DASSAULT SYSTEMES

BIOVIA

ADVANCING RESEARCH ACROSS CHEMISTRY AND BIOLOGY

HOW A LEADER IN DRUG R&D SERVICES IMPLEMENTED A COLLABORATIVE ENTERPRISE ELN

Use Case

Challenge:
Paper-based lab work leads to time-consuming processes with experiments and complicated data entry.

Solution:
BIOVIA Notebook

Benefits:
- Improved support for research across entire company platform
  - 90% satisfaction from users post-rollout
  - 70% of users reported that BIOVIA Notebook saves them time.
- Reduced repeat experiments and track and avoid failures.
- Improved progress monitoring for experiments.

This BIOVIA customer has offered industry-leading drug discovery and development services for over 25 years. Its success lies in its fully integrated, holistic approach to small molecule drug discovery, spanning from target identification to investigational new drug (IND) submissions. The company has global research operations at five sites, with each site specializing in one part of the drug R&D value chain. Central operations, screening services, and in vitro and in vivo biological studies are conducted at one site; medicinal chemistry services, computational chemistry, structural biology, and DMPK studies are based in another; and additional medicinal chemistry support and library management and services occur elsewhere.

In a demanding and increasingly distributed research environment, drug discovery alliance companies can only attract and maintain collaborations by being responsive and providing high quality results as quickly as possible.

What mattered to this BIOVIA customer in meeting collaboration demands, however, was being able to rapidly collect together project information to deliver reports and data, fulfill patent submissions, or leverage and build on past work.

REQUIREMENTS VS REALITY

When the customer began considering an ELN, lab work was documented almost entirely in paper notebooks at all of its research sites. The exception was their medicinal chemistry services site where an in-house hybrid ELN indexed information from paper notebooks for electronic structure searching. Chemists would scan pages of experimental data at scanning locations throughout the facility, and annotate the images with searchable technical details such as chemical structures. This made the paper notebooks searchable, with medical chemistry group leader reporting the system worked reasonably well.

"However, writing up material on paper and then entering information again electronically was duplicated effort," he said. "Overall compliance was poor."

Meanwhile, the biology teams documented their experiments entirely in paper notebooks. Such a system ensured that individual scientists could find their own information when needed, but writing collaborative reports remained time-consuming, as it required those compiling reports to search for information across multiple paper notebooks.

This working practice was captured in their in-house decision making when they began exploring whether to adopt their own ELN. As a result they developed a list of 161 requirements for an ELN. They had several high-level aims including:

- Supporting research across their entire platform, specifically chemistry, biology, ADMET, structural biology, and analysis
- Making experiments searchable to reduce repeat experiments, track and avoid failures, monitor progress, and increase information/knowledge sharing
- Standardizing experimental write ups and making them legible, consistent, and compliant with health and safety regulations

> **"Integrations like these will streamline processes and keep BIOVIA Notebook as a key component in the arsenal of informatics tools to provide better science to our customers"**
>
> — Medical Chemistry Group Leader

The company's final decision hinged on the way scientists reacted to the potential systems. The three short-listed vendors (from a first-draft list of six) were asked to provide demonstration systems that the company's users could try side-by-side, independent of the vendors. After educating itself about electronic lab notebook systems and researching several options, the company opted to implement BIOVIA Notebook. It was the outright winner. One of the group leaders explained that usability and features—both for scientists using the system and the IT staff who maintain it—made it the superior offering irrespective of an extensive requirements list.

"A system may have more bells and whistles than you asked for, but if it's not easy to use and easy to keep up and running, it simply won't get buy in from the scientists," the group leader said. "By keeping it simple, BIOVIA Notebook succeeds—we had people up and using the system within hours of starting. For all of our effort evaluating and preparing requirements, we have ended up with a system that has surpassed our expectations!"

SIMPLICITY RULES

When asked to explain exactly why the BIOVIA Notebook is so easy to use, the group leader replied, "It's just logical in BIOVIA Notebook. The interface isn't overcrowded, the menus are uncomplicated, and the signing procedure is simple." In BIOVIA Notebook, scientists enter information on pages just as they would in a paper notebook. Easy-to-build templates can help organizations enforce standard procedures, but are not a requirement to using the ELN. Plus, as with all ELNs, scientists often find it saves time to record information by cloning an existing experiment and replacing the data.

"With BIOVIA Notebook, scientists can get on and do the science rather than spending time working out which menu to use for chemistry or biology or something else. It's an enabling tool rather than something that hinders them in their work."

BIOVIA Notebook was also easy to implement for this company. "The whole process took five days—from coming in and installing the system to integrating it with our internal systems to users working in BIOVIA Notebook. It was integrated with our existing user/role management system for partitioning access to internal applications and with our reagent supplier and compound management database. It was essential that the ELN tie into these systems, and the ELN provided some simple database links, PL/ SQL, and integration libraries to accomplish this easily," said the group leader.

Training, as well, was accomplished impressively quickly. The company trained 200 scientists in just six weeks in sessions that comprised an initial introduction and walkthrough and a one- to two-hour practical session depending on the user and his/her discipline.

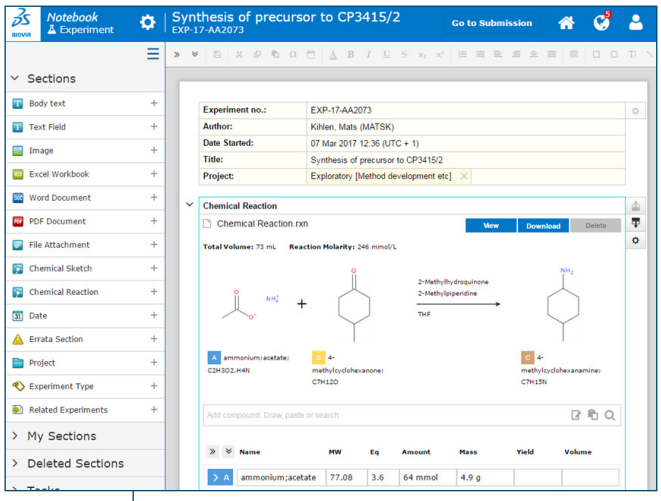

Figure 1: BIOVIA Notebook offers a clean interface that makes it easy to enter experimental data and retrieve results. Searching by experiment number, structure, or other relevant data retrieves full experimental detail, including relevant reaction schemes.

OVERCOMING CHALLENGES IN ACCESS AND ELECTRONIC SIGNATURES

Having used client ELNs for work in the past, the company initially considered whether it should provide collaborators with access to its ELN through a cloud-based system. For several reasons, it opted to host the system internally within its firewall and use the system only for managing project data internally. "We have some collaborators with their own ELNs, and some who are very nervous about managing data electronically," said the group leader. "We wanted to be flexible and able to accommodate collaborators wherever they were."

To ensure the security of client data, the company sets a variety of roles for scientists within their existing user/role management system. Some scientists can only read certain experiments, others can add experiments to projects, and privileges may also depend on whether experiments have been signed or not. Chemistry collaborators, in particular, are very prescriptive, only allowing scientists to see data within a project they have worked on or retrieve results associated with work they have done in the past on other projects. On the biology side, access to data is more flexible, simply because many biologists may be working with data from multiple projects in a single run. BIOVIA Notebook accommodates whatever restrictions a site may have, in this case working in conjunction with their existing user/role management system, but has its own user management system if a local solution is not available.

SATISFYING SCIENTISTS

The company conducted the initial six-month trial with 30 chemists and biologists, before rolling the system out at its other sites. Following the trial, 60% of chemists thought that the ELN saved them time on the job.

> "The introduction of [BIOVIA Notebook] has changed the way that we work, made communication better, and improved the consistency of, access to, and quality of the data that we record in our collaborations."
>
> — Medical Chemistry Group Leader

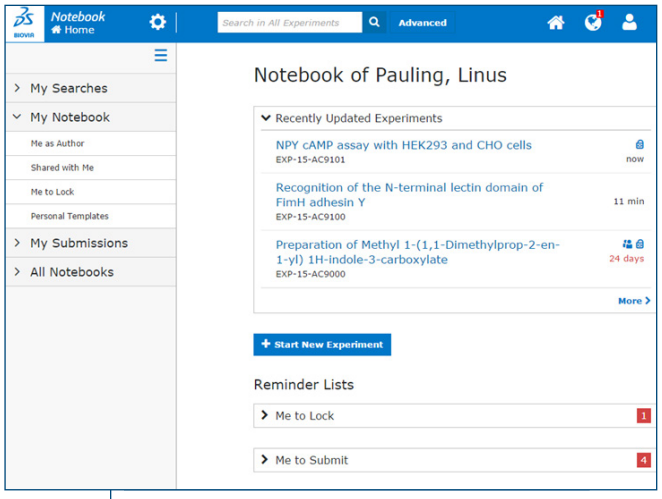

Figure 2: BIOVIA Notebook supports critical lab workflows. The figure shown here provides a look at the clean starting page for users, listing relevant information for initial procedures.

"You could probably do most reporting by using a combination of programs and a lot of print-and-stick in a paper notebook," wrote one user in a survey response. "But you would not be able to share the information as easily as you can with an ELN, and it's much easier to produce a really detailed experiment write up and do it quickly with an ELN."

Six months after the system was rolled out across the company, around 90% of their scientists reported being happy with the ELN. Eighteen months post-rollout, 70% of all users reported that the ELN saved them time, particularly with writing reports and searching for past work. Users across the organization particularly appreciated the ability to clone experiments, automatically import data to speed experimental documentation, and search across their work to gather information for reports. The end result is an electronic system that is higher quality, easier to read, and much faster to locate.

The company is currently expanding the ELN roll out to its laboratories. Further expansion to other sites is also planned. "We currently have more than 460 users of BIOVIA Notebook," the group leader said. Further integrations are also planned, including a system to automatically register compounds into their corporate compound database as they are entered into the ELN. "Integrations like these will streamline processes and keep BIOVIA Notebook as a key component in our arsenal of informatics tools to provide better science to our customers," he concluded.

In a demanding and increasingly distributed research environment, drug discovery alliance companies can only attract and maintain collaborations by being responsive and providing high quality results as quickly as possible. "What matters to our collaborators is that we deliver," said another group leader.

- BIOVIA Notebook serves chemists and biologists conducting research at five global sites and serves additional non-research sites as well.
- Eighteen months post-rollout, 70% of users reported that BIOVIA Notebook saved them time, particularly with writing reports and searching for past work.

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Dassault Systèmes
175 Wyman Street
Waltham, Massachusetts
02451-1223
USA

BIOVIA Corporate Americas
BIOVIA
5005 Wateridge Vista Drive,
San Diego, CA
92121
USA

BIOVIA Corporate Europe
BIOVIA
334 Cambridge Science Park,
Cambridge CB4 0WN
England