How Agilent will use Allotrope Data Format to improve Laboratory Efficiency

Allotrope Fall Connect 2024

Agilent
Trusted Answers

Tony Kappen

Solutions Manager Data, Digital Lab Innovation

Agilent Technologies

Santa Clara, CA

Safe Harbor

This presentation contains forward-looking statements (including, without limitation, information and future guidance on the company's goals, priorities, growth opportunities, customer service and innovation plans, new product introductions, financial condition and considerations, and the continued strengths and expected growth of the markets the company sells into, operations) that involve risks and uncertainties that could cause results of Agilent to differ materially from management's current expectations. The words "anticipate," "plan," "estimate," "expect," "intend," "will," "should" "forecast" "project" and similar expressions, as they relate to the company, are intended to identify forward-looking statements.

Agilent

Executive Summary

Winning Through Improved Integration and Connectivity

The Opportunity: End User demand for increased lab efficiency and reduced capex and operational expenses through lab automation, data management and AI enablement within the laboratory is growing rapidly.

The Data Challenge: The end user is faced with integrating an overwhelming number of data streams not only from a variety of Agilent hardware and software products, but also third-party hardware and software products.

To address this fundamental connectivity problem, Agilent is to developing **an open, flexible, extensible set of tools and technologies** *to facilitate these connections,* **bring these data streams together in a coherent way** *and therefore improve the efficiency of laboratory operations.*

Agilent

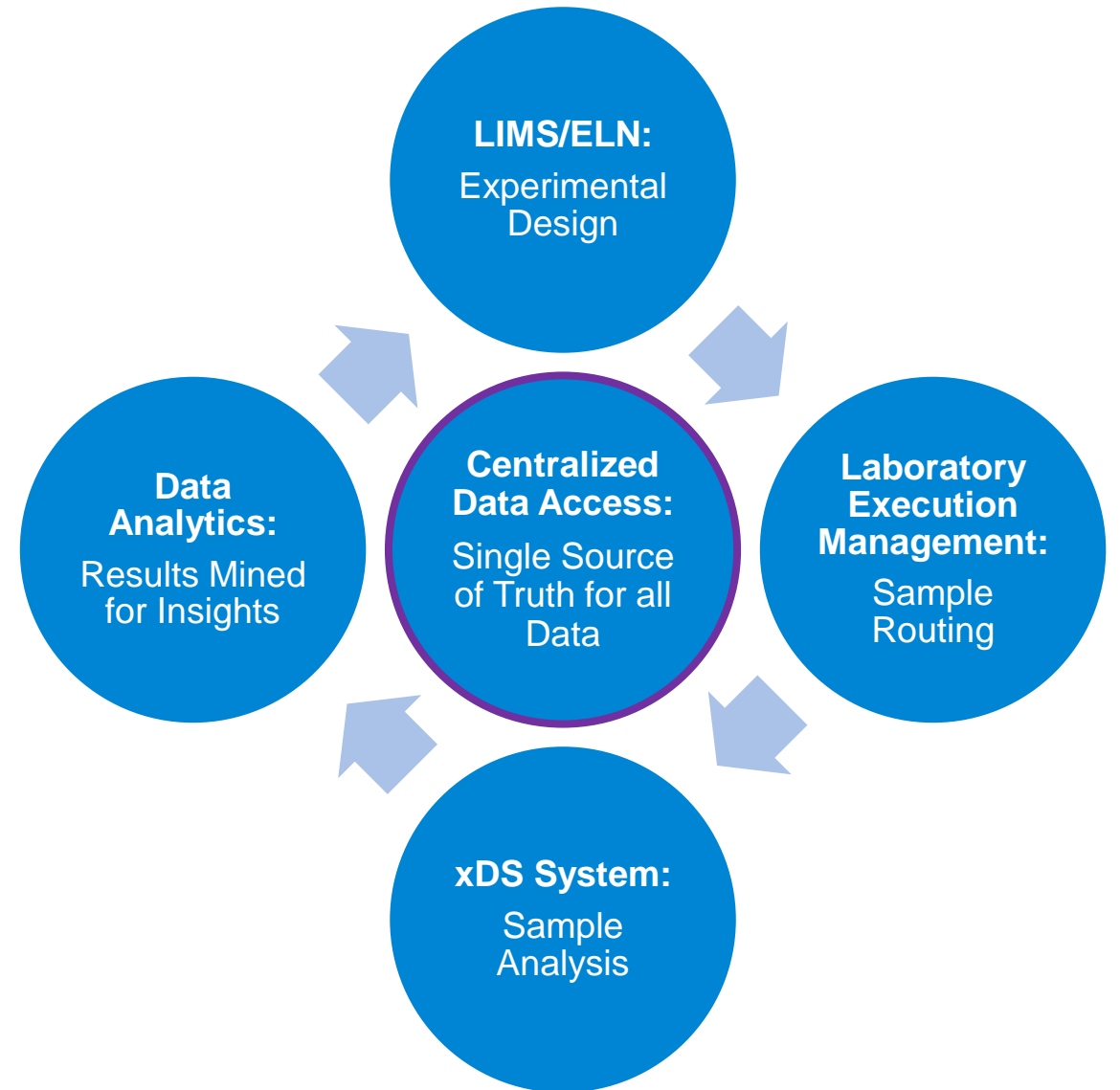# Digitalizing the Analytical Laboratory

The Fundamental Workflow Challenge

The fundamental workflow challenge within all laboratories consists of **four key components**. These components can be driven manually or automatically (digitalized).
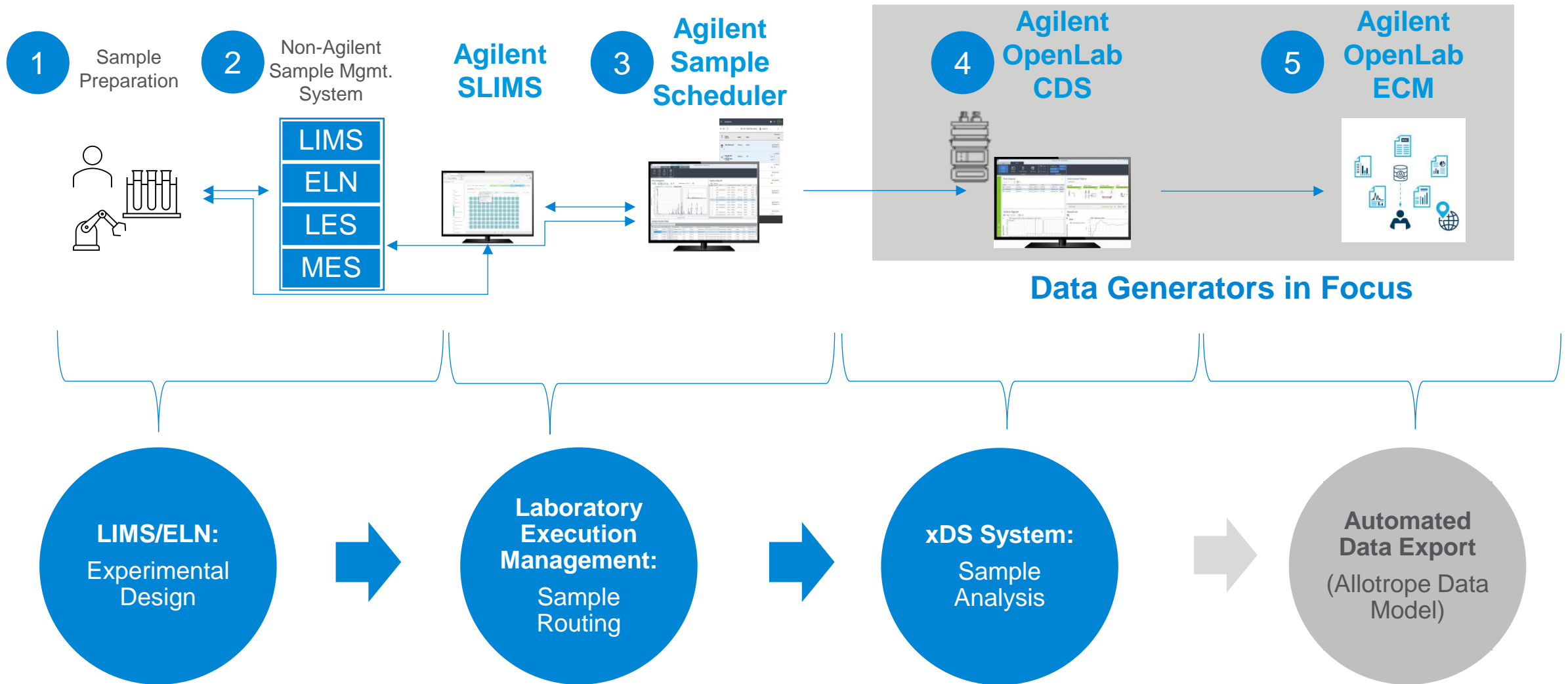
- Experimental Design
- Sample Routing
- Sample Analysis
- Results Mined for Insights

Insights drive experimental design.

To improve the speed and efficiency of the lab, not only do the **operations within a given component** need to be connected and digitalized, but each of the **fundamental components** need to be **connected and integrated** with each other.

LIMS/ELN:
Experimental Design

Laboratory Execution Management:
Sample Routing

xDS System:
Sample Analysis

Data Analytics:
Results Mined for Insights

Centralized Data Access:
Single Source of Truth for all Data

Agilent

An Introduction into Agilent Software Eco System

1 Sample Preparation

2 Non-Agilent Sample Mgmt. System

Agilent SLIMS

3 Agilent Sample Scheduler

4 Agilent OpenLab CDS

5 Agilent OpenLab ECM

LIMS
ELN
LES
MES

Data Generators in Focus

LIMS/ELN:
Experimental Design

Laboratory Execution Management:
Sample Routing

xDS System:
Sample Analysis

Automated Data Export
(Allotrope Data Model)

Agilent

Embracing Allotrope Data Model to support Vendor Neutral Data
Three Fundamental Data Streams

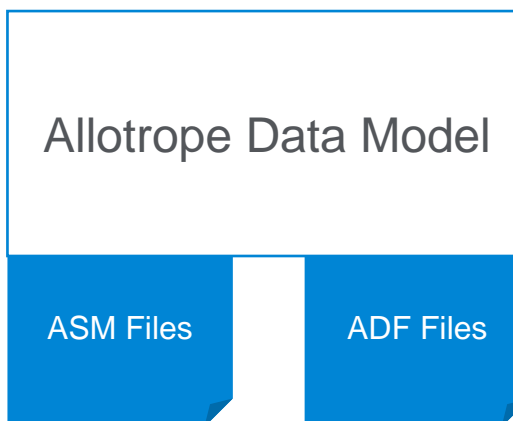**Laboratory Data Stream**
Sample Information, Methods

Instrument Data Stream
Telemetry Data, Run Control

Analytical Data Stream
Raw and Processed Analytical Results

Allotrope Data Model

ASM Files

ADF Files

Outcomes

Integrate

Interoperate

Interconnect

Summary of Approaches in Development
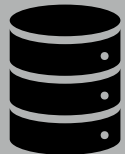## Supporting both Workstation and Enterprise-Level Automated Data Export

As a member of Allotrope Foundation, Agilent is developing Automated Data Export capabilities based on the Allotrope Data Models.

Automated OpenLab CDS Workstation Export (ASM JSON)

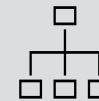**Automated OpenLab ECM 3.X/XT Export (ASM JSON)**

***Proposed* MassHunter Data Export (Custom but well documented HDF5)**

For each type of analytical data made the vendor needs to document the following:

Vocabulary – Collection of terms with agreed upon definition to describe things
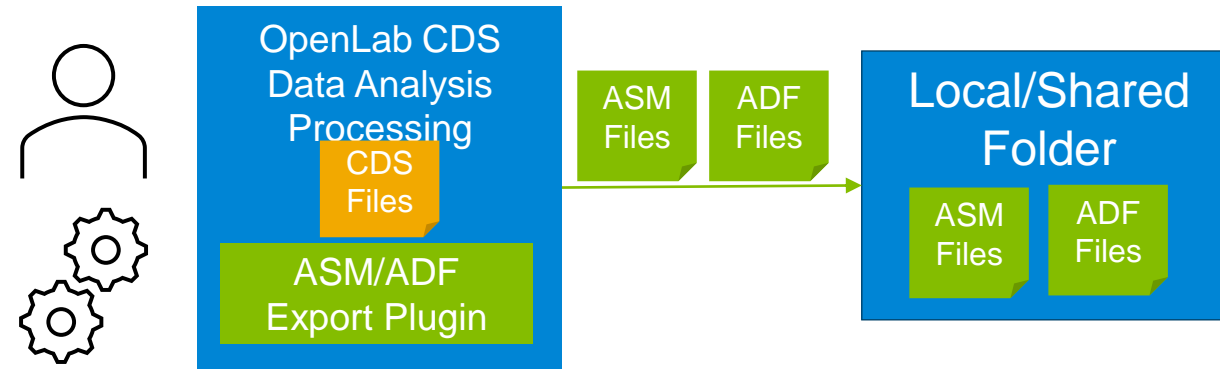
Taxonomy – Hierarchal classification of the vocabulary terms

Ontology – Formal categories, properties, and relationships across taxonomy terms

Automated OpenLab CDS Workstation Export
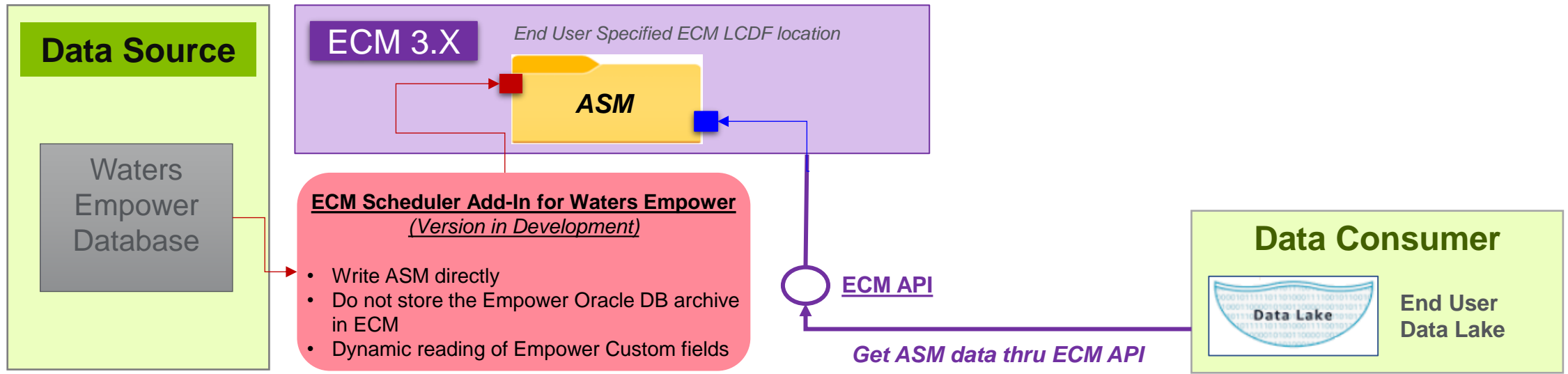## Export for Workstations or Special On-Prem Deployments

1. **OpenLab CDS DA Processing** – Use OpenLab CDS and Data Analysis Tool to generate new Result Sets

2. **ADF / ASM Plugin -** As part of post processing step ADF/ASM Export Plugin coverts Result Set into ASM JSON into a predefined folder

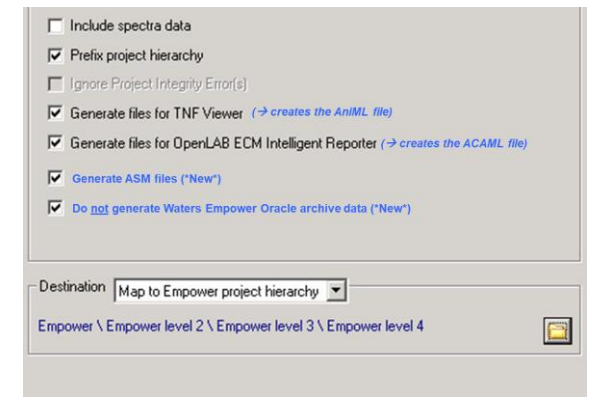**Currently deployed at our Co-Creation partner site – Swiss Cat+**

Agilent

Automated Waters Empower Database Export (ECM 3.X)

Customer Development Project for Exporting Waters Empower Data

Data Source

Waters Empower Database

ECM 3.X

End User Specified ECM LCDF location

ASM

ECM Scheduler Add-In for Waters Empower
(Version in Development)

- Write ASM directly
- Do not store the Empower Oracle DB archive in ECM
- Dynamic reading of Empower Custom fields

ECM API

Get ASM data thru ECM API

Data Consumer

Data Lake

End User Data Lake

New Waters Empower result sets are detected by the ECM Scheduler, automatically converted to ASM objects, and stored in ECM 3.6. The resulting ASM objects can then be extracted from ECM into the End User Data Lake using the ECM API.

☐ Include spectra data
☑ Prefix project hierarchy
☐ Ignore Project Integrity Error(s)
☑ Generate files for TNF Viewer (→ creates the AniML file)
☑ Generate files for OpenLAB ECM Intelligent Reporter (→ creates the ACAML file)
☑ Generate ASM files (*New*)
☑ Do not generate Waters Empower Oracle archive data (*New*)

Destination Map to Empower project hierarchy ▼

Empower \ Empower level 2 \ Empower level 3 \ Empower level 4

Agilent

Looking to the Future - Automated OpenLab ECM ASM/ADF Export

## Proof of Concept: ASM Export from ECM (On-Prem/Cloud)
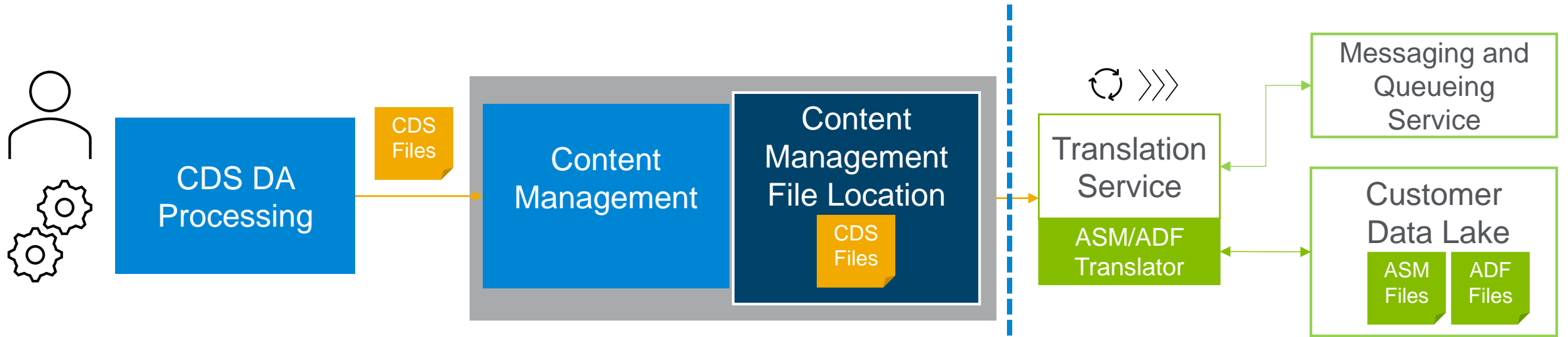
1. **OpenLab CDS DA Processing** – Use OpenLab CDS and Data Analysis Tool to generate new Result Sets

2. **OpenLab ECM** – Versioned Result Set automatically uploaded into connected ECM for compliant Storage

3. **OpenLab ECM –** Provides a notification to the Data Transformation Service that new results are available

4. **Data Transformation Service** – On-Prem/Cloud deployed service which reads versioned results set from ECM extracting the data through the ECM REST-API, and converting the data into an ASM JSON object or an ADF file

5. **Messaging and Queuing Service** – Informs the interfacing Customer Application that an ASM / ADF file is ready for ingestion

6. **Customer Data Lake** – The storage location for transformed data decided by the customer. This can be network drive or a cloud storage location

Customer Success Story - Swiss Cat+

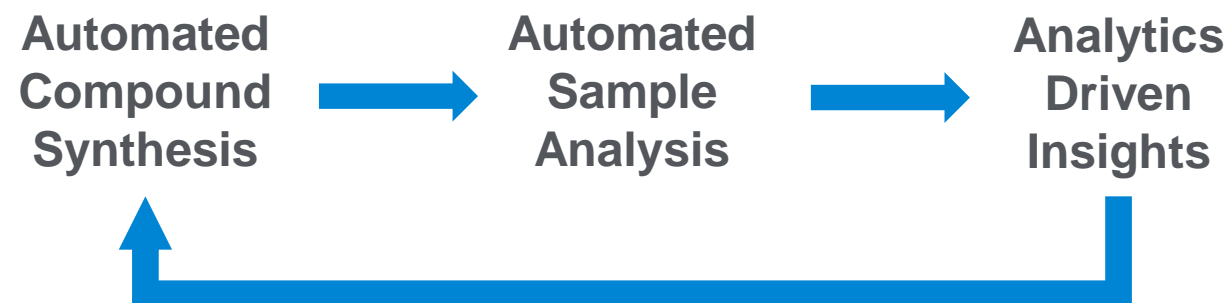## Fully Autonomous Laboratory using **ASM**

The Goal: Design and implement a completely autonomous laboratory for the discovery and optimization of catalysts using robots and artificial intelligence.
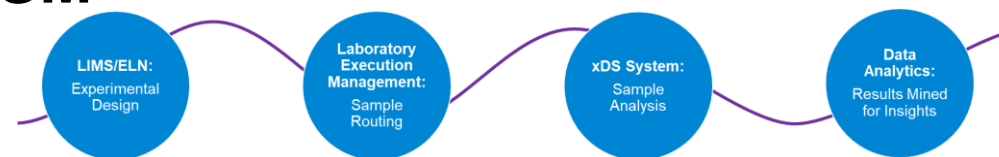
Industry Watchers: *Key pharmaceutical companies* are on the advisory board to support the effort. Additional interest from flavors and fragrances to and other applied domains.

Success here will provide a general template for assembling a fully autonomous discovery and optimization platform across multiple domains and likely trigger multiple projects at other institutions.

LIMS/ELN: Experimental Design → **Laboratory Execution Management:** Sample Routing → **xDS System:** Sample Analysis → **Data Analytics:** Results Mined for Insights

Automated Compound Synthesis → **Automated Sample Analysis** → **Analytics Driven Insights**

Agilent Technologies
Co-Creation Partnership Program

Our Mission:

Identify Key End Users to engage in a co-creation programs **to do a complete build-out of a laboratory** from top to bottom in alignment with Agilent's Strategy.

- Put **the solution in context** to ensure developed components and services are fit for purpose.

- Work with a partner who can **test new capabilities and turn around feedback quickly**.

- Work with a partner using a wide variety of instrumentation and equipment not only from Agilent but from other vendors to **ensure the solution is open and flexible**.

Agilent **OpenLab**

Agilent

Questions