CASE STUDY

Enabling Analytical Lab Automation & Data Harmonization

Michael Arlt
Vice President,
Global Analytical Services

Achim Herrmann
Senior Manager,
Site Analytics Management

Sylvia Friedrich
System Consultant,
Site Analytics Management

Claudia Schwarz
Associate Director of Sales,
Connected Lab

Todd McKenzie
Global Campaign Manager,
Connected Lab

The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the U.S. and Canada.
Executive summary

Acting as a core lab within Merck KGaA, Darmstadt, Germany, the Global Analytical Services group provides customers with a wide variety of customized analytical chemistry methods, processing more than 100,000 samples per year.

After drowning in paperwork and recognizing the huge motion waste created for their from multiple instruments lab staff while handling customer requests, capturing scientific data, generating reports, and uploading information to the LIMS manually, the group decided to go paperless and automate these processes.

The resulting Lab Automation project fully automated how scientific data was captured from various lab instrumentation. The central challenge was overcoming the fact that lab instruments typically do not communicate with one another—in other words, the software in different lab instruments do not natively support a standardized, bidirectional flow of information with different types of instruments. This prevents an automated data stream within a workflow and a sleek LIMS connection. By harmonizing the data across different devices and systems using BSSN™ Software, the newly streamlined communication processes delivered the following results:

<table>
<thead>
<tr>
<th>Benefit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Working Days Saved by FTEs via automation</td>
<td>423</td>
</tr>
<tr>
<td>Annual increase in samples processed</td>
<td>20%</td>
</tr>
<tr>
<td>Estimated ROI from data automation</td>
<td>€400K</td>
</tr>
</tbody>
</table>

Directly Addressing the Challenge of Manual Data Transcription

Let’s start with a number: **3.6%**.
This is the typical range of data-entry errors found in research contexts for each step of manual transcription. In other words: every time we copy something down by hand, we make mistakes.

In your average laboratory, the journey to convey data from its source of origin to the final result is characterized by multiple manual steps, performed by different users over a period of time. Given an average 3.6% error rate per step, how does this impact the reliability of data we capture in a multistep workflow to analyze a sample?

It is estimated that more than 35% of irreproducibility is attributable to manual errors in the performance of experiments and data reporting, which results in unnecessary costs totaling around $28 billion to repeat experimental work.

Here is another number to consider: an average 90 minutes are invested per analyst per day for manually finding data, transferring data, reviewing data, and moving paper.

Nevertheless, most scientific labs still work this way and accept these facts as the costs of doing business.

Why is that? Why do we accept the enormous investment of time and money in processes that can be automated, especially when solutions to these challenges already exist?

Following this line of inquiry, let’s take a closer look into a lab that accepted this challenge and solved for the root cause.
Introduction

Merck’s Global Analytical Services group is an association of 21 labs across the globe that offer a wide variety of needed services in the healthcare and life science industries. Supporting more than 220 analytical methods with a wide spectrum of analytical equipment—such as HPLC, GC-MS, NMR, and so on—this core lab group is unique in the breadth and depth of independent services they provide across all business entities within Merck. Acting as a one-stop shop globally, the Global Analytical Service group not only provides consultancy and support, but also outstanding analytical measurements to their partners in research and development.

What was the challenge?

The generic workflow for an analytical chemistry lab sounds easy: once the order arrives via the laboratory information management system (LIMS), the physical sample will be prepared according to the analytical method needed, the relevant information is measured, the raw data is processed, the results are documented, and the reports are uploaded to the LIMS to be sent back to the requester.

But as usual, reality strikes back: as simple as this process sounds, a great deal of complexity sits just below the surface.

Samples arrive in batches, representing multiple orders and requiring various analytical methods. For each sample, the analyst first needs to download and print out the work order from the LIMS. The next step is to consult a database and search for the correct procedure to do the sample preparation. This gets even more complex if various analysis methods are requested for the same sample. After printing out all the instructions or manually transcribing them to the lab notebook, the analyst starts to prepare the sample. During this process, parameters such as sample weight, solvents used, solvent amount, ambient factors, and so on need to be quantified and documented—most likely by hand. Additionally, after the preparation has been completed, a barcode label needs to be generated that summarizes essential information, like sample ID, analyst name, date, and time, and placed on the correct sample tube. There could potentially be daughter samples prepared from a mother sample for different measurements that need to be logically linked to each other and tracked, which can easily create a lot of extra effort.

The samples are now fed into the chosen analytical instruments, which can be an extremely time-consuming step. For each sample you must type into the system the sample ID, program the desired method, and choose the appropriate experiment parameters for each instrument (e.g., HPLC). Despite the risk of typos, a deep knowledge of programming various instrument software is required.
"You have GC, IR, mass spectroscopy, and all these different data formats, and you have to unify and standardize them in order to have an automated system, and BSSN has solutions for this."

Sylvia Friedrich, System Consultant, Site Analytics Management

After successful completion of the measurement, the generated raw data needs to be transformed into the result. This can occasionally be performed by the instrument software but may also require manual calculations, print screens, and annotations. Next, the scientist transfers important results again into the lab notebook or Excel and generates the report by matching the results obtained from various daughter samples and various methods to the mother sample. Finally, the reports are uploaded (manually in most cases) to the LIMS.

This is as tedious as it sounds. Despite the motion waste that is embedded in the process, the worries regarding the accuracy and integrity of data transfer raises more and more questions.

Given the risk of transcription errors and the massive amount of time invested per analyst, the Global Analytical Services group finally ended up with the following questions:

- Why do we document on paper when we have all the data electronically?
- Why do we type information in analytical instruments by hand via a keyboard when having a barcode label which can deliver all this automatically?
- How can we achieve interoperability and connectivity between different systems?
- How can we link data sets for parent-child samples across multiple process steps and measurement techniques?

Their conclusion was to stop drowning in paper and to instead automate the complete data lifecycle with sleek and clean digitized processes enabled by BSSN™ Software.
What was the solution?

The vision of the project, called Lab Automation, was to create an interoperable and bidirectional exchange of information between all the heterogenous systems and instruments to support the analysts in their workflows. All data would be captured at the point origin, organized, and accessible wherever needed.

The biggest challenge in this process was the fact that most instruments in the lab are not set up to communicate with one another. Basically, they speak “different languages,” and each instrument outputs data in a vendor-proprietary format. Each time you get a new instrument you will most likely get a new data format. Nothing is standardized and that makes it hard to create a streamlined and automated data management framework for multipurpose use.

To tackle this problem, the Global Analytical Services group first decided to address the matter of data standardization.

BSSN™ Software was selected to provide the Lab Automation project with solutions to these challenges. Building on the open-source Analytical Information Markup Language (AnIML) data standard, BSSN™ Software facilitates analytical and biological data management across all types of measurement techniques. By harmonizing experiment data from disparate formats into a single data standard through software APIs and data converters, the data management is optimized to automatically contextualize results with relevant metadata and enable visualization in external systems.

The centerpiece to making this happen are BSSN’s instrument connectors. These connectors create a linkage between the instrument (the origin) and the place where data is stored. All the instruments’ proprietary data formats are automatically converted to the open AnIML data standard and collected in a central database. Additionally, valuable metadata of all kinds (sample-related, static, transactional, and instrument-related) are extracted and stored. This allows a fully automated data flow, automated report generation, and LIMS upload to become the foundation for a well-organized data structure. Furthermore, the challenge of long-term, vendor-agnostic data archiving is also addressed because of the data standardization.

Served from BSSN’s ready-to-use library of more than 300 instrument connectors, a toolbox for the lab group was created. By connecting the lab instruments and converting the data formats, individual workflows can be created on-the-fly and tailored to the scientists’ specific needs, guaranteeing a seamless data workflow. On top of this, customized interfaces and a preselected range of information helped to increase the lab group’s efficiency in working with the data.

All data is captured electronically where it is generated, made available where it is needed, and centrally stored with the BSSN™ Hub tool. The samples are registered in the lab by barcode scan, available in the system and selected for the next sequence. The lab automation solution provides extensive information on the sample, which is compiled from leading systems, such as LIMS or ELN. A preselection offers all samples that are ready for preparation, supported by a wide range of filter and sorting options. Important sample information and measuring methods can be viewed quickly.

After preparation, important sample parameters and values are automatically transferred to the system and a label is printed for the generated sample. The transfer is not file-based. At the end of the sample preparation, a sequence proposal is created for the measuring instrument, including blanks and random sample orders.

The finished sequence list is sent to the measuring device, prepared samples are loaded, the sequence is imported into the instrument control software and the measurement is started. The evaluation of the results takes place in the device software, with data visualizations and analyses enabled via the BSSN™ Workbench application.

“There is no need to look up information in different systems as BSSN Software makes all digital information accessible from one single software platform.”

- Michael Arlt, Vice President, Global Analytical Services
Results and Next Steps

After one year, the Lab Automation project had successfully completed the digital transformation of three different lab facilities with the help of BSSN™ Software’s best-in-class data solutions. This included AnIML data converters for more than 20 different scientific instruments, bidirectional software integration with four different leading systems and 11 different measurement interfaces, a central data store with BSSN™ Hub, and a universal data analysis and visualization tool with BSSN™ Workbench.

The integration of lab instruments, systems, and enterprise applications increased the overall degree of process automation in the lab facilities while reducing the technical burden of IT-supported process steps. By simplifying and standardizing forms, procedures, and the data flow between connected systems and devices, the Global Analytical Services group experienced a significant and measurable improvement in overall efficiency.

The Lab Automation project team closely monitored the group’s output before and after digital transformation to quantify the project impacts over the first year. Most remarkably, they saved a combined 3,386 working hours across all three labs. Put in another context, that’s around 423 working days they earned back, or roughly 2 full-time employees, which could now be devoted to more value-added and creative problem-solving tasks.

The group conservatively estimated a financial savings of approximately €400,000, and a nearly 20% increase in samples processed as a result of the automation of key workflows and data processes. In other words, they recorded a positive return-on-investment (ROI) within the first year of implementing and utilizing their BSSN™ solution.

In addition, by eliminating manual data transcription and redundant entries during the lab workflow, the group experienced a boost of confidence in their data integrity and reporting capabilities, which also meant more satisfied customers in the long run.

The Global Analytical Services group is currently working on expanding the Lab Automation project and BSSN™ Software data solutions to three additional lab facilities, with the intent to continually monitor and enhance their automation processes and configurations as needed.

Learn more at bssn-software.com

References

• Internal research

©2021 Merck KGaA, Darmstadt, Germany and/or its affiliates. All Rights Reserved. MilliporeSigma, the vibrant M, and BSSN Software are trademarks of Merck KGaA, Darmstadt, Germany or its affiliates. All other trademarks are the property of their respective owners. Detailed information on trademarks is available via publicly accessible resources.