

Pressure-Testing a New Solution for Unified Data Handling in Drug Discovery

By Revvity Signals

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Introduction

Merck Research Laboratories wanted to streamline data handling for its drug discovery operations, to reduce complexity and improve data accessibility for scientists. Understanding that these goals could best be achieved through a unified data solution, they conducted a pilot with the Signals Research solution, including Spotfire®, from Revvity Signals.

From the pilot, which involved a broad set of stakeholders, Merck found that the Revvity Signals solution was both highly effective and easy to use. With the solution, scientists and project managers could readily bring together diverse datasets from a wide range of instruments. Modular tools within the Signals solution streamlined data processing, including steps such as curve fitting and data normalization, with powerful options for data parsing, visualization, and trellis functionality.

The end users found the solution easy to use and suited to their diverse needs. Deployment across different departments and locations was straightforward, with options for external users too. The pilot also increased awareness among the scientists of how data can be used more effectively, to accelerate insights and advance projects.

Complex Datasets and Multiple Data Sources and Types

The first step in effective data analysis is to transfer experimental data from analytical instruments to a software solution. The Merck team was challenged by the complexity of this data transfer. The instruments in their discovery laboratories have a range of export options, from no export through the export of multivariate data, covering raw or analyzed data, and sometimes including metadata. Some datasets to be transferred are small and simple, like those from a simple plate reader, while others are large and complex, like graphical data from a high-content imaging instrument.

In this situation, the standard data transfer options all had significant disadvantages. Manual transfer would be time-consuming and error-prone. A template-based workflow would serve some applications, but not all. A hard-coded approach would be inflexible, requiring that

experiments always be run the same way. In addition, all these approaches would require a lot of training.

“So ultimately we want a single unified, streamlined data handling platform for end users. And this is where Signals comes in.”

- Gottfried Shroeder

Associate Principal Scientist Merck

Universal and Flexible Data Capture

Faced with this challenge, the Merck team sought a solution for universal data capture with a single, flexible workflow that could be easily customized to handle its diverse assay requirements.

The Signals Research solution, encompassing the Signals Notebook ELN, was tested against a broad set of assays, covering various multiparametric formats, including single point, screening, and early discovery space experiments. The initial assay set covered kinetic time course, proximity, immuno-, calcium flux, radioligand binding, homogenous time-resolved fluorescence, temperature-dependent fluorescence, microscale thermophoresis, stopped flow, surface plasmon resonance, and high-content imaging assays.

As the team began to see the solution’s flexibility and power, they were inspired to test it with additional instruments seen as “orphans” from a data handling perspective. Thus, they expanded the pilot to include data from capillary electrophoresis, second harmonic generation, cell confluency, acoustic dispensing, and affinity assay instruments.

Through this robust pilot, the Merck team found that the Signals Research solution could seamlessly import data from the full set of instrument types in its discovery operations, managing all the formats and file types.

Streamlined Data Handling

The next stage of the Merck pilot addressed data handling. The team set up a customized protocol for screening data, incorporating capabilities from the modules available in the Signals Research solution.

Using this protocol, a Merck scientist begins by selecting the SciStream parser and importing a file containing experimental data from a plate reader. The Signals Research solution converts the data into a table, which users can check against the raw data right of the screen. Next,

users input the plate map components—well type and concentration. Instant feedback, through color coding, confirms that the components have mapped correctly to the data table. They then drop in a tabular file of compound identifications, which are automatically mapped to the data table.

Scientists can then choose a normalization module, where they can customize the plots and exclude data points if needed. They proceed to curve fitting, which in this case is a four parameter (4P) curve fit. Using these normalization and curve fitting modules, all the quality control is performed in real time. Users can see which compounds should be flagged, and if they decide to exclude a point, they simply click on it; immediately, the curve is redrawn and the new information is incorporated into the large data table. From that data table, users can pick columns to move into a smaller set for specific reports. Easy trellis functionality within Spotfire facilitates data comparisons and identification of trends.

This pilot demonstrated how the modular capabilities of the Signals Research solution could improve the speed and reliability of data processing, enabling individual users, and the Merck team, to advance more quickly to data analysis and insights.

“Definitely implementing Signals Notebook has improved the way we do things—a lot.”

- Salvador Gomez-Carretero
Sr. Data Scientist, H. Lundbeck A/S

High End-User Satisfaction and Flexible Deployment

A critical component of the successful Merck pilot was end-user satisfaction, driven by ease of use and functionality.

Regardless of their data analytics expertise, drug discovery scientists across the organization found the Signals solution easy to use. They quickly got up and running, customizing data visualization formats and harnessing capabilities for filtering, database matching, and graphic-based data parsing. Scientists also appreciated the embedded spreadsheet functionality, particularly for annotating data. They also took advantage of the on-demand availability of additional computational power to handle large screening datasets. And as more scientists began to use these powerful tools, they became more aware of how data can be used more effectively.

The IT team managing the pilot appreciated the deployment options, which were flexible enough to cover the requirements of different sites across the Merck R&D organization. With a cloud-based deployment, the Signals solution can also be accessed securely by external users, facilitating collaboration with research partners.

Active Engagement with Diverse Stakeholders

In the Merck pilot, active collaboration between the IT team and end-user scientists was an essential element of success. The project engaged a diverse set of stakeholders, including software developers, engineering staff, cloud teams, end users, bench scientists, super users, and project management. It also involved a very close coordination with the Revvity Signals team.

A Successful Pilot

The Merck pilot of the Signals Research solution successfully demonstrated its ability to unify and streamline data handling across a large drug discovery operation. By addressing challenges related to diverse data types, complex workflows, and instrument integration, the pilot showcased how a modular, flexible, and user-friendly solution can improve research efficiency. By putting powerful tools for data fitting, visualization, and analysis into the hands of a wide variety of scientist end users, Revvity Signals set the foundation for transforming raw data into actionable insights.

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