

PAPERFREE FROM DAY ONE: ELN DRIVES COLLABORATIVE RESEARCH AT KALEXSYN

A PERENNIAL PROBLEM FOR ORGANIZATIONS IMPLEMENTING ELECTRONIC LABORATORY NOTEBOOKS (ELNs) IS CONVINCING SCIENTISTS TO ABANDON PAPER NOTEBOOKS. KALEXSYN, A CONTRACT RESEARCH ORGANIZATION (CRO) BASED IN KALAMAZOO, MI, AVOIDED THIS PROBLEM ENTIRELY BY NOT LETTING ITS SCIENTISTS DEVELOP PAPER-BASED ROUTINES IN THE FIRST PLACE.



From its first day of business, Kalexsyn has used an ELN, and the company's leaders credit the system with making Kalexsyn a better, more productive partner for its clients.

"Conservatively, our scientists save about 25% of the time spent writing reports and preparing patents relative to a paper system," explained David Zimmermann, CEO of Kalexsyn. "And that 25% translates into more chemistry and very satisfied customers."

FINDING A PRODUCT AND A PARTNER

Zimmermann and ex-Pharmacia colleague Dr. Robert Gadwood, Kalexsyn's president and chief scientific officer, planned to do things differently when they founded Kalexsyn in 2003. Based on their experience working with CROs at Pharmacia, they chose to hire scientists who were experts in medicinal chemistry. "Most of our competitors staffed their firms with synthetic chemists who had happened at some point in their

careers to have made biologically active molecules," said Zimmermann. "We consider medicinal chemists to be scientific artists who integrate information from synthetic methodology, toxicology, ADME, pharmacology, and physicochemical characteristics to create new chemical entities, and we've built Kalexsyn to enable the practice of this art."

Additionally, Zimmermann and Gadwood identified the ability to communicate and collaborate effectively with pharma partners as

a cornerstone of Kalexsyn's business. "We each had over a decade of experience working with CROs while at Pharmacia, so we knew firsthand that many companies fail to deliver in this area," Zimmermann attested.

Experience with a pilot electronic notebook project at Pharmacia had convinced Kalexsyn's founders that paper-based methods were time-limited. "Technological sophistication in the lab has progressed remarkably in the last 20 years, yet scientists still embrace a record-keeping technology that was used by Leonardo da Vinci," Zimmermann noted. "We had no doubt that the future was ELN."

The question for Zimmermann and Gadwood, therefore, wasn't whether to implement an ELN at Kalexsyn, but which one to pick. Kalexsyn's initial choice was "functional," according to Zimmermann, but had a format and organization that didn't always mesh with how scientists wanted to work. Dissatisfaction with the first system led Kalexsyn to engage Symyx and implement an early version of Symyx Notebook in 2004.

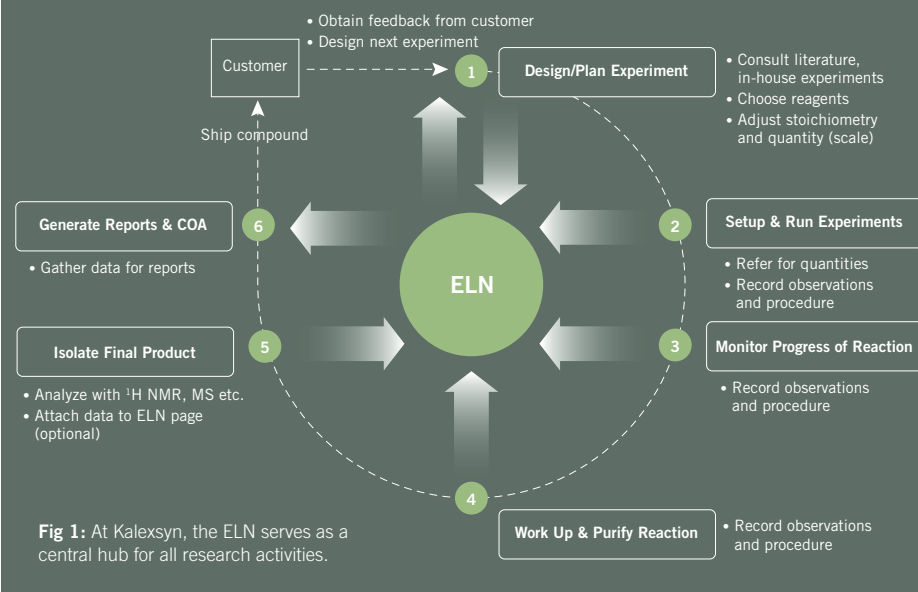
"We realized from the beginning that no software package would be perfect, though we have found the Symyx ELN to be more efficient than our first ELN selection," Zimmermann said. "More important to us was finding a partner that could benefit from our years of pharma experience, listen to our suggestions, and, where appropriate, implement those ideas. Symyx has been that partner—we've not only experienced improved customer support and service, but found a vendor that shares our vision for ELNs."

ELN CENTRALIZES DATA ACROSS THE RESEARCH WORKFLOW

Kalexsyn's ELN serves as the central cheminformatics hub for

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all research activities at Kalexsyn. Scientists use the ELN to record individual research, collaborate with colleagues on projects, and share critical weekly updates and experimental results with clients (see Fig 1). Obviously, projects vary in scope and complexity, ranging from one to two months for a custom synthesis project to several years for a comprehensive structure-activity relationship study. "What's great about the Symyx ELN is that there are no restrictions placed on experimental design," explained Becky Gross, operations manager at Kalexsyn. "We can choose the most efficient protocol for the project, and the ELN adapts to the workflow rather than constraining us to a work process dictated by the software."

The ELN assists at every stage of a project, according to Gross. At the start of a project Kalexsyn scientists can use the ELN to search external chemistry literature and

Kalexsyn's internal archives to design appropriate synthetic routes to targets. The ELN allows a variety of searches, including substructure or keyword searches, and Zimmermann noted that these searches can be for specific materials or methods or for experts to consult. "With the notebook, our scientists can identify who to talk to about a specific synthesis or technology by using the ELN to determine who at Kalexsyn has done the most of those types of reactions," he said (see Fig 2, next page).

Experimental setup is also less onerous electronically. Gross pointed out that the ELN contains a large database of reagents and solvents along with physical data, which scientists can consult as they plan syntheses. And unlike with paper notebooks, ELNs enable scientists to clone experiments, which can be particularly helpful in modifying or optimizing reactions or scaling up a



Fig 2: Kalexsyn scientists Jill Northuis and Tom Belliotti consult about an experiment.

“WORKING ELECTRONICALLY CONSTITUTES A TIME SAVINGS THAT EQUATES TO SAVINGS OF THOUSANDS OF DOLLARS PER YEAR BY PROVIDING EFFICIENCY IN OUR WORKFLOW.”

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synthesis. “It’s easy for scientists to simply cut and paste elements already in the notebook into their plan,” said Gross. “Additionally, stoichiometry and other standard calculations are handled automatically by the notebook, which not only saves scientists time, but reduces experimental errors.”

Perhaps most importantly, the ELN assists with reporting experimental progress to Kalexsyn’s clients. As part of Kalexsyn’s commitment to transparent communication, project teams provide clients with weekly status updates. Gross explained that the ELN has been set up to automatically generate reports, but that most scientists simply cut and paste electronic data into another document to create a report. She noted as well that while the ability to cut and paste has significantly streamlined report creation, the organization of the electronic system has also helped. With paper systems (and even other ELNs), an experimental plan might be described on one page while the data generated from each analytical test might be stored on other, separate pages. In the Symyx ELN, scientists can associate analytical data directly with the experiment that generated it, which saves scientists time tracking down results.

MEASURING ROI IN INCREASED PRODUCTIVITY AND EFFICIENCY

Zimmermann noted that when speaking to colleagues about implementing ELNs, many balk at the initial costs associated with implementation. But he is adamant that an analysis of efficiency and time savings justifies the initial investment.

For instance, Gross pointed out that ELN speeds data entry across the board. “Nearly all our chemists type more quickly than they write,” she said, noting as well that cutting and pasting provides the ability to recreate and modify text in seconds. Faster data entry has another added benefit—scientists tend to provide more detail in their entries.

Overall, Zimmermann has found that the ELN helps Kalexsyn demonstrate consistency in its client communications. “Everyone knows that some scientists do a better job of maintaining a lab notebook than others,” Zimmermann said. “Our ELN levels the playing field and provides standards to ensure we’re keeping complete and consistent documentation on every project.”

Zimmermann estimated that because of the ELN, Kalexsyn’s scientists spend 25% less time on data entry,

which enables them to focus more energy on research. And by being more efficient and productive researchers, Kalexsyn passes those savings on to its clients. “Working electronically constitutes a time savings that equates to savings of thousands of dollars per year by providing efficiency in our workflow,” Zimmermann said.

Zimmermann anticipates that it’s only a matter of time before the majority of pharma and biotech companies have implemented ELNs. “We look forward to seeing a larger number of companies embracing this technology,” Zimmermann said. Zimmermann is confident that more ubiquitous use of ELNs will enable CROs like Kalexsyn to practice even greater collaboration with clients.

“We’d like to see true portability between systems, so that our clients can have real-time access to the work we’re doing for them, and so that they can take what we provide and use it directly at their site,” said Zimmermann. “With that capability, the ELN would become a valuable mechanism to help organizations monitor progress within the CRO.” 