An Executive Summary

How to Achieve a Fully Digital, End-to-End Analytical Workflow

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Realizing the dream of the fully digital lab. Advantages of digital workflow management.

Introduction

Analytical laboratories are extremely diverse in terms of the types of samples they test, the instrumentation and software packages they employ, the skill level of their analysts, and the way they are managed. Ensuring regulatory compliance (e.g., through controls and procedures) adds an additional layer of complexity for regulated labs. Despite these differences, nearly all labs would benefit from reassessing their procedures and transitioning to electronic workflows, which pave the way to more technical controls, increased automation, and, ultimately, improved turnaround time and better quality of results.

Advantages of Digital Workflow Management

While laboratories are very different from one another, there are several common areas within the analytical workflow where glitches and challenges typically occur.

- Many laboratories rely on manual transcriptions, which can easily lead to errors.
- Insufficient communications among operators can cause redundancies or inaccuracies.
- Fragmented staff management tools can lead to a lack of peer-to-peer visibility and sub-optimal resource assignments, which undermine resource optimization and create process interruptions.
- Lack of adequate planning and visualization tools often results in more work or heavier resources utilization.

These issues, combined with demands on labs to do more with less, are good reasons to consider implementing a digital end-to-end workflow solution. Digitization helps laboratories manage complex workflows from start to finish. It eliminates the reliance on paper-based information and keeps it from getting lost while allowing results to be searchable and reusable. It also enables data analytics for useful insights into sample sets. Automated data capture and transfer among different instruments and software packages avoid transcription errors as well. If necessary, a digital system can also be used to validate manual data entry, thereby preventing potential errors.

In addition to simply going paperless, a digital workflow manager can detect sources of errors when results fall out of a specification range so that corrections may be made quickly. Review by Exception accelerates the review time by highlighting any potential

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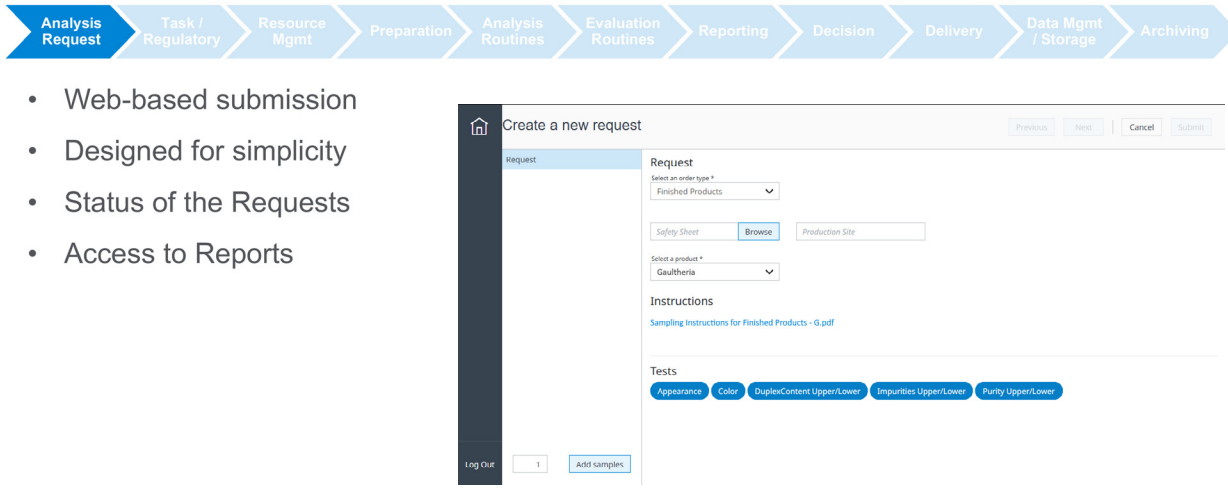
Figure 1: A convenient way for submitting analysis request to a laboratory via a web page.



deviation from the SOPs tolerance, and the system helps identify and navigate through the tasks involved. Also, all past or pending analyses for an inaccurate instrument can easily be retrieved, thus facilitating the impact analysis.

A good digital system that guides users through complex workflows and step-by-step protocols helps operators navigate the processes correctly every time. It also prevents the use of assets that are not fit-for-use such as non-calibrated instruments and expired solvents or standards. Moreover, a modular digital approach offers agility, making changes to a process much easier to implement. Quick dynamic changes, such as instrument integration or routing, are straightforward. Modularity also offers the ability to scale the system in alignment with a laboratory's needs.

Additional benefits of digitization relate to data management and the laboratory's administration. Data can be immediately accessible by lab personnel and management, with automated consolidation of results from different systems, labs, or instruments. Lab managers can see an overview of active projects as well as instrument performance at a glance. Regulatory compliance is streamlined with user assistance, sample tracking, audit trail, and protocol management capabilities. Convenient remote access can be made available to employees working from home as well as external partners.

Agilent SLIMS Solution

To deliver all of the benefits of a digital laboratory, Agilent offers SLIMS, a solution that enables customers to create and manage all of their content and its context with the optimal user experience. The company's software portfolio is built in a way that the different products fit and work together to cover the analytical workflow from the moment the analytical request is generated until the data is archived. This is all connected via OpenLab Services, the backbone of lab operations that hosts administration tools and is the repository for all of a lab's data.

Designed to combine the best of the electronic notebook (ELN) and laboratory information management system (LIMS), SLIMS is a tool that combines sample management and workflow execution for complex laboratory operations. The end-to-end SLIMS analytical workflow begins with a simple way for laboratory clients to submit a request. As it is web-based, analytical labs simply provide clients the URL so they can immediately start submitting requests, including details about the samples and which tests they need. The screenshot in **Figure 1** illustrates the simplicity of the request screen. There is no obligation for clients to install any software and its intuitive interface requires no training. After submitting the form, the client will have direct access to the status of the analyses as well as the final report when it is ready to be shared.

Next, the testing laboratory uses SLIMS to confirm the sample reception and start planning relevant activities. This could include checking to see if their instruments are fit for purpose, assessing inventories of consumables, assigning tests, and allocating tasks to operators.

At the bench, there are many places that a sample could get lost. SLIMS can track samples precisely, and even decide the best location for a particular sample, based on its type and rules set by the lab. SLIMS manages the relevant metadata about any kind of sample the lab is handling. In addition, SLIMS' barcode label designer for sample identifiers and barcodes simplifies the tracking process.

When the samples are ready for analysis, the analytical method describes what specific actions must be taken.

Figure 2: Visual indicators of a laboratory workflow.

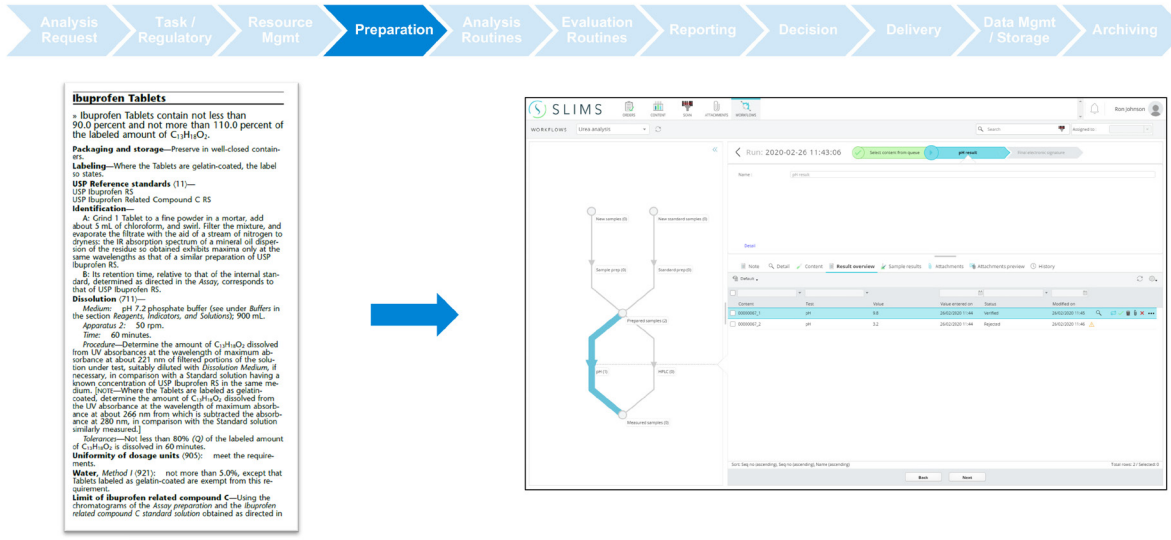
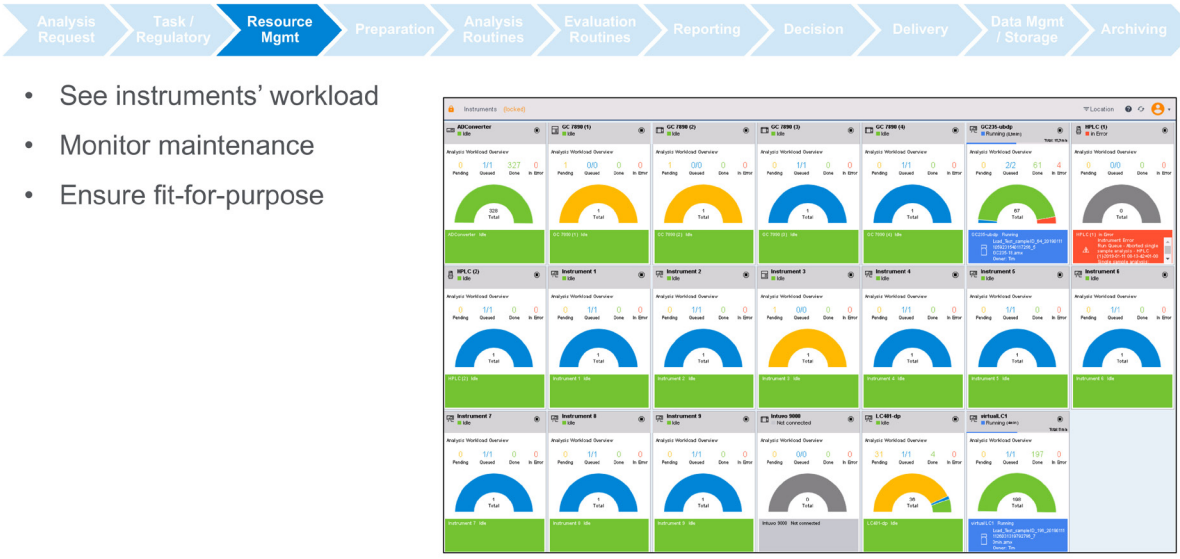


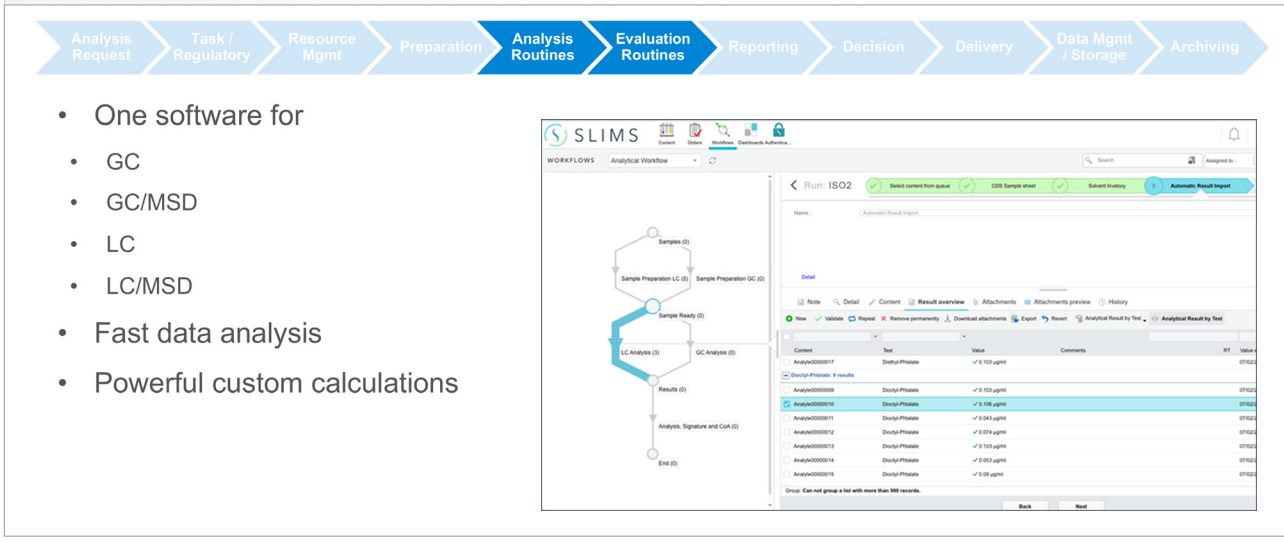
Figure 3: Laboratories can monitor all their instruments' status and usage at a glance.



The method can be broken down into several protocols which can each span multiple steps or be as simple as a single workflow element. **Figure 2** shows an example that depicts SLIMS' visual indicators of a workflow. The arrows represent a protocol, while the circles denote samples in the queue waiting to be acted upon in subsequent protocols. This visual provides a helpful overview of the status of the lab to manage its complexity. The different steps bind the content together, derive samples into new samples, and give context. All of the steps follow standard operating procedures (SOPs) developed and tied to specific projects, experiments, and users.

For a digital workflow to function properly, the handshake between different applications is crucial. The SLIMS solution conveniently allows users to operate instruments without having to launch their chromatography data systems (CDS). Instead, it automates the sample route to the appropriate instrument. **Figure 3** shows how easy it is to monitor instrument usage and maintenance needs with the software. The screenshot shows the live status and workload of an entire instrument fleet. This

Figure 4: Agilent SLIMS software connects seamlessly with a laboratory's chromatography system such as OpenLab CDS.



helps laboratories decide which instrument to use for a given analysis. It is especially useful when team members are not always in the lab. When sent to OpenLab CDS, the samples are placed in the context of the sequence. From there, both Agilent and non-Agilent instruments can be controlled. Data processing is then performed and reports are generated. **Figure 4** illustrates the seamless integration of SLIMS with a CDS. Results are imported into SLIMS expeditiously and without manual transcriptions. All of the pieces of information are kept in one repository, ready to be harvested when necessary and retained for the required data retention time.

SLIMS Implementation

There are several key concepts that can reduce the complexity of the implementation process and promote its successful execution. A laboratory must have a clear vision of the desired end state. Terminology should be unified, ensuring a common understanding with all the stakeholders in the organization. Standardization of protocols is helpful, instead of attempting to implement every individual circumstance. The journey to digitization is a great opportunity to review procedures and see how they can be kept in smaller, simpler steps that could be reused. Huge monolithic protocols should be avoided, as they cannot be modified easily.

It is important to strive for a system that is adaptable and easy to maintain. Implementation takes time; labs can start with something small and achievable and build from there. Acceptance of the system by laboratory staff should also be considered. Although it takes time and effort to build a complete solution, the positive impact on lab operations is immense.

There are five major steps of the SLIMS implementation journey:

- **Launch:** In this step, labs must take the time to define a common vocabulary, ensuring that all people in the organization share the same definitions. Return on investment (ROI) key indicators must be defined, such as reduced cycle times, data quality improvements, or a reduction in error rate.
- **Scope:** For the scoping step, laboratories should involve the users early so they will be empowered by the project. It is essential to understand their requirements and expectations. Small, continuous successes will lead to efficacious adoption of the system. A phased approach is advised for easier transitioning. Digitization could be implemented in one lab first, then rolled out to others. Also, a generic workflow could be implemented to capture manual inputs first, and subsequently converted to full automation and instrument control.
- **Installation:** Installation is typically straightforward, as it simply involves deploying a software package. However, there are matters to be addressed, such as infrastructure aspects, multisite deployments, and cloud vs. on-site installation. A scalable architecture is recommended, as it allows the system to grow with the laboratory. Labs must consider remote access, backup strategy, validation, connectivity of all the instruments, and end-user deployment options. Fortunately, most recent software packages are web-based, dramatically simplifying deployment.
- **Implementation:** The actual implementation is the most visible part of the digitization journey. Although there is no single turnkey solution available that will perfectly fit a lab's needs, the SLIMS Store

enables the fast construction of a comprehensive digital solution. It is a website where customers can download logical components and build out an entire workflow. The SLIMS Store's collection of preconfigured, yet customizable, packages simplify the digitization process for faster implementation. The modular approach offers flexibility to tailor the system to the specific requirements of a lab and make modifications easily, enabling straightforward integration and expansion to other labs.

- **Maintain:** Once SLIMS goes live, laboratories may believe they have reached the end of the journey and fail to consider maintenance of the system. However, by its very nature, a digital lab combines elements that were not initially designed as a whole. Thus, it entails extra care, particularly when the system is integrated into a lab's daily activities. As users become more familiar with the digital system, Agilent gives them the capability to manage their own software. The flexibility of SLIMS allows analytical labs to adapt to changing circumstances without having to hire an outside consultant.

Digital Transformation Stories

There are many ways in which digital workflow management can improve the performance of a laboratory. For a recent Agilent client, throughput was significantly increased while maintaining regulatory compliance. A real-time quantitative polymerase chain reaction (qPCR) lab managing biological samples approached Agilent to set up a digital compliance solution during a worldwide travel ban. With just three weeks' notice, they were required to increase their sample throughput five-fold.

A cloud solution was proposed to accelerate the initial setup. For additional time savings, the Agilent team handled the entire implementation, all of which was done remotely. They concurrently assisted with the validation of the system as well. In less than two weeks, the lab's objective was fulfilled. With the engagement of Agilent engineers, a system was up and running 24/7 with trained users. The lab can now manage their samples from registration, to qPCR results import, to analysis sign off.

Another recent example in which adherence to compliance was critical illustrates the importance of starting with realistic ambitions and iterating step-by-step. A customer was lacking a clear overview of the activities within their labs. They sought a global solution to connect to their LIMS and manage their samples and procedures at the bench level. With obvious compliance needs, they required integration with their instruments, especially with their non-Agilent CDS.

Agilent's engineers established the project in close association with the customer's regulatory team to ensure an appropriate solution was developed. An agile, iterative approach was taken while goals were reviewed throughout implementation. For different stakeholders to gain knowledge of the digitization process, they started a simple generic workflow solution that covered all of the methods in the lab.

The customer now has plans to expand, working in a mixed mode with both internal and Agilent resources on the later phases of the project. This is focused on creating more specific workflows to capture all of the details of specific techniques.

The final example illustrates how the complexity of the lab can be managed in a long-term relationship with the vendor. An environmental testing laboratory wanted to offer their clients a digital experience, so they asked for a portal to manage analytical requests and share the results. The new system from Agilent generates barcoded stickers during request creation, which are adhered to the sample by the customer before being submitted by mail. Once received in the lab, the sample is processed through multiple workflows with integrated instruments and complex automation.

Using preconfigured packages from the SLIMS Store, Agilent provided the initial setup, training, and configuration in conjunction with a local client team. Since then, the local team's knowledge has grown enough that they can now build their own configurations. This allows further customization and flexibility for future changes in the laboratory's needs.

Conclusion

Digital laboratories realize significant benefits via automation and insights that provide ultimate productivity. However, there is no universal off-the-shelf solution to help labs achieve their goals. As no two labs are identical, a flexible, adaptable digital system is necessary for end-to-end workflow management. To this end, Agilent's SLIMS digital workflow solution features a modular approach by offering preconfigured, configurable packages that can be combined to create a unique, compliant digital workflow for any laboratory. Combining the best of LIMS and ELN, the scalable system incorporates and automates instruments from Agilent, as well as other vendors. Thus, SLIMS delivers comprehensive digitization that maximizes operational efficiency from sample submission all the way through the analytical process.

FAQs: Achieving a Fully Digital, End-to-End Analytical Workflow

Here, Nicolas Louvet Software Product Manager for SLIMS at Agilent Technologies, answers several questions posed during a recent *LCGC* webcast, "How to Achieve a Fully Digital, End-to-End Analytical Workflow," sponsored by Agilent.

Is it possible to integrate data from gas chromatography (GC), high-performance liquid chromatography (HPLC), and inductively coupled plasma mass spectrometry (ICP-MS) into your application?

Yes, SLIMS can send data to the data system that will be used to run the analysis, including method parameters or any relevant data about the samples. Afterward, SLIMS retrieves the results and either use it in calculations or reports and store everything. We worked on the optimal user experience when using Agilent chromatography software, but we also have experience in connecting all the software packages in general, including chromatography data systems from third parties.

What type of training is available for lab and IT personnel who are implementing SLIMS?

We have a training program for users in the lab who are willing to do configuration work such as getting packages from the store, basic automation, creating workflows and software maintenance. For more advanced needs such as connecting to specific instruments or software, we have a training program to help experienced key users use our Software Development Kit (SDK) or our application programming interface (API).

Can you manage standard operating procedures (SOPs) in SLIMS?

Yes, we have specific tools to manage SOPs. You can have your own rules, and you can assign specific access rights so only authorized persons can use and/or change those SOPs. You also can define specific groups and roles and align them with, for example, training records so only the appropriate people have access to the proper equipment.

What does Agilent do and what is expected from lab personnel during and after deployment?

During the first step of the digital-lab journey, personnel can be involved in the early discussions with our team to specify and describe the expectations, and after, provide feedback on how the solution is configured. After the rollout, if the customer decides to take the lead on the configuration, then Agilent will assist with the transition to the team. Thereafter, it will be up to that team to lead the developments and the changes in the software.

How do we get results data from simple equipment that only have limited access points?

For small instruments without network capabilities, there are small devices that would help convey the data from small instruments into the digital solution.

If there are test failures during any of the instrument runs, do you have the capability to perform deviation reports for such failures?

Yes, and it will be up to you to decide the rule to apply when setting up the specific workflow for that test run.

What types of data can you export from SLIMS?

Basically, everything—there are many different ways to export and share data. For example, end users can provide direct links to an instrument or an experiment and share that within the organization. They can also share the reports that are generated by the system. There are also advanced Excel import and export functions available to the users. If you think about exchanging data with other systems or software such as analytics software, or a data lake, the system provides advanced APIs to do so.

How does SLIMS manage training records and employee qualifications?

Within SLIMS, you can restrict access to certain modules or certain workflows to specific groups based on their qualifications. If you already have an in-house system that is managing training for your team, we can potentially integrate with that platform to match SLIMS with the instruments or protocols.

Can the system store training records and staff authorizations to meet the requirements of ISO 17025?

Yes.

Can data from an analytical scale be sent directly to OpenLab CDS?

Not directly. SLIMS would be the perfect solution to handle that data from one system to the other. Other potential integrations are also possible.

What types of tasks can I do with a tablet?

SLIMS can be used on tablets for relevant and specific steps of the global workflow when the user focus should be on the task at hand such as having a balance measurement. We don't see the workflow experience being completed with a tablet.