EXECUTIVE SUMMARY

Integrated Laboratory Informatics Systems Deliver Greater Efficiency and Improved Data Integrity

Simplifying laboratory management across multiple workflows and techniques.

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INTRODUCTION

Although the benefits of a paperless lab have been discussed for years, several challenges have stood in the way of many labs taking complete advantage of a fully digital lab. Labs are complex and heterogenous, working with many different types of samples (e.g., batch release, cleaning validation, and environmental), procedures, software packages, data formats, instruments, consumables, and analysts. Mapping this complexity into an end-to-end electronic or digital workflow solution has often led to frustration.

For instance, informatics systems have expanded or were added over the years in an attempt to create efficiency. Some systems were integrated piecemeal, while others haven't been integrated into the ecosystem at all. This environment created a fragmented lab ecosystem, leading to potential sources of redundancies and errors. These pain points are underscored in FIGURE 1, which highlights several areas that customers said stood in the way of them becoming more efficient.

WHAT IS A DIGITAL LABORATORY?

Efficiency is closely related to the value of the lab, and eventually is measured by a lab's throughput, reliability/quality, and cost efficiency. Digital lab tools support these critical areas. Such a system would improve lab communications, optimize the use of resources, offer live visualization and control of the processes, manage all content and context, and focus on high-value activities, with automation and review only when necessary.

Figure 1: Common pain points for laboratories.

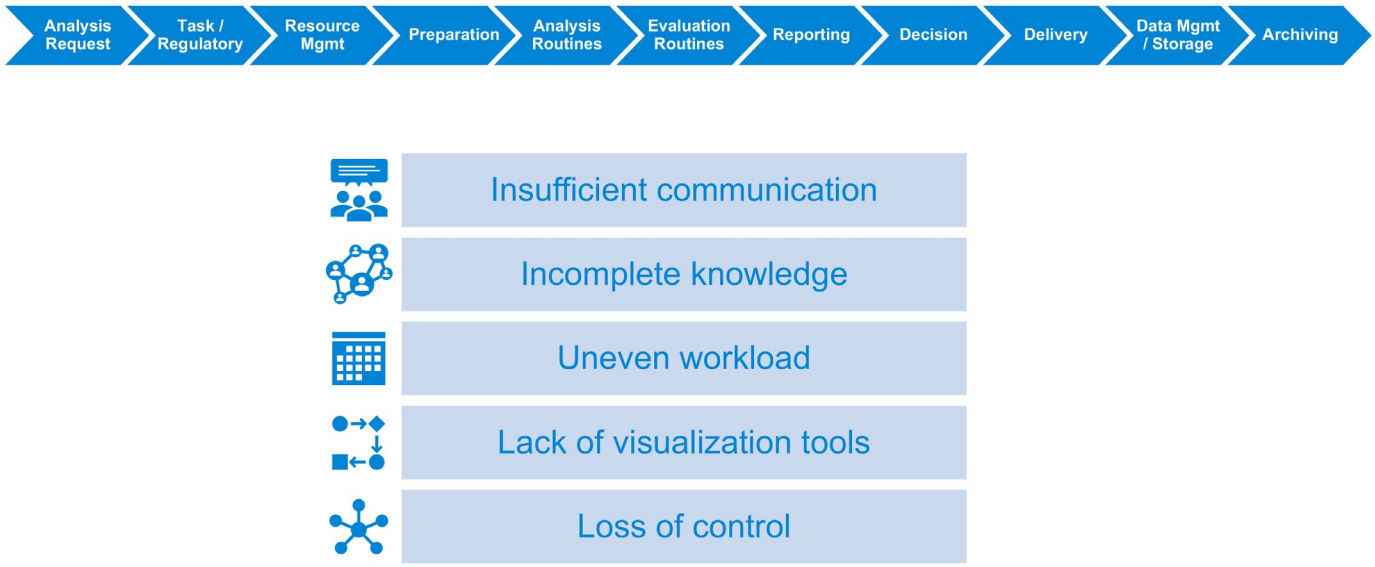
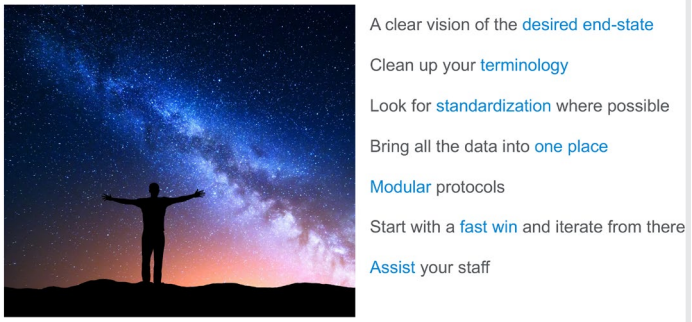


Figure 2: How laboratories can prepare for digitization.



A digital lab is more than simply being paperless. An effective digital lab system might:

- Capture steps and actions without transcription
- Use technology to facilitate processes
- Use touchless authentication
- Allow for sharing of data via web
- Present only assets that are fit for use (e.g., calibrated/maintained instruments, non-expired solvents or standards)
- Readily provide the status of any instrument or sample
- Quickly notify lab personnel of any problematic issues

Important tips for preparing a lab for digitization are shown in FIGURE 2, and include defining what you want to achieve as the result of deploying a digital lab, standardizing relevant terminology in the organization, subdividing analytical methods into multiple protocols, and bringing data into one place. Note that being overambitious makes implementation difficult. A better approach is to start with a fast win and expand from there.

END-TO-END DIGITAL WORKFLOW

Because all labs are different, there is no turnkey solution for laboratory workflow management. Agilent offers a solution that can handle the complexity and heterogeneity of any lab. Based on Agilent's OpenLab Software backbone, the SLIMS workflow management system was developed with sample management, workflow requirements, and lab employees in mind. It manages a lab's samples, experiments, and results from start to finish (see FIGURE 3). This solution includes the business intelligence that connects to instruments, accessories, and chemicals inventory so that all aspects of sample

Figure 3: An end-to-end analytical workflow broken down into unit operations.

Figure 4: Customers can submit their own analysis requests with SLIMS to the laboratory.

analysis are incorporated into one easy-to-use system.

The digital workflow begins with a convenient way for a customer to submit their analysis request and related information to the lab through a simple web page (FIGURE 4). Customers can check the status of the analysis and access the final report once it is approved. With the ability to track different sample types and metadata, the system is flexible enough to handle the specificity of a lab without customizing the software code.

Once the samples are received, the software allows laboratories to confirm receipt, assign tasks to operators, verify availability of assets to fulfill the request, and assign assets to requests. Then, the digital system's resource management capabilities enable labs to track the location of samples as well as manage sample derivatives and their context. Instrument calibration and maintenance are monitored to verify they are fit-for-purpose, while reagents and standards are surveilled to ensure they are still valid and not expired. The use of barcodes is encouraged whenever possible, as they avoid manual transcription errors. The software allows users to read and create barcodes.

Next is sample preparation, the heart of the lab operation, where typically most errors occur. SLIMS allows tasks to be organized as users run multiple samples in the same protocol or run multiple protocols on one sample. Analysts receive step-by-step guidance through procedures, employing only assets that are fit-for-use.

Connections to small lab devices play a key role in the process. Every method is divided into a series of simpler protocols that either cover one or many workflow elements. FIGURE 5 depicts the workflow for a complex analytical method. Each arrow represents a separate protocol, including the current number of samples it is processing, while each circle indicates the number of samples in a queue for one of the subsequent protocols. By clicking on any arrow or circle, the user is routed to corresponding detailed information. This straightforward visualization tool allows users to easily track the process of complex operations in the lab.

A distinct advantage of the Agilent solution is its bidirectional, seamless integration with Agilent and non-Agilent chromatography instruments. Samples can be routed to any suitable instrument in the network, thus eliminating the need to transcribe information between the workflow management software and the chromatography data system (CDS).

Figure 5: The workflow for a complex analytical method.

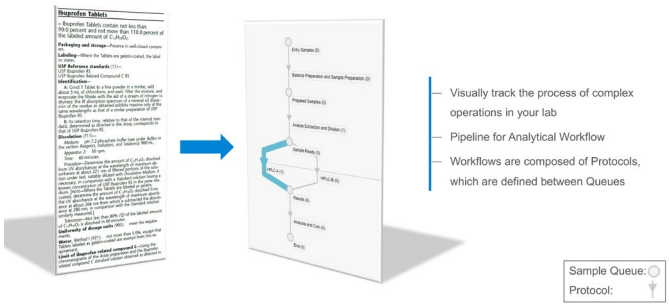


Figure 6: Instrument status at a glance.

Conveniently, the status of every instrument's condition in the laboratory can be observed at a glance (FIGURE 6). Accessible on a computer or mobile device, this web-based tool aids in instrument selection and provides an immediate alert when an instrument is in an error mode.

Advanced data analysis and reporting capabilities are built into the CDS. The scalable architecture enables centralized data and instrument management, while the advanced data integrity ensures quality. The CDS software can show an overview of the entire sequence as a helicopter view and a detailed view of a chromatogram within the same interface (FIGURE 7). The tool helps users quickly identify issues such as missing or additional peaks, retention time shifts, or integration problems among hundreds of chromatograms.

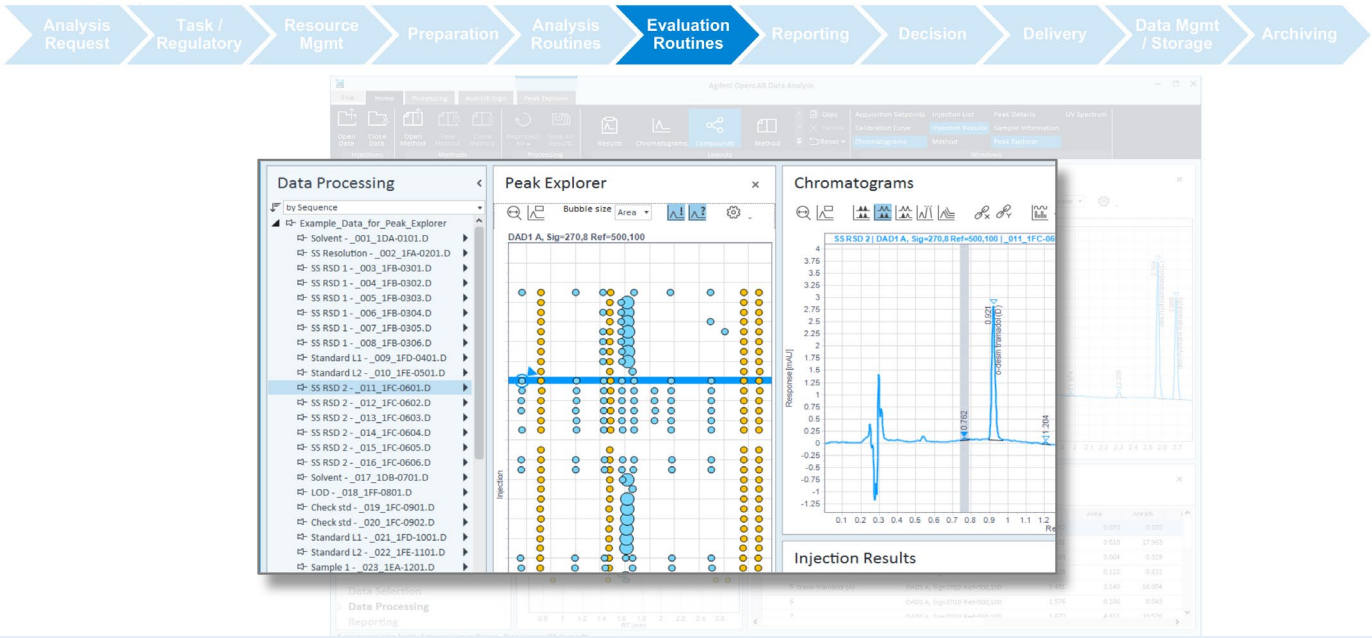
Agilent's OpenLab CDS also offers a powerful custom calculation engine that supports calculations similar to what is provided in Excel, but negates the use of these external software/files to avoid transcriptions and potential errors. Calculations can be made at the sequence level, injection level, or peak level (FIGURE 8).

OpenLab CDS allows users to conduct audit trail reviews directly in the context of the reviewed electronic record. Compliance reviews are typically focused on specific events that might be indicative of erroneous or potentially fraudulent activity, such as re-processing or manual integration. To streamline the review, audit trail categories have been included in the software. Entries are tagged and categorized, enabling quick perusal. Full text searching is also available, allowing rapid retrieval of relevant audit trail information. The audit review can be conducted along with the data review in the same user interface, which obviates the need for keeping other records, printing the documents, and signing them.

The scalable architecture enables centralized data and instrument management, while the advanced data integrity ensures quality.

The seamless communication between the workflow management software and all the laboratory's instruments makes the relevant information and results available where needed, again with no manual transcriptions. Results are

Figure 7: Simultaneous helicopter and detailed views of a chromatogram help uncover anomalies quickly.



automatically imported from any instrument in the lab (see FIGURE 8) into the workflow management software.

SECURE CONTENT MANAGEMENT SYSTEM

The digitalization journey would not be complete without a secure place to store the data for effective use and reuse. Agilent's informatics system provides a single back-end for all of the information. It automatically collects, organizes, stores, and archives data transparently. Beyond chromatography data, the central secured repository can be expanded to store and organize any type of file, such as reports or logs. Labs can be confident that they have stored every report and file produced and know exactly where to find them. The various functions of the OpenLab software suite come together to make the end-to-end solution work. Importantly, as the operations and workload grow, the system can scale to support expansion.

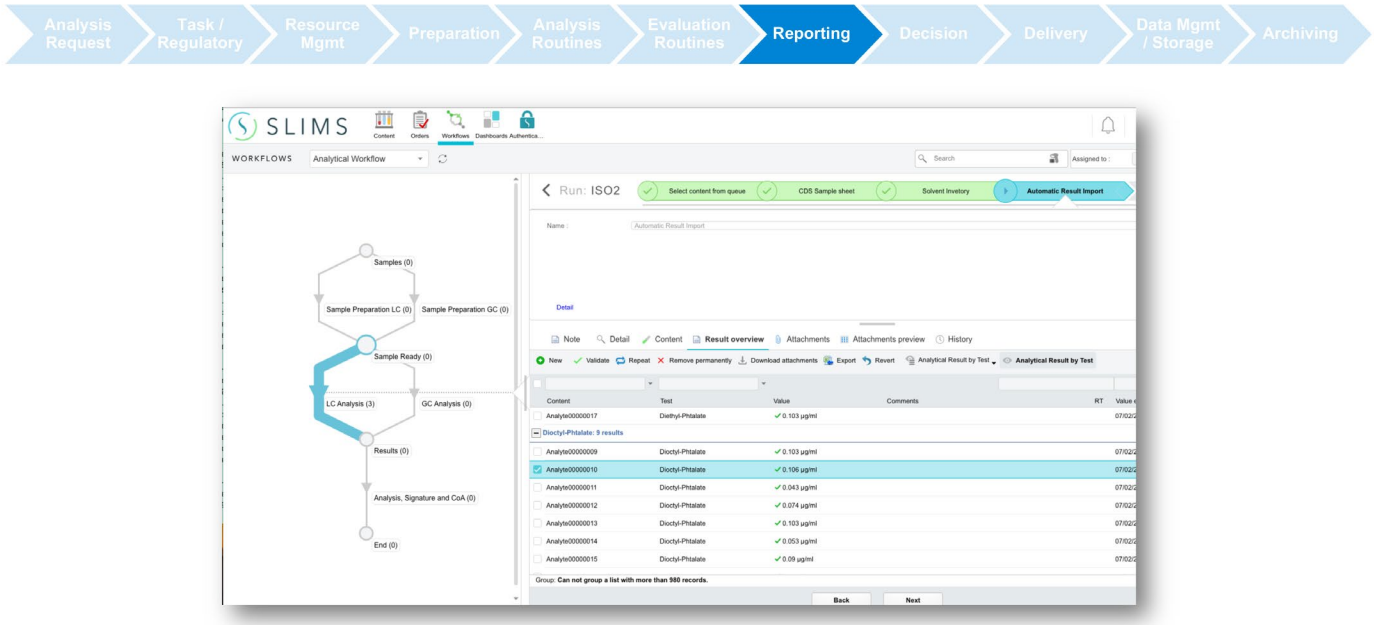
CONCLUSION

A modern, integrated workflow informatics solution allows laboratories to monitor and manage the analytical process from sample submittal through reporting and archiving. Agilent's OpenLab software suite seamlessly benefits the entire workflow and guides analysts with automated process checks to reduce mistakes.

The software package automatically captures essential data, stores it in a single repository, performs custom calculations, and generates reports.

Focused on high efficiency and data integrity, the software package automatically captures essential data, stores it in a single repository, performs custom calculations, and generates reports. To support auditing, the system is paired with a secure content management system, and allows labs to

Figure 8: Embedded calculations at the sequence level, injection level, or peak level.



store, version, and sign all laboratory data, results, and reports in one place. The searchable data is readily available for analytics or secondary use. Customers of the lab have the convenience of easy sample submittal, status checks of their sample during its lifecycle, and access to the report when it is ready. Implementation of this comprehensive digital solution offers labs the advantage of easy compliance, reduced errors, maximized efficiency, and assured data integrity.

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FAQs: Integrated Laboratory Informatics Systems

LCGC recently held a webcast on "Integrated Laboratory Informatics Systems Deliver Greater Efficiency and Improved Data Integrity," sponsored by Agilent. Here, Thomas Schmidt, Director of Product Management at Agilent, answers several questions from the audience.

Who implements the workflows?

It is the customer's choice, but a typical scenario is that we start by implementing and configuring the workflows. Our goal, however, is to give you the capability to extend the system to meet more and more of your needs in the lab over time. Our strategy is to start with a fast win and not run a long project. Then, we evaluate the first win, iterate, and go from there to "give the power to the lab."

What is the value beyond compliance with centralizing data storage and content management?

Centralizing data and content opens up a lot of different use cases. Compliance, auditing, and inspection are critical. Beyond that, users can find information about samples and methods they've used in the past and look across data sets for trends. Labs get a lot of value out of looking at deeper trends to optimize their operation.

How do you see the role of the Allotrope Standards in the future?

The Allotrope Standards will play a prominent role in the future in three areas: providing a common standard for long-term archiving (i.e., a data format that is readable over the retention period), supporting labs in their collaboration efforts, and in harmonizing analytical methods. The lab is very heterogeneous, especially when we look at the data, and Allotrope is a means to mitigate this heterogeneity.

My lab does not analyze pharma samples. Is data integrity still important?

Yes, having data that is valid, that you understand, and that you have confidence in is critical for any lab.

Can I realize the benefits of data integrity without the burden of pharma compliance?

Absolutely. The way in which data-integrity and compliance controls are implemented in OpenLab CDS is granular. Customers can choose to configure it differently depending on whether you need to comply with pharma regulations or ASTM, food, or environmental methods. You can tailor it to the needs of your lab without having to go through a fully compliant workflow the way a CFR 21 Part 11 lab must.

Can I connect the scheduler to production or logistics to update the priority or due date?

It depends on whether you're referring to the scheduler itself or the laboratory execution system, as the purpose is to connect the lab to a leading system, which could be a production and logistics system. From this perspective, yes, because our solution also comes with comprehensive programming interface capabilities that allow other systems to submit and update information.

What if I already have a laboratory information management system (LIMS)?

LIMS is a business application; it's about numbers and typically does not have workflow execution capabilities to transform your paper-based lab into an electronic workflow.

As a business application, LIMS knows what kind of samples you analyze and the specifications, but hands over this information to a laboratory execution system that combines what's needed from the sample management capabilities and the workflow capabilities into a holistic solution. This means, for example, SLIMS and the LIMS can interact in a complementary way.

Is this an all-Agilent approach? What if they already have lab software from other vendors?

In a perfect world, it would be an all-Agilent approach, as there are benefits to a single-vendor approach, but we have to give it a reality check. As mentioned, the lab environment is very heterogeneous, and this refers to the instrumentation and software packages. So whatever solution you have, it must be able to deal with the heterogeneity of the lab. Agilent can interact and exchange information with software packages or data systems from other vendors as well.