ENSURING INSIGHTS FROM DATA

A view beyond ELNs, LIMS, and SDMS

Connect to the Future with Enterprise, Automated Scientific Data Management

ACD/Labs

THE 3 USES OF ANALYTICAL DATA IN R&D

1 **To understand a material or process:** Analytical experiments are undertaken to collect each of data a, b, c with interpretation x, y, z. Information extracted from the data (in various systems) leads to decisions about next steps and knowledge for the future.

2 **To understand materials or processes, and their relationships:** Decision support across analytical experiments requires assembly of data from the various systems used in data consumption.

3 **To reveal limitations of/enhancements to experiments, materials, or processes:** Insights from trend analysis of analytical data; expose the unexpected from analytical data—predict and classify—with data science.

Is the need simply many IT systems for data?

THE SMALL DATA PROBLEM

- R&D doesn't necessarily have a Big Data problem, rather it is challenged with storing and accessing the volume of a variety of small data.
- R&D materials, from compounds in discovery, to API, and the final drug product, need to undergo various tests. Those tests/analyses use diverse equipment to generate that 'variety of small data'.
- Scientists use this data to identify and characterize materials throughout their lifecycle. The experimental goal is to assess material quality and/or ensure processes are understood and controlled. Good data reveals process variations and/or material identity, quantity, or purity.
- IT groups need to provide and maintain appropriate systems for transmission, storage, and enterprise access to this essential data, in a secure environment.

Where does automation offer the greatest advantages?

AUTOMATION IN THE CONTINUING EVOLUTION OF R&D INFORMATICS

- There are a multitude of systems for collecting and managing data
- Decoupling analytical from data source can afford greater accessibility and usability. But then, how is analytical data properly identified?
- Digitalization* is being pursued to help with data marshalling and collaboration
- Digital data lends itself to re-processing with new methods or hypotheses
- Cloud-based technologies are also expected to increase data access
- The thirst of data science for AI and machine learning is further driving automation in the handling of data

Future-proofing IT stacks is being able to federate, automate, and communicate

*Disambiguation of Digitalization vs Digitization can be found in the Gartner Glossary of IT terms

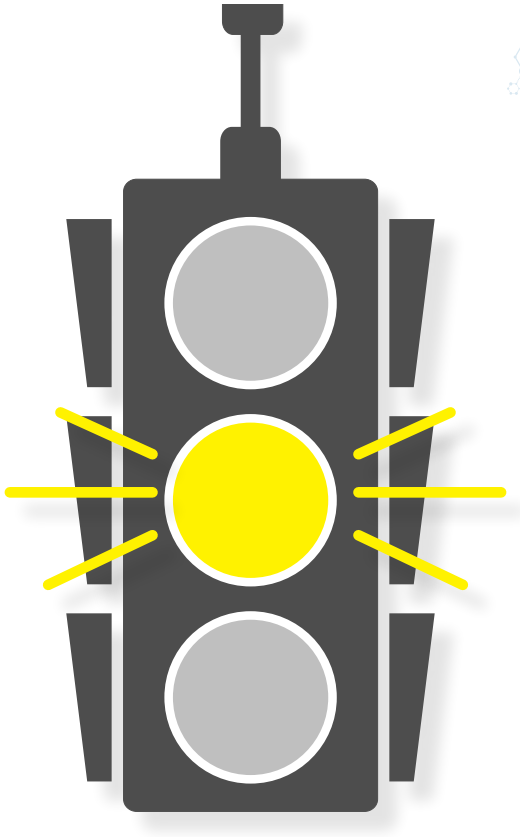
RISKS ASSOCIATED WITH INCOMPLETE "SMALL" ANALYTICAL DATA MANAGEMENT

- Lack of data integrity—data transcription and transposition
- Lack of insight for decisions (for future applications within the organization or in response to regulatory requests)
- Difficulty collaborating with partners/colleagues in other labs/geographies
- Critical data scattered without context or connection to the data's intent
- Repeated experiments required due to lack of data accessibility

RISK-MITIGATING DECISIONS RELY ON ANALYTICAL DATA

Analytical data is essential for ensuring the identity and quality of materials

If the systems in your stack only manage abstracted text and images, you're delivering **limited insights**



Click here for "The state of scientific analytical data management" survey results

In the pursuit of building an informatics ecosystem that fulfills scientific and business requirements, it is important to remember that —

data on its own is usually not very useful.

A line of inquiry and context is needed to gain **valuable insights** from data.

So ask, for systems deployed in your R&D organization:

- What data do they house?
- What insights are needed?
- What else can be expected?

MEETING THE SCIENTISTS NEEDS

Context gives meaning to data and metadata provides context.

Marshalling of **contextualized analytical data is essential**, because the data is:

1. Scattered in disparate systems
2. Assembled from multiple experiments that use a variety of techniques and formats
3. Abstracted results that are tangibly rendered as numbers, text, and/or images
4. Information about the materials, processes, samples, sources, transformations, abstractions, and results that are key to revealing insights

An ecosystem needs to support inclusion of contextual information, and specialized tools are also often necessary for scientists performing operations on and (re)interpretation of data, to generate results.

Systems that help standardize and homogenize analytical data facilitate marshalling.

There is no single accepted data standard that suffices for all data, yet.

Click here to download white paper "Looking Beyond Analytical Data Standardization – the Fourth Paradigm"

MEETING DATA SCIENCE NEEDS

Data must be:

- Relevant to the line of inquiry
- Structured
- Normalized
- Cleaned to good quality
- Of sufficient quantity to be statistically relevant
- **Contextualized** with metadata

WHY AUTOMATE?

Reliability & consistency in processes

While GxP environments in pharmaceutical development demand reliability and consistency, so automating these processes seems obvious, there are many complex repeatable processes that can benefit from being executed the same way, every time. Data handled in this manner are also more amenable to comparative studies and data science.

Increased efficiency

Since automation can work 24/7 there is an opportunity for increasing efficiency by reducing reliance on manual data marshalling, processing, interpretation, reporting, and storage.

Reduction of tedious, repetitive tasks

Not only can automation reduce the risk of error from transcription/transposition, it also allows scientists to concentrate on innovation and tasks better aligned with their expertise.

Aligned with Digitalization Efforts

ENTERPRISE INFORMATICS WITH ACD/LABS SPECTRUS

	FEDERATE	AUTOMATE	COMMUNICATE
Chemically intelligent tools	x		x
Query data	x	x	
Preserve data (short & long-term)		x	x
Access data	x	x	x
Multi-technique data sources	x		
Vendor agnostic	x		
Re-process and re-interpret data		x	x
Contextual information			x
Structured and unstructured data	x		x
API and Integration tools		x	x
Implementation Services		x	x
Configuration/Customization	x	x	x

An ecosystem of complimentary informatics systems is necessary to support innovation in R&D

*GxP compliance-ready features and capabilities

BENEFITS OF AUTOMATION WITH SPECTRUS

- Minimize manual processing & interpretation to increase efficiency and consistency
- Reduce the time and difficulty of cross-experiment assembly
- Make data more easily accessible for review, reporting, and decision-making
- Derive structured datasets for:
  - Training of and analysis by ML/AI applications
  - Longitudinal trend analysis/insights
    - Instrument utilization and performance reports
    - Historic overview of material supply quality
    - Comprehensive material characterizations & predictions

Digitalize analytical data that streams from sources and facilitate its processing, interpretation, and abstraction to results that are **assembled for decision support and data science**

BECOME R&D DATA-ENABLED

NOT JUST DATA-DRIVEN

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