

THE ENTERPRISE LAB NOTEBOOK

Leverage the enterprise ELN to optimize the capture and reuse of information, protect intellectual property, streamline laboratory workflows, enhance partnerships, and accelerate the productivity of virtual teams.

By Trevor Heritage, Ph.D., President, Symyx Software

The scientific R&D landscape is undergoing historic changes. Driven by globalization, demands to do more with less and the constant need to demonstrate return on investment, scientists are under tremendous pressure to increase efficiency and improve productivity not only at the experimental level but across the organization. Along with this pressure, scientists are faced with numerous challenges resulting from industry outsourcing and increasing company consolidation driven by mergers and acquisitions. As organizations expand partnerships, extend into different geographical regions, and outsource projects to contract research organizations (CROs), the number of globally dispersed “virtual teams” increases—as does the likelihood of workflow communication and information-sharing breakdowns. Combine these challenges with the pressure to deliver breakthrough results at lower cost and we find ourselves in an environment where scientists require new informatics and workflow solutions that help them work together more effectively and be more productive.

“By centrally and consistently capturing scientific information, an enterprise notebook fosters workflow optimization, process consistency, collaboration, and improved productivity through knowledge sharing.”

- Trevor Heritage

Over the last decade, electronic lab notebooks (ELNs) have emerged as one of the primary scientific informatics solutions for helping scientists design, execute, analyze, and report on experiments in a more efficient and secure manner. ELNs help scientists focus on science rather than documentation. They also enable scientists to share experimental results, orchestrate workflows, and learn from the knowledge of others to improve experimental throughput and results.



Figure 1: An enterprise electronic lab notebook fosters improved collaboration and decision making within and across project teams, including contract research organizations.

Domain-specific ELNs like those used specifically in discovery, process, or formulations chemistry create silos of information that are difficult to manage, access, contrast, and compare. More and more, scientists in pharmaceuticals, biotechnology, chemicals, and consumer products are

demanding a single, enterprise lab notebook that works the way they do and helps them collaborate more effectively with colleagues in other disciplines, laboratories, and partnering organizations.

Symyx Notebook: An Enterprise ELN

Symyx Notebook is a single, flexible, multi-disciplinary ELN that can be used internally across the enterprise or worldwide across business ventures. By offering a centralized data repository and infrastructure for capturing, accessing, and sharing experimental information while also supporting the diverse needs of different disciplines without extensive customization, Symyx Notebook makes it possible for scientists to collaborate effectively on multi-stage projects while simultaneously building upon the successful methodologies and collective results of others. Customizable workflows complemented with fine-grained security enable scientists in different organizations to drive workflows more effectively by coordinating and reviewing experiments in the virtual team. Symyx Notebook's flexible, highly configurable, and secure infrastructure significantly increases organizational agility, enabling R&D organizations to adjust resources dynamically, collaborate effectively with global partners and CROs, and accomplish more with less in today's challenging R&D environment.

An enterprise notebook for improved collaboration

A single notebook deployed across the enterprise can be used across multiple scientific disciplines, as well as across the entire R&D spectrum—from early discovery to late-phase development, and on into early manufacturing. By centrally and consistently capturing scientific information, an enterprise notebook fosters improved productivity by enabling different disciplines within an organization to learn from others within the organization. To enable information re-use, both the information and the process used to capture the information across the organization, must be consistent. An enterprise ELN drives this consistency while also ensuring minimal delays in transferring information to the next step in the R&D process.

An enterprise ELN facilitates collaboration with CROs and partners by supporting:

- Workflow coordination across geographic and business boundaries

- Authoring of experiments by multiple scientists
- Data capture and data access across the globe and between business networks
- Secure control of read/write access at experiment and experiment section levels
- Regulated and unregulated lab documentation procedures, as appropriate

Building virtual research teams

The challenges involved in successfully integrating CRO and partnering scientists into a virtual global research team are significantly lessened when the outsourcing organization extends and leverages its own ELN into the CRO. Virtual research teams work best when there is operational transparency between the outsourcing organization and the CRO or partner. This means outsourcing organizations should engage CROs in long-term partnerships, get them involved early in the R&D process, and establish clear protocols for exchanging information and materials through work requests and tasks that are built and managed using the shared ELN infrastructure. Such engagement and partnership streamlines the exchange of information, activities, and materials, enabling scientists at both locations to respond with agility to changing experimental conditions and requirements because they are sharing consistent experimental procedures, processes, and results in real time. Embracing such informatics partnerships today will ensure that scientists gain full advantage from the considerable gains made within R&D informatics over the past 20 years in consolidating, capturing, and making information re-usable.

Effective CRO/partnership enablement requires an informatics infrastructure that can be “turned on” to enable CRO collaboration and then shut down at the end of the engagement, one that ideally requires a minimal footprint within the CRO. This approach helps the CRO, which gains advanced scientific informatics technology and access to information for more efficient research without the burden of added infrastructure costs. The approach also benefits the outsourcing organization, which gains the ability to select different CRO partners depending on its research needs and the centers of excellence it wishes to employ. Outsourcing organizations need the flexibility to

collaborate with best-in-class CROs that can shorten the path to a more robust, promising pipeline.

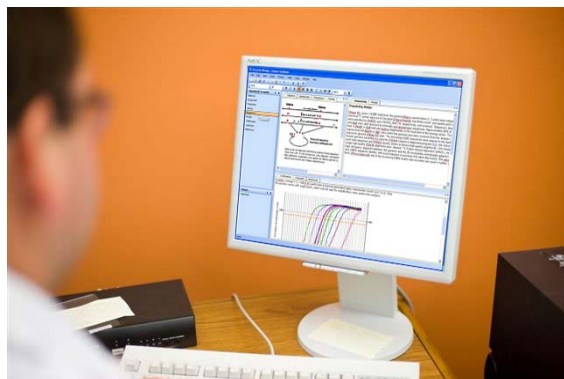


Figure 2: The enterprise ELN supports rapid experiment design, execution, analysis, and reporting, as well as real-time data access and sharing.

Integrated global workflows and data access

A single, globally deployed, enterprise ELN streamlines the exchange of information, activities, and materials with multidisciplinary CRO scientists. The following simple example illustrates how the enterprise ELN enables secure, authorized workflows while also minimizing information exchange delays from data capture through analysis and reporting.

In this scenario, scientists at the outsourcing organization initiate an experiment and clone it into the CRO repository after clearing out any proprietary information that is not appropriate for the CRO scientists to see. A synthesis request can be created using ELN messaging or a document workflow, enabling the CRO scientists to access the experiment directly from their inbox. The CRO scientists check out the experiment, execute the reaction, and record the procedure. The CRO scientists can access any section of the experiment and add new sections during editing to capture relevant analytical data as needed; meanwhile, scientists at the requesting organization can monitor progress at the CRO.

When the experiment is complete, the CRO scientists check it back into the CRO repository and route it back to the requesters. The experimental protocol enables the scientists at the outsourcing organization to mark the CRO

experiment as complete and remove the CRO scientists' permissions to the experiment, thereby protecting intellectual property. The outsourcing scientists can then take advantage of configurable reporting templates to create and distribute required reports supporting project team collaboration. The result is efficient scheduling and notification, real-time access to results, and instant feedback and adjustments—leading to increased results, decreased costs, and improved efficiency.

Centralized data storage and security

Deploying a single, enterprise ELN benefits globally dispersed partnering teams by maximizing IP capture, reducing infrastructure costs, and simplifying deployment, maintenance and management costs. The outsourcing organization defines consistent business rules for managing experimental protocols and data capture and deploys the resulting experiment templates to the CRO via a central server. The outsourcing organization then has the freedom to push additional projects to the CRO with the assurance that they will be carried out in a consistent manner. On the other side of the virtual divide, the CRO always has instant access to the latest templates without having to waste time with costly, time-consuming software reinstallations. In addition, the CRO can depend on the secure infrastructure of the outsourcing partner.

ELN cost and maintenance are critical issues for most CROs, which typically function with reduced operating margins and lean IT resources. CRO desktop installations utilizing a virtual desktop emulation environment such as Citrix® server can minimize deployment and ongoing support costs for both CROs and their outsourcing partners. Cost savings are realized as a result of less hardware, fewer software licenses, and reduced administrative staff across facilities worldwide. A virtual desktop emulation environment also facilitates remote access where bandwidth is limited, as the emulation environment transmits screens/keystrokes instead of data files. More importantly, this configuration enables outsourcing organizations to maintain their intellectual property at the corporate location and provide as-needed access to CROs.

Implementing appropriate security details is another essential requirement when deploying an enterprise ELN to a CRO site. The enterprise

ELN must enable operation in a 21-CFR Part 11 compliant environment that supports electronic signatures, good laboratory practices, and audit trails with secure document versioning. The ELN security model must also be capable of restricting CRO scientists to only appropriate repositories and folders. For example, outsourcing scientists may have permission to view all corporate repositories including the CRO repository, while CRO scientists can only access repositories associated with specific contract research projects. Such fine-grained security restricts projects, experiments, and field-level data to appropriate eyes, once again protecting critical intellectual property.

Boosting decision support in virtual teams

To further facilitate better collaboration within and between virtual teams, companies can integrate the ELN with advanced data access, analysis, and decision-support software like Symyx ISENTRIS. This enables scientists to leverage corporate, commercial, and local database information in a self-service research environment. As well as helping virtual teams manage unstructured data better (i.e., the files, documents, reports, etc. that make up approximately 80 percent of the information that passes between researchers), systems like ISENTRIS also provide access to structured data—the remaining 20 percent of lab information that is captured, stored, and retrievable in software applications like inventory systems, data warehouses, registration systems, laboratory information management systems, and chromatography data systems. By enabling

researchers to build better queries, filter data more quickly, sort results more effectively, and compare/contrast information across the enterprise, ISENTRIS helps research teams drive more quickly and easily to smarter decisions.

As R&D organizations accelerate the pace and extent to which they partner and outsource R&D operations, their primary strategic issue is how to increase productivity, not just to reduce costs or offload work. An enterprise ELN offers the opportunity to reinvent and streamline outsourcing relationships and make global partnerships more productive. When coupled with an effective decision support solution, such an ELN enables virtual research teams to share information efficiently, communicate effectively, and, most importantly, work off the same virtual page. ■

Trevor Heritage joined Symyx in 2007 as a result of Symyx Technologies' acquisition of MDL Information Systems, where he was serving as chief scientific officer and senior vice president of software product management and strategy. Previously, Dr. Heritage was senior vice president, corporate officer and general manager of Tripos Inc.'s discovery informatics and software consulting services business. He has a Ph.D. in organic chemistry from the University of Reading, England.

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