



Allotrope Connect Virtual Workshop

MassSpec ADF: a full data “round-trip” - From raw data conversion from Sciex Analyst to reopen ADF

5 October 2020

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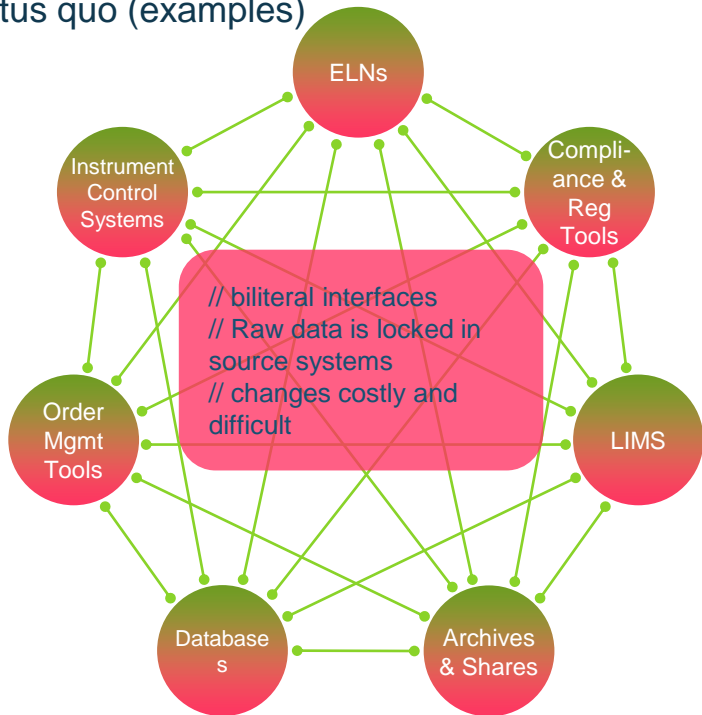
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 - Henning Kayser | Digital Transformation Lead | Bayer AG



Data-centric System Architecture

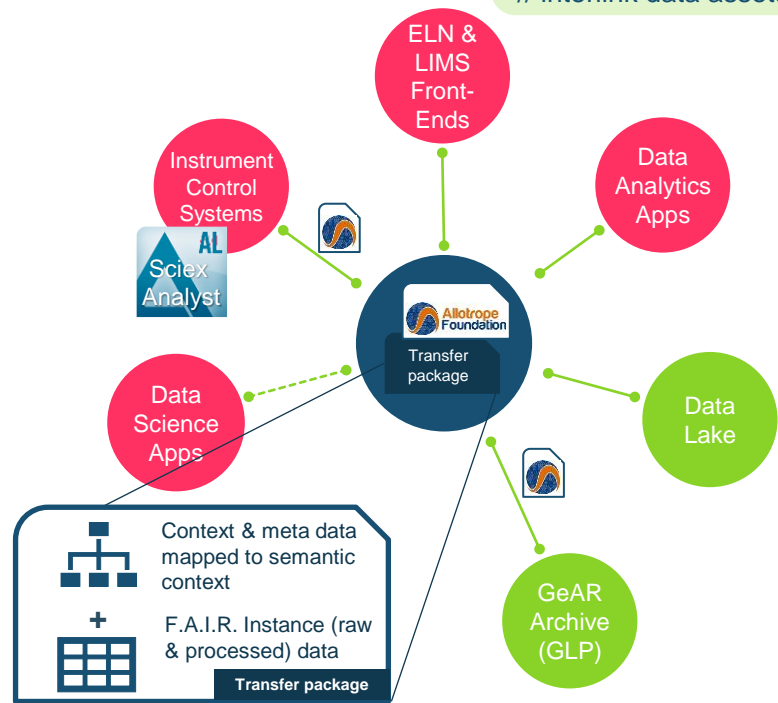
Escape interfacing gridlock in **Data hostage Apps** – Unlock **Data** from **Apps**

Status quo (examples)



Target state

// separation of apps & data
// standardizing data access
// streamlined interfacing
// interlink data assets



SCIEX ADF Viewer

- Stand-alone application
- Creates ADF files from SCIEX Analyst® mass spectrometry data
 - Includes:
 - Raw spectra
 - Method information
 - Quantitated data
 - Audit trails
 - Native files
- Uses SCIEX Analyst® -specific model

SCIEX ADF Viewer

- Reads (SCIEX) ADF files
- Displays data in tabular and hierarchical format
- Displays Total Ion Chromatograms, Extracted Ion Chromatograms
- Exports data description to Turtle (ttl) and XML format

SCIEX ADF Viewer

- Uses SCIEX-specific vocabulary
- Vocabulary is customizable
 - Allows administrative user to customize URIs
 - Vocabulary URIs
 - Unit URIs

- Demo

Work planned or in-process

- Integration with ADF Explorer
- Harmonization with MS Data Shape
- Documentation
- GLP Support (e.g., software validation)
- Support for SCIEX Multiquant, SCIEX OS software





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