	LCQuan: workbook in study folder	sequence file (.csv)	Folder: Imports



Next steps

- Send detailed BA workflow for peer review:
 - Within EBF
 - Global BA community
- Discuss with Allotrope and EBF the possibility of a Focus Workshop on Bioanalysis
- Start Integration Project to get MS data hooked on the Allotrope Framework
 - Budget required
- Agree with vendors to collaborate with Allotrope
 - Develop adaptors to convert data to ADF format

Summary

- Started an EBF – Allotrope collaboration
- E-Data Topic Team reviewed the Allotrope Taxonomy and described the BA workflow
- Possible next steps:
 - Organize a BA Focus Workshop at Allotrope
 - Integrate LCMS/MS data in the Allotrope Framework
- Ultimate goal:
 - Exchange e-data with partners (CRO-Sponsor)
 - Long-term Readability

Thank You

EBF-team

- Martina Wein – Boehringer Ingelheim
- Stefan Blech – Boehringer Ingelheim
- Rachel Green – LGC Group
- Tobias Haslberger – Abbvie
- Alex Attema – PRA Health Sciences
- Marco Heldoorn - PRA Health Sciences
- Hans Mulder – Astellas
- Philip Timmerman – Janssen (Sponsor)

Allotrope

- Gerhard Noelken – Allotrope Foundation



THANK YOU – Q&A

