



Rethinking scientific data

Allotrope@Bayer



**Driving measurable
outcomes for labs via
digitalisation and
standards**

Wed, Nov 13th 2018 // Henning Kayser //
Lab of the Future //
Wellcome Genome Campus //
Cambridge, UK





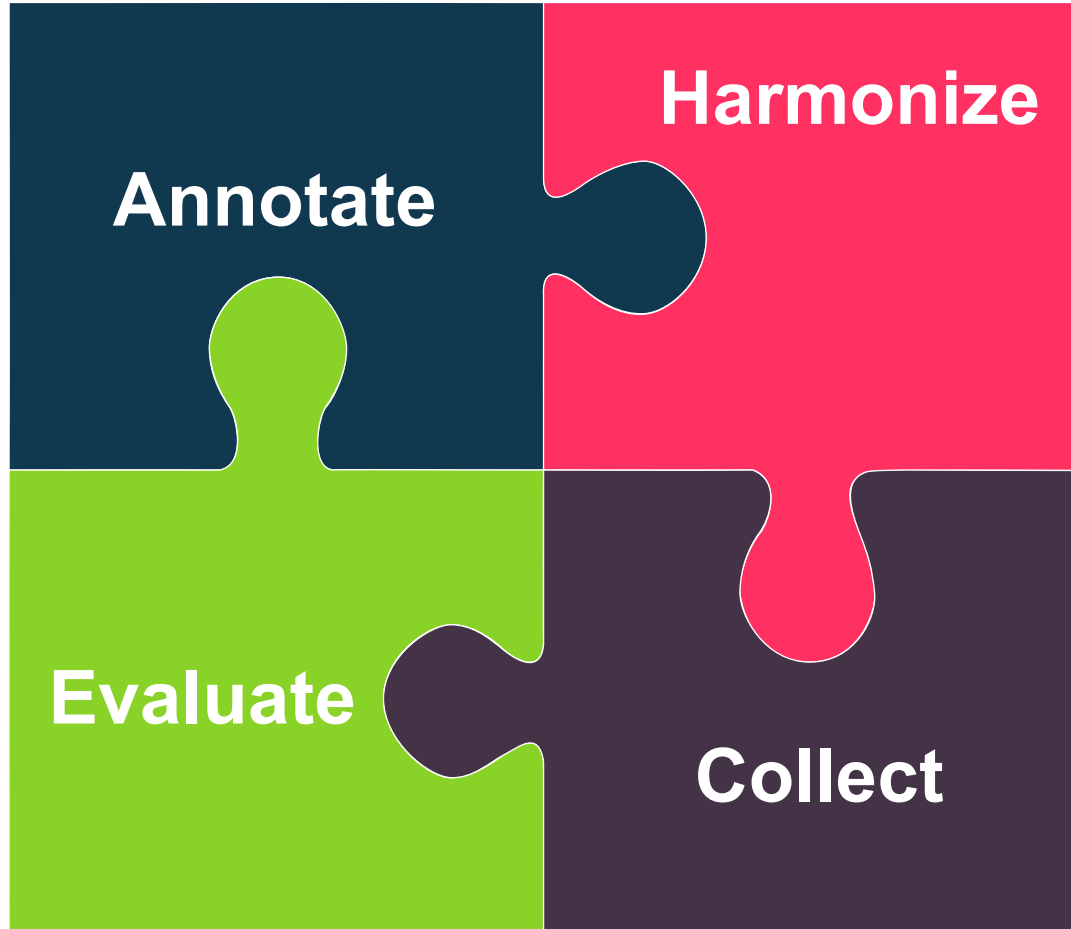
Industry-wide challenges in R&D



- // R&D productivity challenges
 - // Data Silos / Manual transfers
 - // Implicit Know-how
 - // Accessibility of data
 - // Find vs. reproduce data



Data life cycle in a „Digital lab“



- // Required enablers
 - // Harmonize, curated data
 - // Annotated context, meta data
 - // Data-centric collection
 - // Commoditized labs
- // Cross-correlation of scientific data
 - // Automated evidence generation



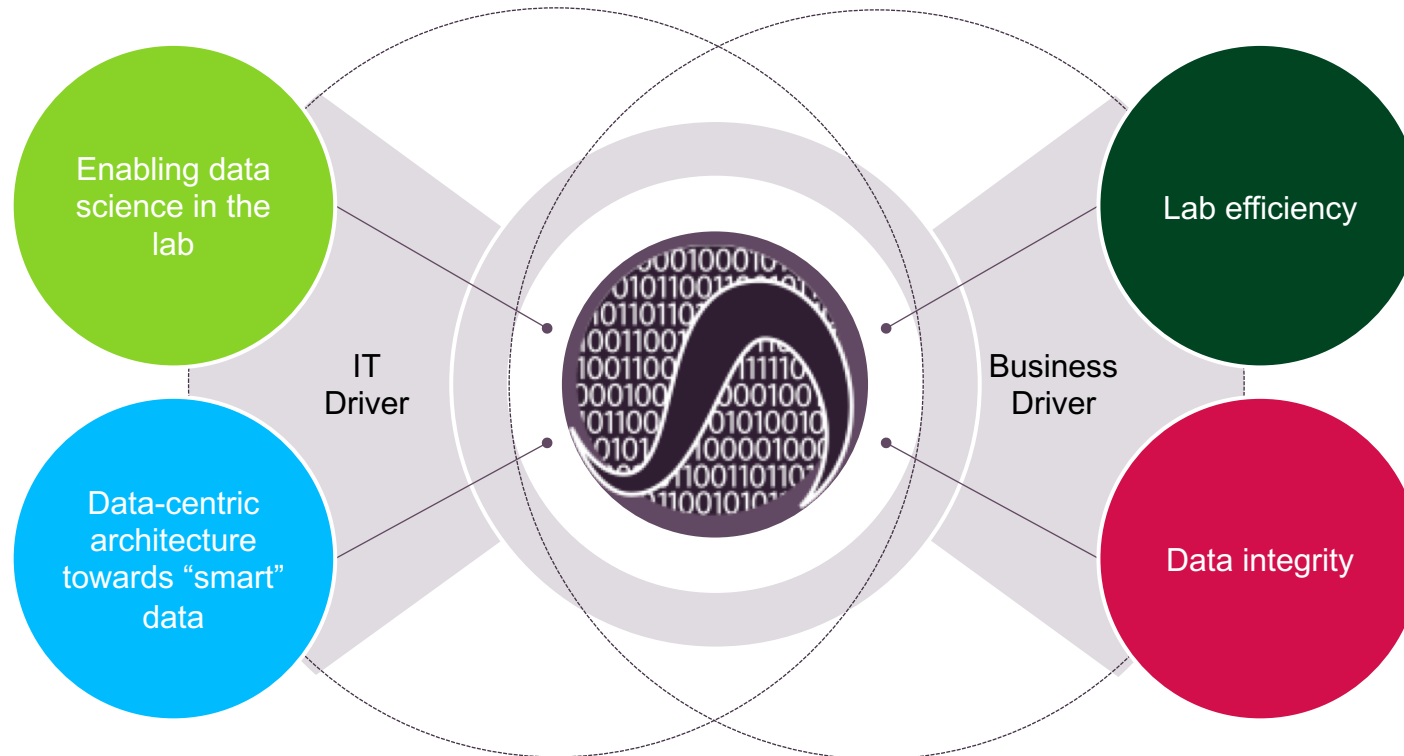
Transfer MS Method Information using ADF

*Annotate
data*



Motivation for “smart” analytical methods

Why using standards?





Managing analytical methods

As-is: Interrupted Process for Setting up MS Analytics

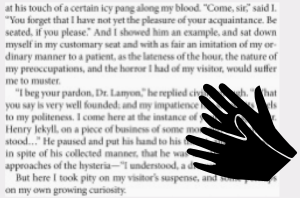


**Labware &
STARLIMS**



LIMS




MANUALLY
assigned analysis




TEXT-BASED
Analytic (HPLC-MS) Method



MANUALLY
transcribed text-Method
to MS software

HPLC-MS 
Workstation 1

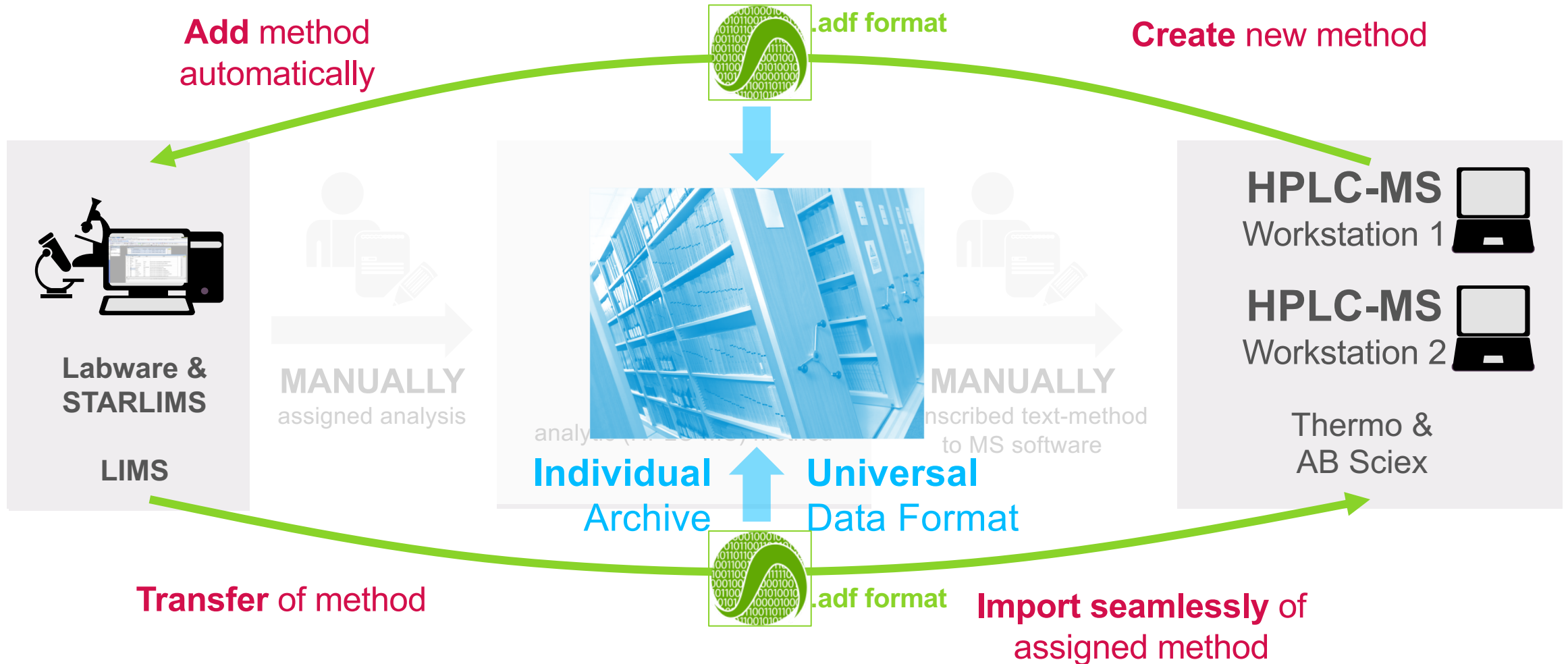
HPLC-MS 
Workstation 2

Thermo &
AB Sciex



Managing analytical methods

Now: Simplified process, universal machine-readable methods





Analytical Method Management

Text-based to machine readable



...A small aliquot (25 μ L) of the inbound sample was removed and diluted with 325 μ L of methanol for initial analysis. The diluted sample was injected onto an analytical LC-MS system consisting of Shimadzu LC-10 series pumps, variable wavelength UV detector (SPD-10Avp), and autosampler (SIL-10Avp), and under control of Shimadzu ProminenceVP v 7.32.0.190 software, with a Waters model ZQ mass detector running MassLynx version 4.1 data acquisition software. Injections were made onto a Waters X-Bridge C18 column (4.6 \times 50 mm, 5 μ m particles) using mobile phase of (acetonitrile/water +10 mM ammonium acetate, with a linear gradient elution mode from 5% to 95% organic over 4 min at a flow rate of 4 mL/min. Samples were detected by UV absorbance at 220 nm and by mass spectrometry including the extracted ion chromatogram for the target (M + H)⁺ ion.

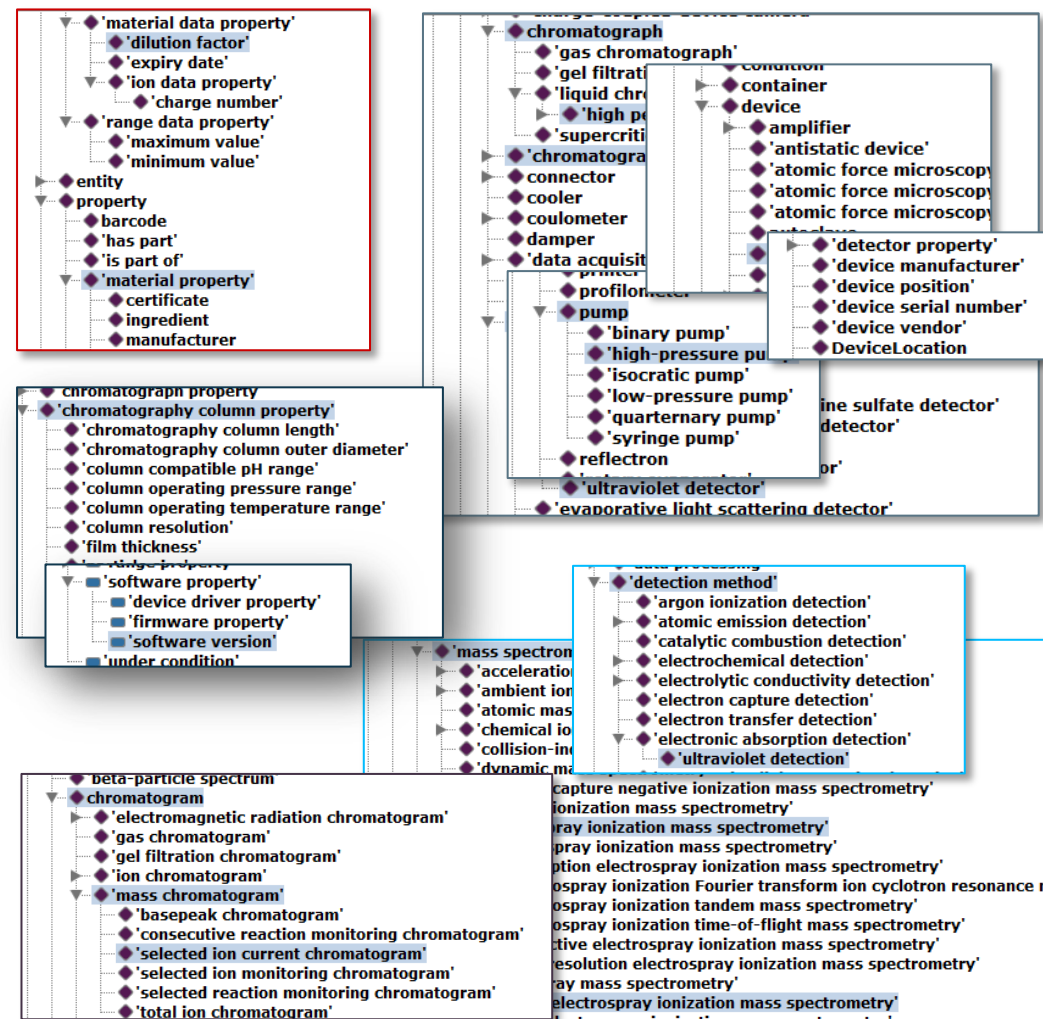
Material

Device

Properties

Process (method)

Results





Analytical Method Management

Benefits on various levels



**INTEGRATE
MS-WORKSTATION**
from stand-alone system
into a lab landscape



AVOID ERRORS
through checks, enabled by
Parameter reporting



**HIGHER DATA
INTEGRITY**



**BETTER WORKFLOW
INTEGRATION**



**CENTRAL METHOD
REPOSITORY**



**EASY METHOD
TRANSFER**
from machine A to B



OK

GxP-COMPLIANT
information transfer



**GENERIC
INTEGRATION**
instead of bilateral
integration into LIMS/ELN



Harmonized Data

**Selected implementation
examples**



Allotrope Foundation

**How does Allotrope help us
implement these strategic
patterns?**

The Allotrope Community



abbvie

AMGEN

Baxter



OSTHUS
success with R&D



Architect

Genentech
A Member of the Roche Group



Lilly



Drinker Biddle



COGNITIVECHEM



TETRASCIENCE



SYNTHACE



COGNITIVECHEM



HALO DIGITAL



Waters
THE SCIENCE OF WHAT'S POSSIBLE.



accenture

PANGAEA
Bringing it together to make it happen



University of Strathclyde Glasgow



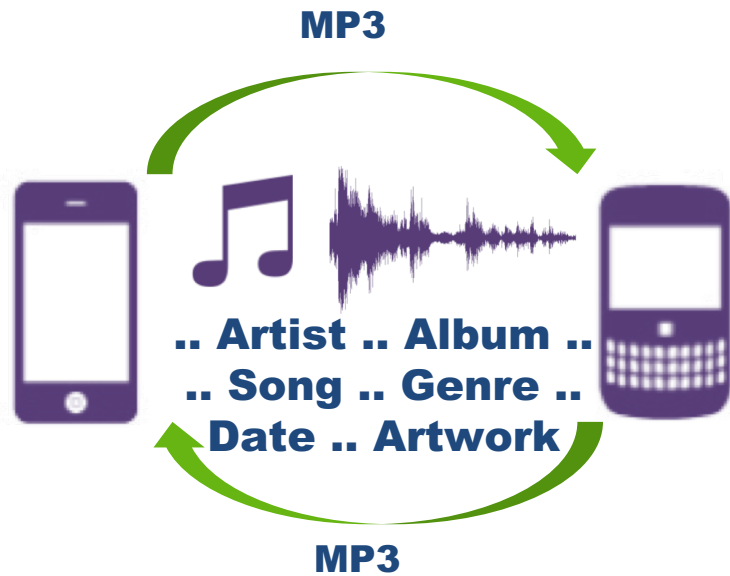
BSSN Software • Erasmus MC • Fraunhofer IPA • L7 Informatics

Mettler Toledo • NIST • SciBite • Stanford University • University of Illinois at Chicago • University of Southampton

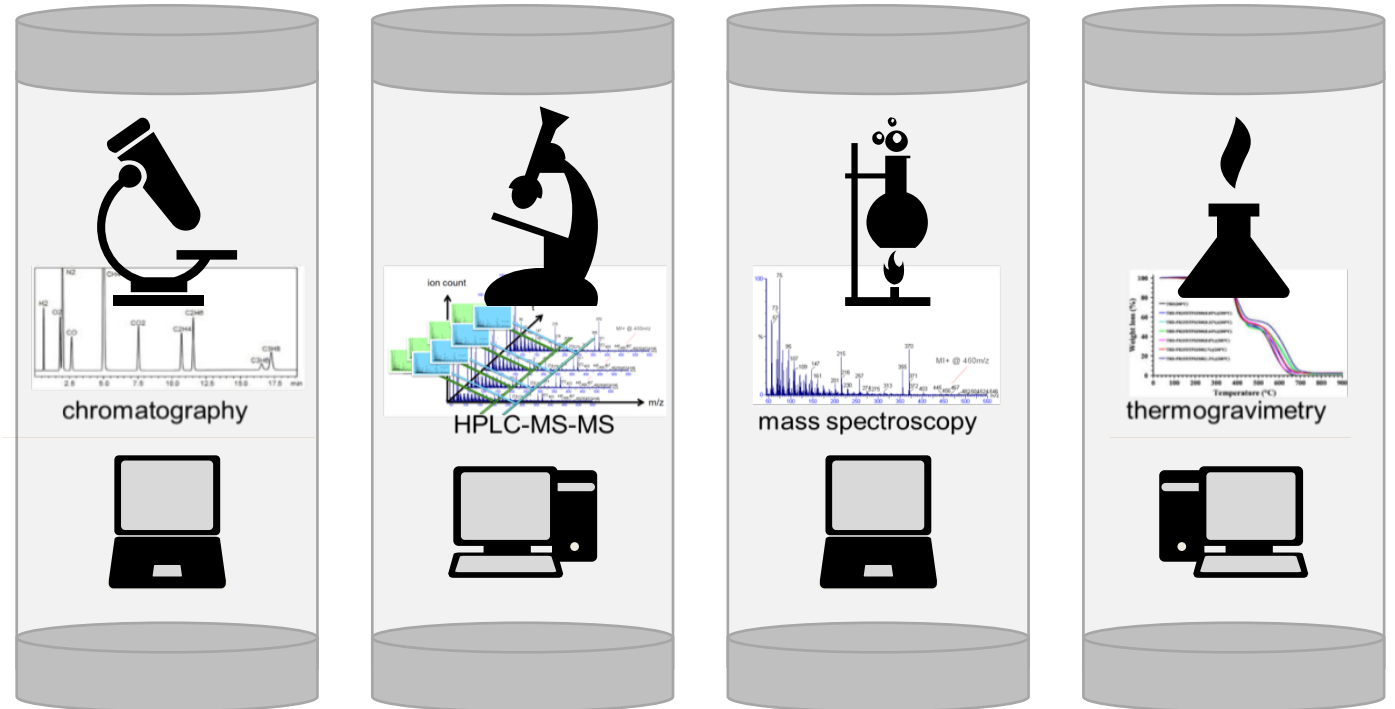


FAIR Data for the lab

In our private environment...



- In the scientific environment...

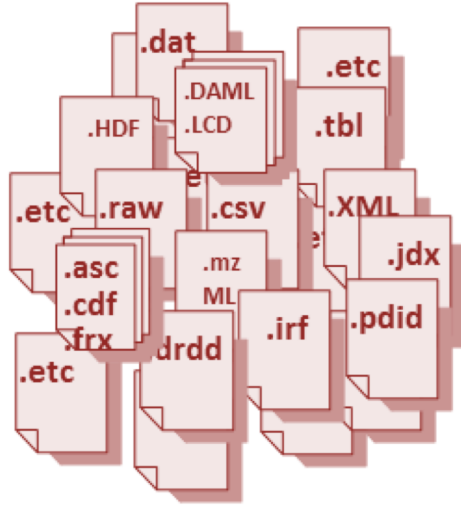


We generate data in every minute.
Why not use its untapped potential?

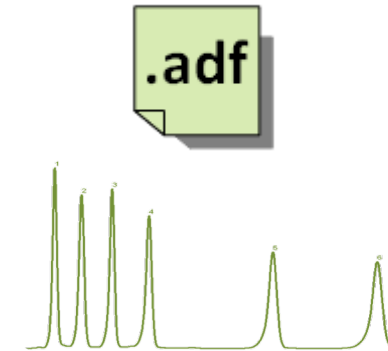


Addressing the root causes

Vendor/instrument-Specific Formats



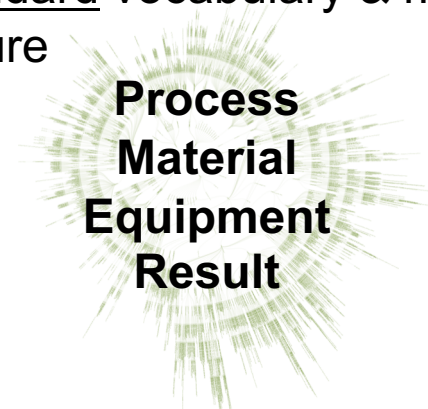
Data in Standard Format



Paper-based and unstructured text for methods, regulations, recipes, observations, etc

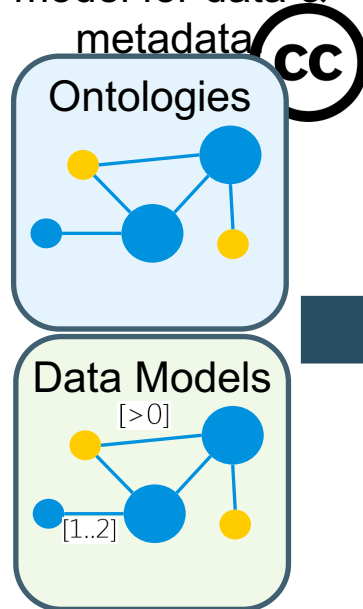


A Standard vocabulary & metadata structure

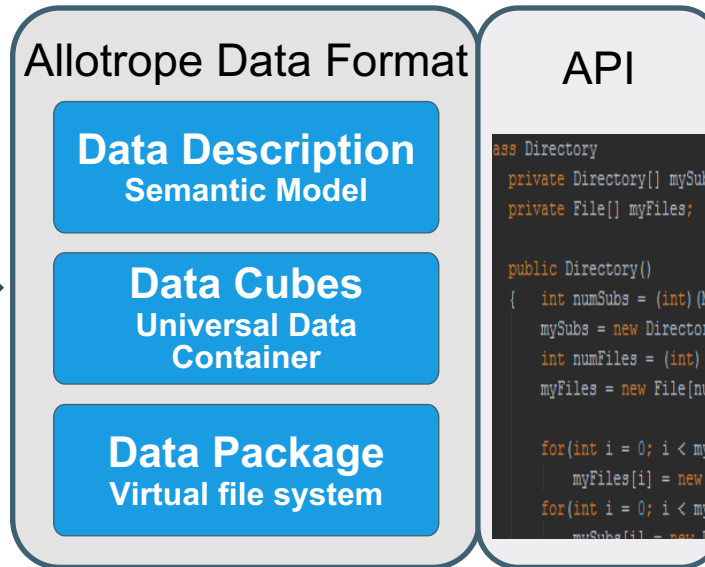


The Allotrope Framework

A standardised semantic model for data & metadata



A set of constraints on the semantic model using data shapes.



A high-performance binary data format. Instrument, vendor, platform agnostic.

An API to allow consistent creation & reading of ADF files.

ADF Explorer



ADF Explorer allows browsing of existing ADF files.





Harmonized Data - Examples

Bayer is a founding member of the Allotrope Foundation



// Successful instrument integration into electronic lab notebook using Allotrope Data Format (ADF)

// idbs ELN: ADF importer

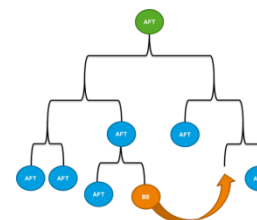
// YSI Bioanalyzer: Rest service



// Use of Allotrope Ontologies (AFO) as master data in Biologics Development project

// 19 Assay techniques added

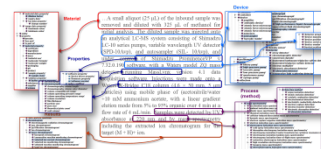
// Increased Allotrope taxonomy by >4350 Terms



// Transfer of analytical methods between LIMS and mass spec instrument control software using ADF

// MS Method to/from ADF Converter

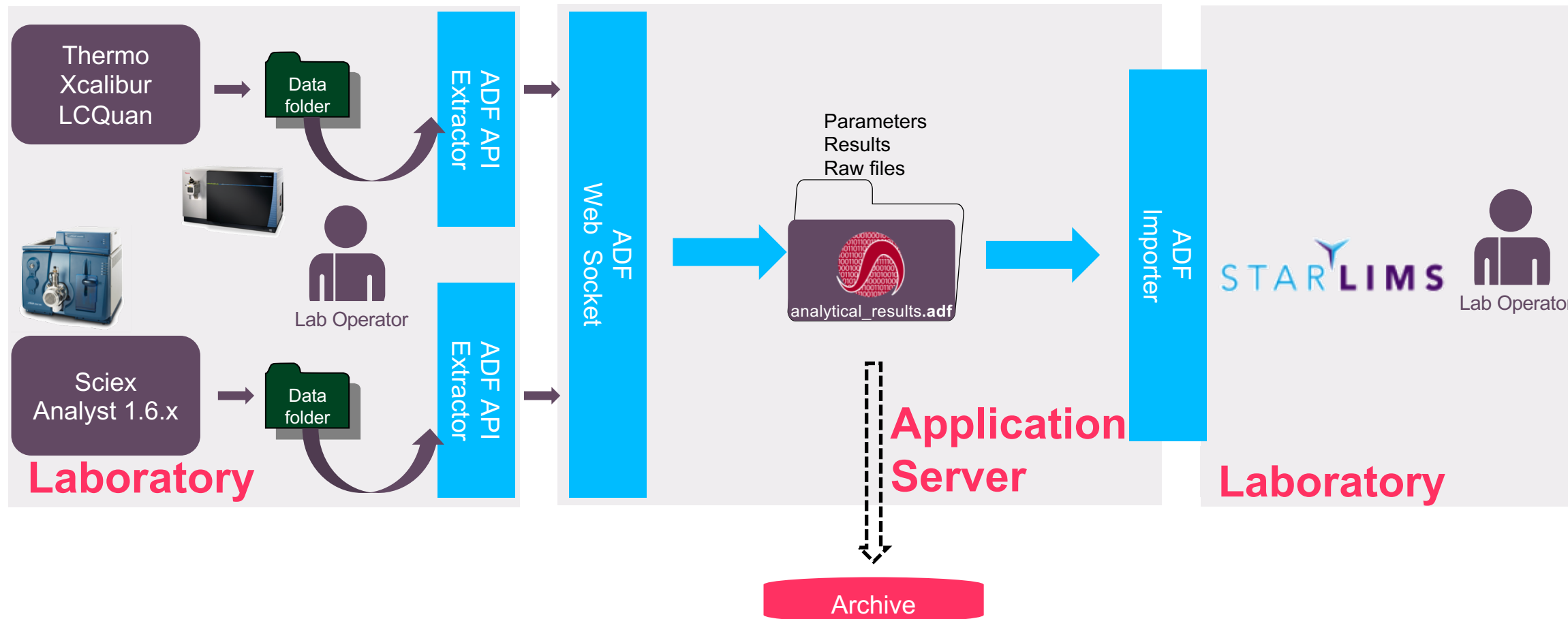
// Sciex Analyst & Labware LIMS





Mass Spectrometry - Crop Science Implementation

ADF Adapter





Allotrope enabled archiving



Allotrope-
enabled
eArchiving

Scalable
Platform

Long-term
FAIR data

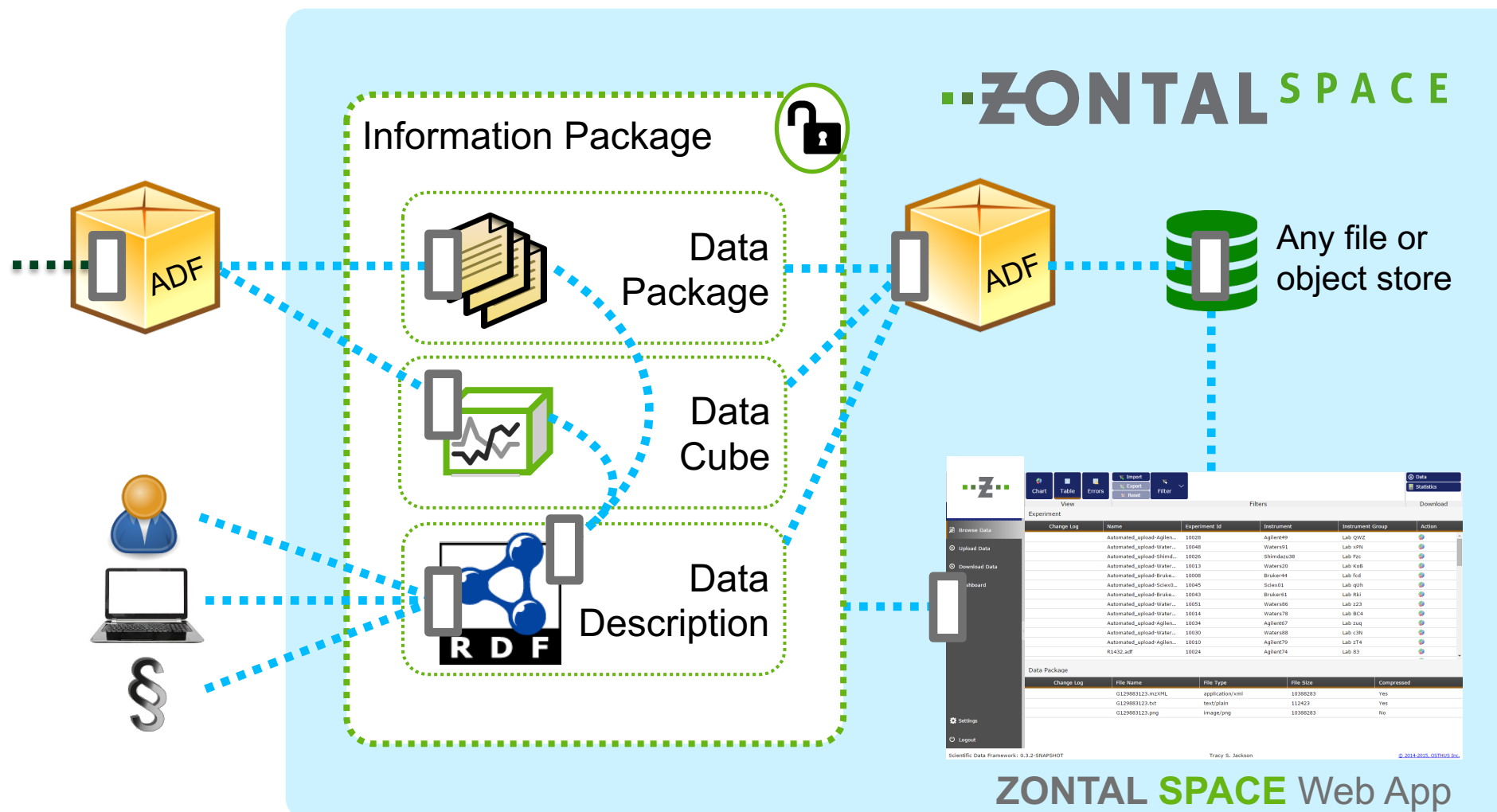
Decouple
Producer &
Consumer
(OAIS ISO 14721)

Self-
descriptive
Foundation for
advanced analytics
& ML





ADF CAPTURE & METADATA Enrichment





Towards digital labs

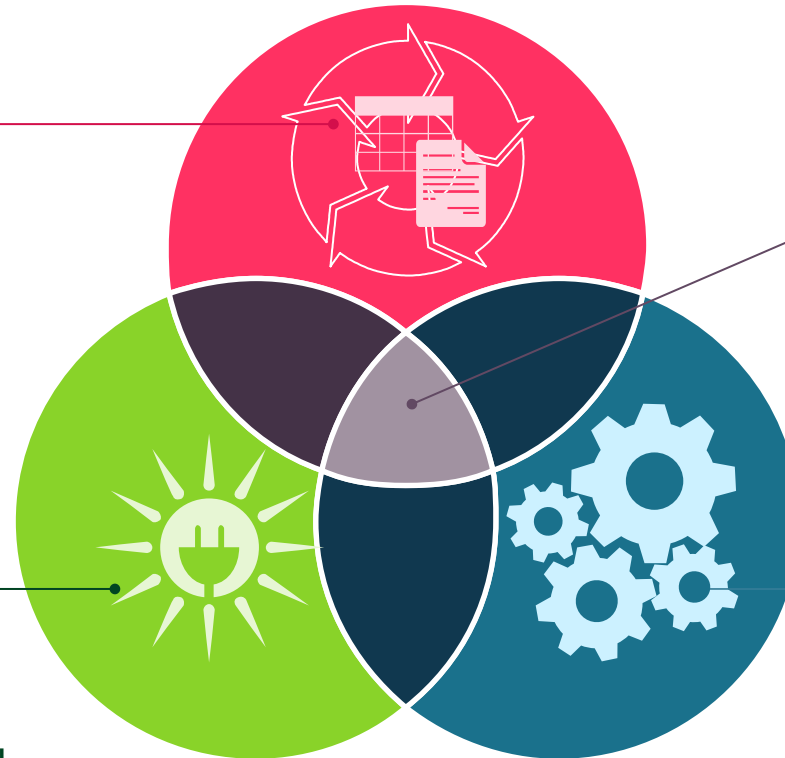


Data-centric architecture

- Decouple data and process
- Use standard interfaces
- Use standard data formats
- Enable a living archive

Accessibility

- Make laboratory data company-wide accessible
- Enable smart collaboration (internal & external)
- Reuse data beyond initial purpose



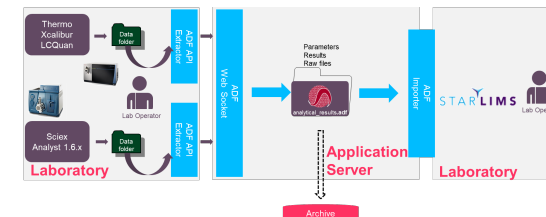
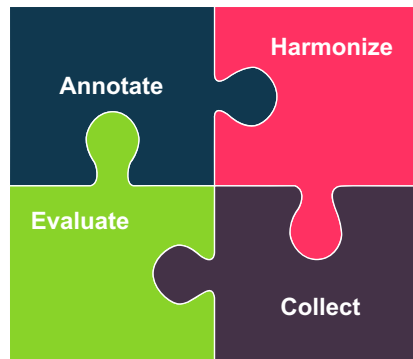
Digital labs
// Scalable, integrated processes

Semantics

- Use ontologies to add context to master and meta data
- Enable implicit documentation



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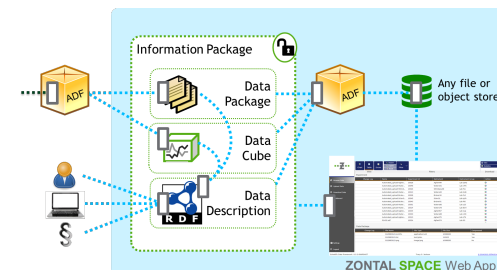
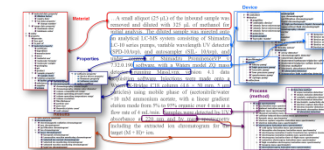
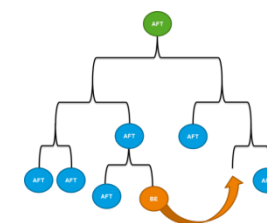
// Enablers through Allotrope

// Accessible Data (FAIR)

// Data centric approach

// Explicit knowledge through semantics

// Towards automated scientific evidence





Forward-Looking Statements

This presentation may contain forward-looking statements based on current assumptions and forecasts made by Bayer management.

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The company assumes no liability whatsoever to update these forward-looking statements or to conform them to future events or developments.



Thank you!



Bye-Bye

