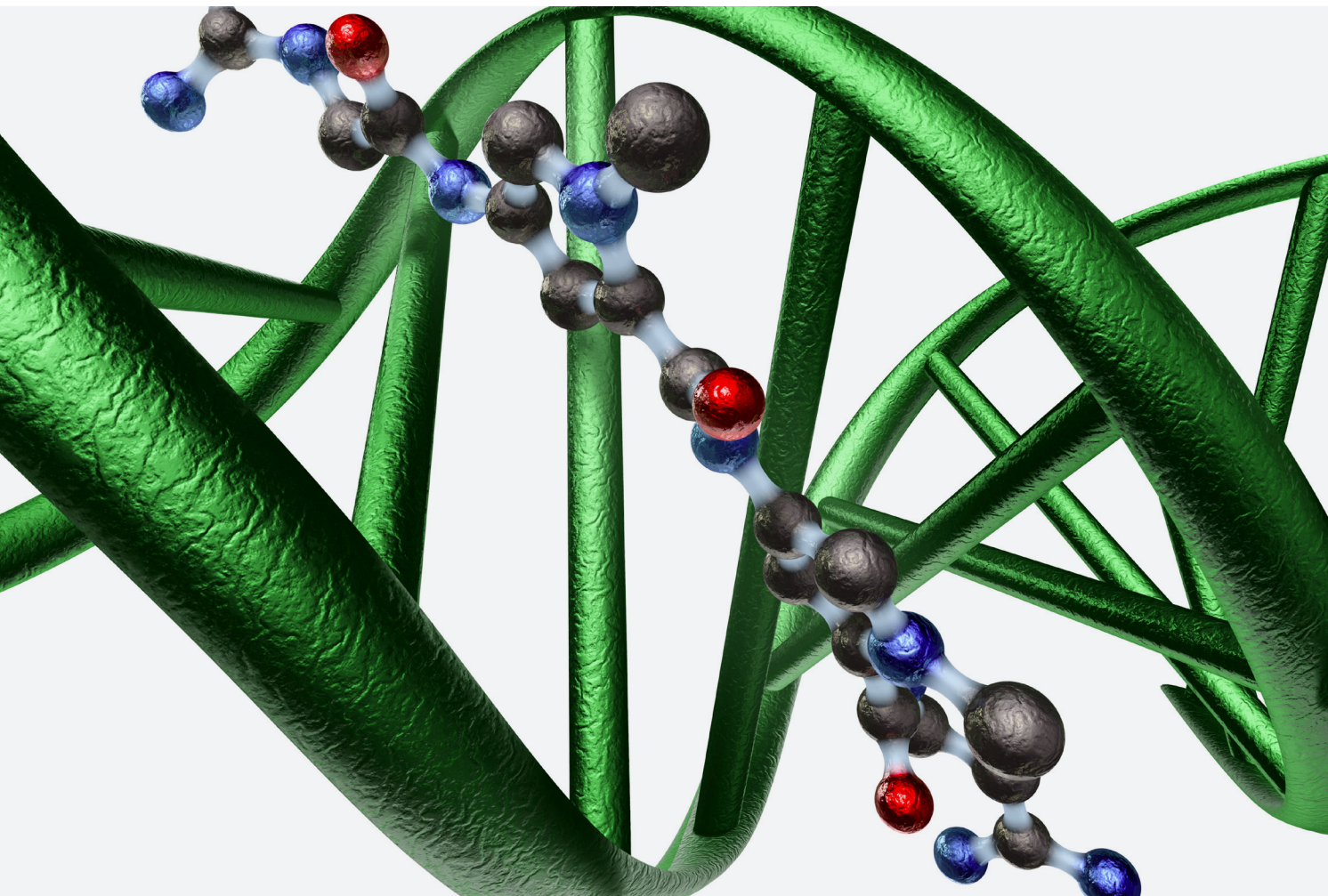


# MILLENNIUM'S ELN EMPOWERS CHEMISTS AND BIOLOGISTS

CUSTOMER STORY



Conventional wisdom holds that biology is not just more complex to manage electronically, but actually more resistant than other areas of discovery to electronic systems such as electronic laboratory notebooks (ELNs). But Millennium, the Takeda Oncology Company, found that by clearly defining workflows and implementing a highly configurable notebook, it could begin moving its entire discovery organization—encompassing both chemists and biologists—to a single ELN system.

### Challenge:

Collaboration hindered and drug development slowed by disparate information management systems used by chemists and biologists

### Solution:

BIOVIA Workbook (previously Accelrys Electronic Lab Notebook, formerly Symyx Notebook)

### Benefits:

- Improved collaboration and productivity with chemists and biologists using the same ELN system
- Drug candidates move faster into pre-clinical/clinical review
- Scientists save time by leveraging previous work (50% of reactions are clones of previous reactions)
- Higher quality experimental records, streamlined chemistry workflows

“Most of us have heard drug discovery described as the ultimate team sport, requiring individuals from disparate groups to share data and work together,” said Craig Tulig, associate director of R&D Systems at Millennium. “Someone doing an *in vivo* study is going to want to reference the chemist’s original formulation or the summary results from the analyses captured in LIMS. Plus, from an informatics perspective, the ELN is increasingly becoming a key enterprise system. It’s impractical for a small team to maintain two systems for different parts of discovery. That’s why we’re moving toward a single ELN system for all of discovery, if not for all of Millennium.”

### INCREASING THE VALUE OF PROPRIETARY INFORMATION

While the result of Millennium’s ELN implementation is a nearly paperless lab, Tulig is quick to note that “paperless” was never a business goal. “For us, going paperless was a means to an end, not an end in itself,” Tulig explained. The primary driver for both the chemistry and the biology projects was having a way to search and retrieve information buried in paper notebook records.

Millennium first tackled chemistry, probably, Tulig mused, as much because of vendor comfort with solutions as a pressing need in that area. “Most research informatics vendors had their beginnings in chemistry—compound registration, screening, reagent inventory, chemical drawing programs,” Tulig said. “When we first started looking at options in 2000–2003, everything was skewed toward chemistry. It’s different now, though; we’re really seeing the market maturing to provide more general-purpose capabilities for a broader range of disciplines.”

An ironic reality motivated the chemistry project. Millennium, like most pharmaceutical companies, subscribes to online databases that let chemists search reactions described in the literature. But chemists could not search across Millennium’s

own proprietary chemistry, which, said Tulig, was arguably much more valuable than what could be found in the public sources. Millennium initially assumed they would need some type of chemical information system to store and retrieve proprietary reactions. However, the project scope quickly changed to an ELN, because, as Tulig stated, “Once you’ve made chemists go through the effort of entering experimental details into an electronic system, you’re not going to get them to do more work entering all that same information in paper notebooks.”

ELN implementation began in 2003. To the surprise of the R&D Systems staff, Millennium’s legal team was an early advocate of the project. “The legality of ELNs as a repository for intellectual

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Millennium: The Takeda Oncology Company

property was very controversial at the time, but our legal team determined early that an ELN would be less risky than paper for two reasons,” Tulig explained. “First, our IP would be easier to find, and second, our IP would be legible.” Tulig also pointed out that ELNs tend to result in an overall boost in the quality of records. The standard PDF produced serves not just to institute best practices for documenting research, but creates peer pressure that encourages chemists to ensure that their work is as well documented as their peers’.

The ELN also streamlines the chemistry workflow in several ways. In benchmarking done before the implementation of the biology ELN, Millennium discovered that 50% of reactions created in the ELN are clones of other reactions. Tulig said that proves that chemists are searching the ELN before they experiment and leveraging the results of previous work to save time. Additionally, prior to implementing the

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ELN, Millennium required chemists to engage with a variety of electronic systems including a reagent inventory system, a reagent catalog database, a compound registration system, and various analytical tools. Millennium configured their chemistry notebook to integrate seamlessly with these systems.

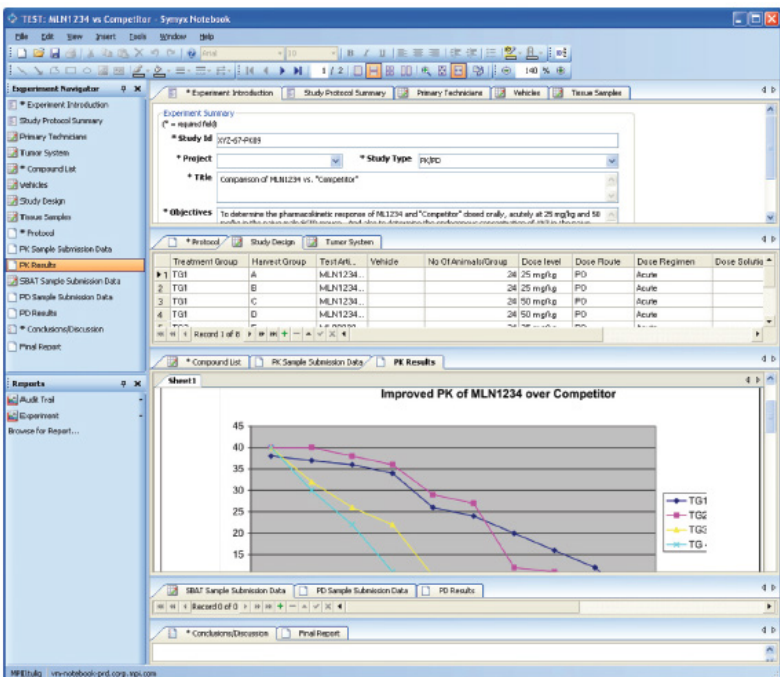
“We took all the integration behind the scenes, creating the appropriate hooks to needed systems so that scientists could focus on their experiments rather than navigating the various

## OVERCOMING REPORTING HEADACHES AND BOTTLENECKS FOR BIOLOGY

As in chemistry, the need for a searchable biological archive prompted Millennium to consider a biology ELN. In 2008, Millennium Discovery Research began reviewing its paper notebook processes and policies to see how they mapped to the company’s organizational goal of getting development candidates more quickly into preclinical and clinical review. “If you want to declare a development candidate or file an IND [investigational new drug] application, you need to be able to assemble everything you know about that compound—quickly,” said Tulig. The process was inefficient and paper-based even though the team quickly discovered that biology was already handling key data electronically. High quality electronic images, for example, were being printed out, cut with scissors, and pasted into paper notebooks by biologists. Plus, it was often difficult to search for study findings in paper notebooks. “You had to know what you were looking for so that you could identify which notebooks to look in,” Tulig said. “And if you couldn’t find the right data, it was often easier to just repeat the study.”

“We’d heard about the inefficiencies of paper notebooks in biology, but it really hit home when we saw what scientists were keeping in their notebooks,” Tulig said. “When everything else you’re doing is already electronic, an electronic notebook makes a lot of sense.”

More problematic was the diversity of biological workflows that the ELN would need to expedite. The chemistry implementation required the IT group to deal with one set of researchers working with one set of systems. Biology, on the other hand, comprised ten different departments doing widely different kinds of work and using different types of hardware and software. Rather than serving as the “center of the universe” like the chemistry notebook, Millennium’s biology notebook is more of an information hub that collects critical summary data from other informatics systems in the ELN and provides drill-down access to experimental details.



**Figure 1:** Millennium’s standard template ensures that biological data is traceable by collecting information from chemistry, DMPK, and pharmacodynamics in a single location. Study designs are completed within the ELN and, with a mouseclick, executed in LIMS. Associated data is similarly imported back to the ELN with a click.

systems,” said Tulig. For instance, chemists setting up an experiment at the bench use a barcode reader to scan the samples they plan to use, and the ELN automatically looks up the reagents in the reagent inventory and brings all related chemical structures and data into the ELN. Tulig noted that the integration has also made it easier for IT to consolidate systems without disrupting scientists’ routines. “As a result of our ELN implementation, we actually tossed out our older reagent inventory and reagent catalog systems, but from the ELN perspective, there was almost zero impact to the chemists,” said Tulig.

“From the beginning, we saw the chemistry ELN as the center of the universe for the chemistry lab,” said Tulig. “We used the ELN to tie together diverse systems—including those that were not particularly well loved by our chemists—and create a purposely tailored workflow within one application that matched how our chemists work in the lab.”

**“We didn’t want the technology to be a driver in and of itself, but when you look at the original evaluations, the ELN was the system preferred by both our scientists and our technical teams and that spoke volumes.”**

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“Many of the systems biologists use when doing their jobs are really good at executing an experiment, but those systems don’t typically provide a lot of context about why the experiment is being done or what the conclusion of the experiment is,” said Tulig. “That’s the real value to the broader organization, and we’re using the biology notebook to serve as that final repository where all of the related results associated with biological research come together.”

Tulig pointed out that the electronic system has helped biologists stay on task in preparing IND documentation. “They can plug in search criteria and retrieve the appropriate information almost immediately—often including information that they may have overlooked if they were working solely with paper,” said Tulig.

## IMPLEMENTATION STRATEGIES

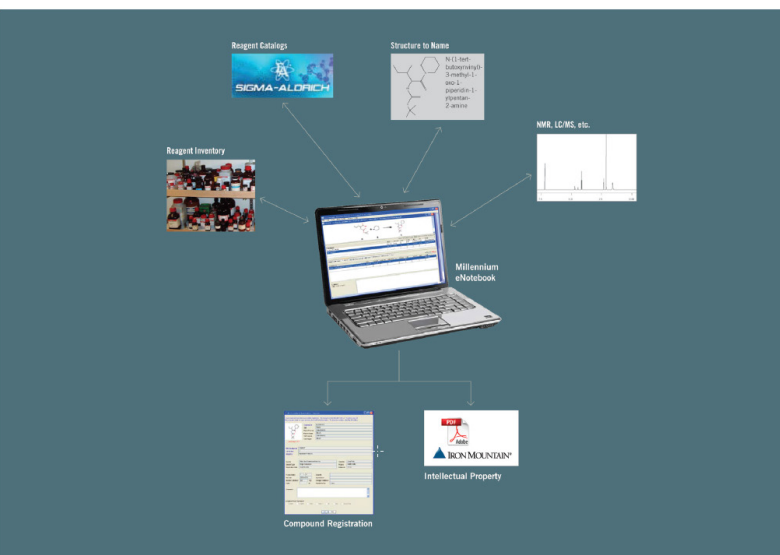
The relative maturity of ELNs combined with Millennium’s own experience with systems of this type led to somewhat different implementation strategies. The company relied on its robust software development life cycle (SDLC) to manage both efforts, but piloting is where “the rubber really hits the road,” said Tulig.

“The pilot team is the gateway before you roll the system out to the entire department,” Tulig continued. Piloting was particularly important in biology, where the workflows were

a lot more complex. “We did a lot of up-front analysis where we mocked up what we thought an experiment would look like and used Word to create little mini-forms and images and workflow diagrams of what was happening in each lab,” said Tulig. The prototyping ultimately helped Millennium specify requirements and evaluate vendor solutions. “You bring in Vendor 1, hand them the paper prototype and implement it, and then you do the same thing with Vendor 2 and so on—and you are able to make apples-to-apples comparisons,” Tulig explained.

In both implementations, Millennium used an agile approach that created an almost immediate feedback loop between IT and users. Tulig noted that agile development not only helps IT develop a more “right” system, but secures buy-in from users. “My favorite anecdote from the chemistry implementation is when we were halfway through the pilot and wanted to implement a few more features before the final roll out,” Tulig recalled. “The response from the chemists was, ‘No! You’re not going to make us go back to using paper, are you?’ Even at this early stage, they were saying, ‘Please don’t take the electronic notebook away from us.’”

One challenge in the biology implementation has been defining vocabularies. Tulig explained that chemistry mainly revolved around chemical structures and project descriptors. Biology, on the other hand, involved a wide variety of experiments that were often described in different ways by different groups. “The tradeoff has been balancing when to make the scientists change their routines and when to make the software smarter,” Tulig said. “We hope that as the software matures, it can use ontologies to standardize vocabulary and recognize automatically when one descriptor is equivalent to another – but sometimes, this isn’t possible.”



**Figure 2:** Millennium’s ELN serves as the center of the universe for chemistry lab systems. Most tasks can be completed directly in the ELN without needing to switch to another system. Millennium used a service-oriented architecture (SOA) approach to integrate these diverse systems, which has been successful in letting IT staff swap system components without disrupting the scientific workflow. This same approach was employed in the biology rollout.

## TULIG’S ELN IMPLEMENTATION TIPS

Tulig credits several factors as key to Millennium’s success with its chemistry and biology ELN implementations. Here are his tips:

- Set goals and make sure you follow them through the project. For example, knowing the most common searches we wanted to do influenced how we designed the templates and which vocabulary we spent time on.
- Pilot. Pilot. Pilot. You just can’t pilot enough. It helps you define requirements and it’s key for vendor selection. In our case, even though we’ve made our selection for our Phase 1 group, we’re going to pilot again with a Phase 2 group just to make sure that the templates are correct and to get a proof of concept before we roll out the ELN to entire departments.
- Hire and retain staff who truly understand both the technology and what the scientists are trying to accomplish with it. The ability to marry the two is invaluable.

Both the chemistry and biology implementations took advantage of subject-matter “point people” to define workflows and provide feedback during the initial pilot. Based on its experience with the chemistry implementation, Millennium introduced a tiered training program for biology rather than the classroom training it deployed for chemists. Online eLearning will be offered to introduce basic functionality of the ELN. Additional custom lessons will also be designed to explain Millennium’s specific business rules associated with ELN use. Finally, pilot team members from each department will formally present to their colleagues the templates developed and how and when to use them.

## MEETING ORGANIZATIONAL NEEDS

Some of Millennium’s scientists and managers initially questioned the need for a single ELN system. A common assumption was that most scientists would only want to search for information within their own individual departments. But Tulig points back to the “team sport” metaphor.

“We knew it would be valuable for our scientists to be able to consistently find information on compounds, studies, and project status across the whole organization,” he explained. And while the most weight was put on how scientists liked the systems evaluated, the ability of the system to accommodate enterprise requirements easily was also important. “We didn’t want the technology to be a driver in and of itself, but when you look at the original evaluations, the BIOVIA ELN was the system preferred by both our scientists and our technical teams—and that spoke volumes.”

## About Dassault Systèmes BIOVIA

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