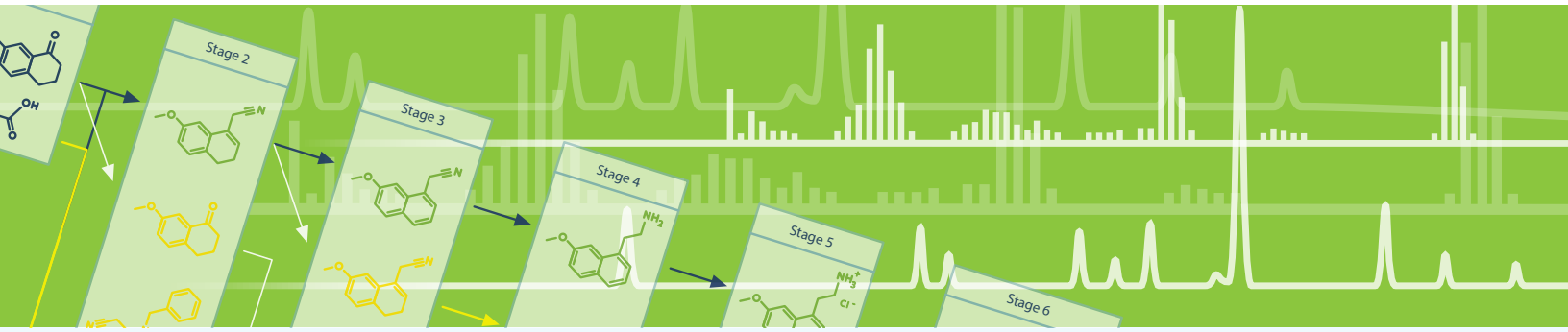
Case Study

Real Results from Bridging Gaps in Data Management

How a Major Biopharmaceutical Company Improved Process Development and Regulatory Submission Efficiencies



Summary

In 2019, a top US biopharmaceutical company began working to improve the synthetic route of an API. In addition to route development, the process development team wanted to streamline chemical and process data management and simplify regulatory submissions. The team used Luminata®, a chemistry manufacturing and control tool from ACD/Labs, to achieve these goals. The software reduced the time spent organizing spreadsheets and tracking analytical files during both the experimental and regulatory submission phases of the project. Luminata also contributed to a broader shift in philosophy, where scientists have become more open about sharing data between colleagues.

Luminata®

Key benefits of Luminata included:

- Improved result interrogation and decision making
- Efficient data tracking
- Reduced time compiling regulatory documentation
- Simplified batch comparison for company management
- Reinforcement of a data sharing culture

ACD/Labs

Background

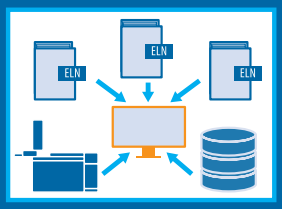
Pharmaceuticals are one of the most tightly regulated industries in the world. While it is clearly necessary to test the pharmacological effects of a new medication, it is equally essential to verify the consistency of the manufacturing process. For this reason, process control chemists and engineers prepare extensive regulatory documents. These reports accompany New Drug Applications (NDAs) to the FDA and span hundreds of pages, covering impurity levels, process conditions, and control strategies.

A team of development scientists at a large US pharmaceutical company began optimizing a novel chemical reaction in 2019. This process was updated from a previous method, but it would require substantial effort to gather the necessary data to meet regulatory approval. The project would also take place at an accelerated pace to meet scheduling needs.

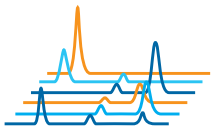
"It was a fast-moving project," explained the process chemistry lead for this project and a veteran process chemist of 14 years. "We were making some big decisions about what the synthetic scheme was going to look like… We made some changes to certain elements of the process late in the game, and we had to make sure we knew the consequences of those decisions."

The Challenge and Goals

Goals

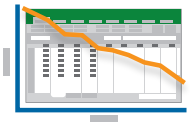


Bring together data from across ELNs



Simplify review of results

Accelerate regulatory submissions



Reduce reliance on Excel

The process development team wanted to improve data management practices and make report compilation faster and easier. Previously, they used Excel spreadsheets to share experimental results between groups. Unfortunately, Excel is poorly suited for sharing chemical, process, and analytical data. Team members were forced to jump between spreadsheets, manually transcribe data, and chase down analytical files to verify results.

A development team member explained that tracking Excel spreadsheet versions is challenging, even when best practices are followed. "SharePoint becomes a dumping ground," they observed. In the past, the process development team would often need to contact the supervising scientist to verify methods because it was too time-consuming to locate the correct entries.

The process development team wanted to streamline the review of experimental results to simplify decision-making. "We are trying to get into the nitty-gritty details of what happened to 'Impurity A,'" one scientist explained. "If you had all [the details] in one package, where you could directly compare to see exactly what happened to 'Impurity A,' I would have a lot more insight."

The team also wanted to reduce the time they spent compiling information in the regulatory submissions process. Different departments within the company use separate Electronic Laboratory Notebooks (ELNs). Data was spread across multiple systems and analytical devices, creating extra work when scientists reviewed results or compiled regulatory information.

"For each experiment, you could have multiple ELNs where that data is located," explained the process chem team lead. "As you go across multiple experiments, I run the experiment and then hand it off to one of my colleagues in engineering to work it up. Well, now I've just multiplied that again and again. Inside Excel, you can track ELN information, but it is difficult to track which ELN the experiment was done in."

Implementing Luminata

Process development had invested in Luminata to help manage analytical data, but this was the first project where the CMC decision-support software would be used from the outset. One team member had already worked with Luminata and was impressed by the program's ability to consolidate streams of analytical data with synthetic route information.

Most team members would be using the program for the first time. Getting them accustomed to the software required some adjustment. There were "a whole range of reactions," remarked one researcher. "The folks that got it, that understand the power, they were willing to work with it."

There was a learning curve, but the team understood that all complex software required an adaptation period. Management helped reinforce the commitment to Luminata by offering support and encouragement to the team as they implemented the software.

Impurity Data Management in Software Designed for Chemical Information

Team members became more enthusiastic about Luminata when they saw data in the software. "When we got the data in there, that was cool," remarked a process engineer on the project. "Taking all our batch history and being able to overlay that on each other and see what happened… being able to overlay front runs with plant results. These are things we would have done in a PowerPoint slide before, but now it is much easier."

Luminata became part of the team's day-to-day operations, aggregating project information and allowing team members to compare results. Teams could continue to use their preferred ELN and analytical instruments without the need to retrofit their equipment. Researchers were impressed by the software's ability to help interrogate analytical data. "There are frequently these low-level impurities, and we kept asking the question 'Have we seen this?' Instead of relying on somebody's memory, we go into Luminata, see all the experiments that have been run, and see if that peak was there."

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Before Luminata, "it would take a lot of time to go fishing for that information." Previously, if there were questions about an impurity peak, the team would often spend as long as an hour searching for an answer. With Luminata, an experienced user could address such questions in a matter of minutes.

Data for Regulatory Submissions Accessible in One Place

Months later, when it was time to write the Process Control Justification (PCJ) report, researchers could collect data directly from Luminata to prepare the document. Since Luminata tracks the data's origin, it was possible to trace each piece of data to an ELN, which would act as the source document. A member of the team involved in compiling the regulatory documentation observed that "Luminata bridged those different gaps, where we can have all that data from the very earliest starting materials through the process to make the drug substance, we can also now link to the process for the drug product."

Luminata also allowed the team writing the PCJ to quickly filter through files and find entries that best represented their results. Previously, this had been a time-consuming endeavor. "There's a reason why whenever [report authors] run into a problem, the first thing they do is pick up a phone and call the lead chemist," explained a researcher. "Because that's the easiest thing to do."

Overall, it was felt that there were substantial time savings and relief about the reduced need to juggle spreadsheets. "I felt like I was a lot more efficient. I wasn't going back and trying to manage 'Which Excel file was that data in? Where was [the original data] actually located? Was this completely filled out or not?' I'd say that I was 33% more efficient… because I didn't have to keep going back, searching for something."

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A Shift in Culture Around Data

Luminata also brought some unexpected benefits. According to one scientist, "One of the groups that were surprisingly receptive to Luminata was at the management level. Now, suddenly, they can see the process that's being run in our pilot plant, and they can look at our front run and compare it to the actual data from the run. That was not a trivial thing for them to be able to see previously. Now you can actually bring those pieces of information together and do overlays."

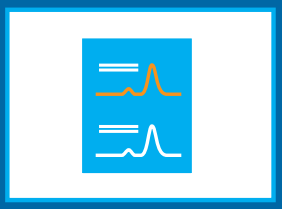
Beyond the time savings in regulatory submissions, it was felt that Luminata helped shift the company culture around data accessibility and digitalization. Team members no longer had to email back-and-forth to chase down analytical results. "It's a change in the philosophy," said a team member. "The data was now everyone's data, versus it's my data which I'll share with you either when you request it, or I just want it off my desk."

Another scientist observed that Luminata could contribute to a change in the attitude towards data. "A lot of companies are doing 'digital transformations' because it is so clear that data is like gold. No one wants to waste time generating the same piece of data a second time… There is not a lot of cross-talk sometimes between different functions. If we have a better way to share our data—to be collaborative across our organizations—it's going to make us move faster as a company."

Benefits

Quickly interrogate impurity information

Data tracking



Simple batch comparison

Reinforced culture of sharing data

Conclusions and Future Deployment

Overall, the software met the expectations and goals of the team. Luminata streamlined data from multiple ELNs, improved the efficiency of preparing reports, and strengthened a culture of data sharing. It helped the team reach project objectives and develop an efficient chemical process for drug manufacturing.

In addition to these benefits, there is interest in getting more from Luminata in the future. One team member was interested in tracking the quality of starting materials through the development process. "Do you have a lab experiment where you are seeing an impurity you didn't expect? A lot of times, we'll ask, 'Was there something in the starting material?' Having that connection—having it all outlined in Luminata, or in a system where you can see everything—was something we could have used more readily."

"We didn't use it to its full extent," they said. "We'd love to see more use of the software. I've seen it develop and change over the past few years that we have been using it, so the more we can get experience with it, have some training opportunities with the software, it will help bring people up to speed on how to use it. Because I know there are so many things in that software that we are just not using right now."

About Luminata

Luminata is the only Chemistry, Manufacturing, and Controls (CMC) decision support software. It lets researchers store, search, map, process, and reuse their chemical and process data in one application. Uses of Luminata include process development, impurity control, forced degradation studies, formulation, and supply chain management.

Learn More About Luminata ▷

About ACD/Labs

ACD/Labs creates software for chemical research and development. Our software brings together data from multiple instruments and sources, so scientists can manage their data. Using ACD/Labs' software, scientists can design and automate experiments, process analytical data, and report results. We support customers in many industries, including pharmaceuticals, biotechnology, chemicals, consumer goods, agrochemicals, petrochemicals, government, and academia.

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