Scientific Decision Support for Advanced Materials Research

The PerkinElmer Signals™ Research Suite

Introduction

Digital transformation has been emphatically proven to benefit the bottom line by improving speed-to-market through data agility, and higher confidence in the results of R&D experimentation. For example, in early 2020, the consulting firm, Accenture, surveyed 1550 top executives in companies with $1 billion or more in revenues regarding the impact of their digital transformation efforts. They discovered that those companies that championed transformation had revenues that outperformed their industries' averages and showed a better than average growth trajectory.[1]

Working with hundreds of companies involved in chemistry-based research, the PerkinElmer Informatics team have seen four most common challenges to digital transformation of the R&D process across industries as diverse as specialty chemicals, agro-sciences, food and beverage and oil and gas.

CHALLENGE 1: Difficulty analyzing experimental data because too much information is captured on paper.

CHALLENGE 2: Inability to identify the best solutions to meet performance requirements because data captured across multiple testing methodologies and parameters is not structured for analysis.

CHALLENGE 3: Difficulty in R&D collaboration (e.g. searching experimental data from other researchers, sharing test results) due to the lack of advanced platform.

CHALLENGE 4: Inability to demonstrate the superior value because highly fragmented data is locked-up in siloes.

Addressing these challenges produces the following benefits:

- Faster ability to respond to customer requests
- Improved efficiency and speed of research
- Better collaboration, communication and intellectual property control

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Best Practices to Digitally Transform the R&D Process Using Analytics Technology

PerkinElmer developed the following guidelines for companies looking to digitally transform their R&D processes. These approaches are not meant to be sequential. We can together identify where companies are on their digital transformation journey and select the approach that deliver the best results to their business.

GUIDELINE 1 - Capture, Organize and Explore Data Digitally

It's difficult to analyze data captured on paper. Scientific data needs to be captured and recorded digitally. Because science is not a solo endeavor, researchers, project leads and test engineers need to share information with colleagues, anywhere, any time. Capturing the data in an electronic lab notebook removes unproductive hours getting data ingested and wrangling it so it can be analyzed. When choosing an electronic lab notebook, consider one that offers the following capabilities:

- Provides access from anywhere
- Delivers dedicated workflows for synthetic chemistry
- Integrates task and request management workflows for sample characterization and testing
- Supports all types of data and the ability to share, collaborate, and retrieve data rapidly
- Includes the power and flexibility of an advanced analytic application like TIBCO Spotfire®

PerkinElmer Informatics Signals Notebook delivers these features in a modern user interface that's like learning to use your smartphone – simple, intuitive. Signals Notebook including ChemDraw®, the leading chemical drawing software, will provide you a powerful solution for capturing, organizing, sharing and exploring your data.

GUIDELINE 2 - Structure Data So It Can Be Analyzed Scientifically

There is a common misconception that if data is captured electronically, it is structured for analysis. It is not just about moving data capture from paper to glass. Another misconception is that Microsoft Excel can easily analyze unstructured data. It's a giant leap forward when rather than trying to make sense of an incoherent collection of data in Excel, researchers and engineers can structure data into tables with defined column names and define relationships between the tables. When choosing an analytics platform, consider one that allows users do the following:

- Quickly filter down the entirety of a R&D workflow to a targeted subset of interest
- Mine and visualize scientific and business data across experiments and research projects
- Spot actionable insights without requiring IT intervention

PerkinElmer's advanced analytic application TIBCO Spotfire® provides the ability to jumpstart and accelerate this process, structing data and making it ideal for reuse. TIBCO Spotfire® delivers a powerful capability for ingesting, structuring, visualizing and exploring your data.

GUIDELINE 3 - Ensure Scientific Data Can Be Searched Easily and Organized in the Best Way

The ability to analyze enormous volumes of heterogenous scientific data is a foundational requirement. Embedding intelligence like chemical structure information is also. These capabilities help chemists and test engineers gain faster insights into chemical structure activity relationships. However, some research teams rely too much on standard charts and graphs in Microsoft Excel or general-purpose business intelligence applications. These tools lack the foundational data management capabilities mentioned above. Choose a solution that offers the following capabilities:

- Rapid search of massive amounts of scientific data involving multiple testing methodologies and parameters
- Create on-the-fly frameworks for tests of individual materials to studies involving many different dimensions at once
- Guided search and analysis workflow that queries and represents data both intuitively and intelligently

The PerkinElmer Signals Data Factory provides a user-driven application that adapts to the needs of scientific concepts and is fully integrated with the latest data visualization, machine learning and AI techniques..

GUIDELINE 4 - Demonstrate a New Solution Meets Business Requirements

To demonstrate a new solution addresses customer needs and meets manufacturing requirements cost effectively, researchers not only need to demonstrate their own lab results, but also incorporate manufacturing data, cost data and sometimes data inputs from customers. For most companies, this data is locked in siloes. The data stored in these disparate systems needs to be unlocked, ingested and structured for analysis. Choose a solution that offers users the ability to do the following:

- Import data from disparate sources
- Ingest data with minimal IT involvement
- Reformat data (i.e., wrangle the data) so it can be analyzed meaningfully
- Analyze product performance options by comparing cost, quality and specification options

TIBCO Spotfire® and Lead Discovery can unify the data from various sources and deliver these features with a powerful capability for accessing, structuring, visualizing and exploring your data.

Figure 1. An example of a formulations dashboard.

Summary

PerkinElmer Informatics solutions utilize a modern software architecture to accelerate scientific discovery. Scientists, test engineers and project leaders recognize that more rich visualization or more comprehensive presentation of analyses provides a better representation of the complexity of their world. That's is the goal of the PerkinElmer Informatics Signals Research Suite – a smooth, integrated workflow employing future-proof technologies to empower your best research and development.

Reference

1. https://www.accenture.com/us-en/insights/industry-x-0/cross-functional-collaboration

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