Are ELNs Really Notebooks?

The new generation of electronic laboratory notebooks offers tools for collaboration, productivity enhancement and data protection

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For hundreds of years, scientists have painstakingly journaled experimental results into paper laboratory notebooks. This often-tedious process has been vital to scientific invention and intellectual property protection. Paper works — it's a medium that is easy to use, doesn't require much training and is ingrained in our culture. However, in the modern age of research teams and multi-site R&D centers, the traditional paper notebook is fundamentally flawed in the ability to share and manage data. Knowledge is lost to the filing cabinet. Experiments that previously failed are doomed to be repeated again.

To create a "paperless" laboratory, attempts were made in the 1990s to develop electronic versions of traditional notebooks. For the most part, these systems were market failures. Why? Maybe they were ahead of their time or the computing technology wasn't yet available. Or, maybe the reason was that they were just that — attempts to replace paper. These early market systems did not address the real collaborative shortcomings of paper.

Scientists often felt that the burden of using them outweighed any benefits.

Today, there is a "rebirth" of the electronic laboratory notebook (ELN) market. New systems are emerging that offer new tools for collaboration, productivity enhancement and data protection. There also is a renewed demand from the market, as companies look to reduce the time to market for new compounds and increase scientific effectiveness. This new generation is not just an attempt to reduce paper. The ELN of today is about the *usage* of data and information and the creation of a *knowledge repository.*

What is an ELN?

Like a famous person once said, "it depends on what your definition of is, is." You can ask 10 people "What is an ELN?" and there is a good chance you will get 10 different answers.

This is for good reason. An ELN can have a different definition depending on the environment in which it will be used. An ELN for drug discovery is much different than an ELN used in quality assurance. One is targeted at intellectual property protection and collaboration, while the other is for compliance and traceability. An R&D director of a major pharmaceutical company describes their ELN as: "A secure system that assembles content from multiple sources that are related to each other, allows for textual annotation, and packages it in a legally acceptable document which can be searched, mined and collaborated." *Whew!*

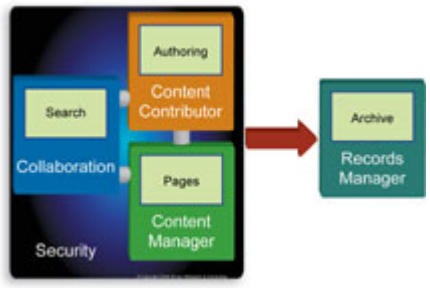

Figure 1: The basic components of an ELN

There are, however, common components to an ELN regardless of where it will be used. These components allow for content creation, management and collaboration, all of which are "wrapped" in a common security layer. The security layer restricts access to intellectual property and assigns privileges and roles to users. For legal reasons, most companies still print final ELN R&D data to paper and store it remotely, although this trend is slowly changing toward a fully electronic archive. Major ELN components include the following:

• **Content Contributor:** creates the ELN content. Usually, this is a journal entry authoring tool with text entry, templates, electronic signatures, witnessing and data importation. However, in more chemistry-oriented systems, the authoring tool is often tightly coupled with specific applications, such as modules for synthesis, formulation or reaction chemistry.

• **Content Manager:** provides the management of contributed content and has bi-directional communication with contributors. Most often this is a relational database, but it also can be several integrated data management systems. For example, documents can be stored in a document management system, instrument data in a scientific data management system, compound data in a registration database, and so forth. Data from these multiple sources are gathered and assembled into an ELN document.

• **Content Collaboration:** A basic requirement of an ELN is the ability to search and locate information such as text, molecular structures or publications. Workflow management is an important aspect, as manual processes can be highly automated. Tools for sharing and commenting on results, discussion groups, common workspaces and portals take an ELN far beyond being the replacement for a paper notebook.

Beyond the paper replacement

Many of the larger life sciences companies are taking an enterprise view of a Research ELN (RELN). This is a broader electronic R&D vision that is synonymous with frequently used terms such as digital R&D, eR&D, collaborative R&D, and so forth. Here, the ELN has specific tools for functional areas, such as medicinal or process chemistry, that are integrated into a R&D-wide collaborative framework. Generic authoring tools are provided for areas with less-defined processes, such as biology. This vision imagines a common user interface, IT-friendly backend architecture, and authoring module tightly coupled with biology and chemistry-specific tools. Today, this is only a vision, as companies are faced with an integration challenge of implementing multiple vendor offerings with no supported standards for system interoperability.

Vendor Offerings

As ELN budgets and the interest of end-user companies have grown over the last two years, there has been an increase in the number of vendor-developed ELN products. The

approaches and the strategies differ, but there are two categories of systems on the market: nonspecific and specific.

Nonspecific ELNs are systems designed with a backend content management architecture, generic content authoring, searching, collaboration and security which can be used across many markets such as pharmaceutical, food, academic, packaged goods and specialty chemicals. The philosophy of a nonspecific ELN is summarized by Steven Arpie, director at NoteBookMaker who said, "The more complicated you make the plumbing, the easier it is to clog the drain." These systems are designed to be used by chemists, biologists, engineers, material scientists, and so forth. As these systems mature, look for a few of the nonspecific ELN vendors to add more application-focused modules targeted to the needs of end users. Nonspecific ELN vendors include CambridgeSoft, GenSys, Kalabie, LABTrack, NoteBookMaker and Waters.

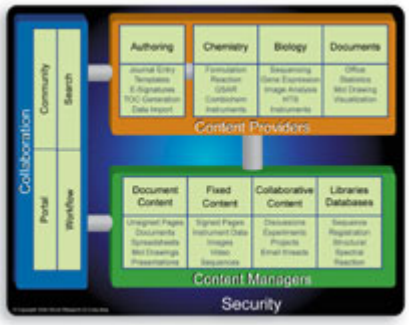

Figure 2: An R&D-wide ELN view with example components

In the past few months, Waters has been making significant investments by expanding their information management portfolio with acquisitions of Creon Lab Control, which is developing an ELN for content creation and collaboration, and NuGenesis Technologies, the market leader in scientific data management (SDMS). Waters' strategy is to provide ELN solutions integrated with applications such as their SDMS, Empower CDS, and MassLynx LC-MS software for life science and industrial analytical organizations.

CambridgeSoft, a longstanding leader in desktop systems for chemistry, provides a notebook solution from a single CPU to an enterprise-wide deployment. Their generic authoring tool also has been integrated with their structural analysis products to make the system "chemistry aware." According to Joshua Bond, CambridgeSoft ELN projects manager, they are often asked to integrate their enterprise ELN with other systems, such as registration databases.

GenSys focuses on enterprise deployments, emphasizing their architecture, search, authoring tool and template capabilities. GenSys has developed a robust API to integrate with application specific systems.

Specific ELNs are systems that are very feature-rich in one or more functional areas, such as reaction chemistry or compliance. These are targeted at enhancing the productivity of the scientist but are not sufficiently generic enough to be used across multiple markets. Generally, these systems are targeted at the life sciences market. Specific ELN vendors include Cheminnovation, DeltaSoft, Ingenovis, IntelliChem, MDL, Rescentris, Synthematix, Tripos and VelQuest. For example, VelQuest has developed their ELN around a method execution engine for GXP and 21 CFR Part 11 compliance in late-stage development and QA/QC. MDL and Tripos develop custom ELNs based on their existing chemistry and biology tools. Look for several of these vendors to branch out across

multiple application areas to develop a more enterprise-wide platform.

Synthematix and IntelliChem are two companies that have a strategy to move into multiple application areas. Synthematix, which has an ELN offering targeted at discovery chemistry, has plans to develop additional applications. Tom Laundon, COO of Synthematix, says that their "vision is to have scientific domain expertise in every segment we serve. Our strategy is that we must understand and support each area of application in depth, and then expand from there." IntelliChem, which started out in process chemistry, has developed additional applications for analytical, bioprocess and medicinal chemistry. Matt Wallach, vice president for marketing and product management at IntelliChem said, "Our strategy is to have an underlying platform, which is very broad, and to create best-in-class applications in every single area."

Laboratory data is growing exponentially and available ELN systems offer the ability to manage it and to create a searchable knowledge repository. As Pat Martell, director of informatics marketing at Waters put it, "The issue is not data generation. The challenge is accessing the appropriate data collected, analyzing, visualizing and having the appropriate tools to turn that data into useful knowledge." The tools are here and the time has arrived to finally put away those paper notebooks.

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