

# The Right LIMS Delivery Method

By J. Thomas Kent

Until recently, a commercial Laboratory Information Management System (LIMS) was beyond the reach of most small and medium-sized labs. So labs often resort to “home-grown” solutions to save costs—only to find they’ve spent 2-10 times as much as a comparable commercial LIMS would cost. A number of commercial LIMS vendors are now offering “hosted”, “rented”, “SaaS-based”, or “in-the-cloud” LIMS aimed directly at small to medium-sized labs. While the vendors make these products sound appealing, it is often difficult to read between the lines of vendor advertisements to determine the precise features, functionality and benefits—as well as the differences among the various offerings.

## COMMENTARY

### Many Options

**Purchased commercial LIMS** are, in general, large, complex, feature-rich products that were designed to be sold to large labs for in-house deployment. The lab purchases licenses for the LIMS software, and also buys the servers, storage devices, peripherals, and other software licenses (such as databases, load balancers, backup software, etc.). The lab installs the software in a test environment, performs a thorough evaluation, and often pays hefty fees for the vendor or another professional services group to perform customization. Once in production, the software is updated and patched, and hardware is maintained, as needed. Most small and medium-sized labs cannot afford this expense.

**Rented commercial LIMS** represents an effort by LIMS vendors to appeal to small and medium-sized labs. A rental approach is almost identical to the above purchased approach, except that the lab rents the software rather than purchasing the license outright. All the other purchases—hardware and additional software—remain the same, as do

other costs (testing, customization, updating and maintenance). The major difference is a staged payment for the software.

**Hosted LIMS** is a commercial LIMS provided to customers in a different way. Rather than requiring the customer to purchase hardware and software, the customer simply uses the software that is running at the vendor’s site. The vendor will have built a front-end to the product that allows the lab to connect to the software through the Internet and run the product. In general, hosted software providers do not rewrite their products to take advantage of new, Internet-based technologies, but simply put a different front-end onto what is often a very old technology base. In addition, the provider often must create a unique instance of the underlying product and infrastructure for each user organization. This can represent either a slight increase in cost to the vendor, or a financial nightmare for customers. Each instance of the software requires its own hardware infrastructure, and the services burden is even greater. Imagine trying to upgrade dozens or even hundreds of instances of software and hardware without causing massive user disruption and trying to synchronize versions for all the different customers.

**“In-the-cloud”/Software-as-a-Service (SaaS)** is a relatively new software delivery model for deploying business services on-demand, in a cost-effective manner. While it bears some resemblance to a hosted model, there are very specific requirements. True SaaS-based offerings are usually built from the ground up to take advantage of service-oriented architecture, Web 2.0, and other relevant technologies that are designed to deliver sophisticated capabilities on-demand. SaaS offerings are built for multi-tenancy, where only a single instance of the application is required, with a single database that can manage the data for multiple customers, while keeping customer instance data separate from all other customers. Done correctly, this model provides

security, confidentiality, and brings excellent economies of scale, since the vendor does not need a massive investment in hardware and services to provide the latest version of the product. For this reason, true SaaS vendors can often sell services at a lower cost than traditional vendors. And SaaS offerings often embrace the idea of an online community where users can share best practices, collaborate, and easily purchase third-party software to meet their emerging needs.

### What’s Best for Small Labs

There is no one-size-fits-all approach to LIMS, but budgetary and resource pressures often preclude purchasing or renting a LIMS solution. Labs are looking for vendors who will deliver robust LIMS solutions in a less expensive manner. Today, we are seeing several LIMS vendors who provide solutions based on either the hosted or SaaS approaches defined above (including Sciformatix, Bika, LabLynx, and Promium).

The advantage of such LIMS is that, if designed properly, they can provide superb capabilities at a fraction of the cost of purchased or rented systems. And they can, if built on new technologies, provide improved ease of use, robust reporting and compliance capabilities, 24x7 availability, easy upgrades, and access to a community of users who can enhance the LIMS over time.

Whenever a new idea such as SaaS arises, many traditional suppliers adopt the terminology without making the necessary changes in products, services, or delivery mechanisms. It is very difficult to retrofit SaaS into a product that was built ten or 20 years ago. It takes domain expertise, technology skills, and time. Lab managers should be careful to separate fact from marketing hype in making such a critical decision.

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**SYMYX**

## Operational agility and productivity with an enterprise Notebook

Recent industry reports indicate that many pharmaceutical and biotech organizations are in the market for a single, enterprise electronic laboratory notebook. And with good reason. A single notebook fosters workflow optimization, process consistency, collaboration, and improved productivity through knowledge sharing. A single notebook deployed across the enterprise also solves many of the information challenges within R&D, including data silos, information access bottlenecks, inconsistent data, and high costs of ownership.

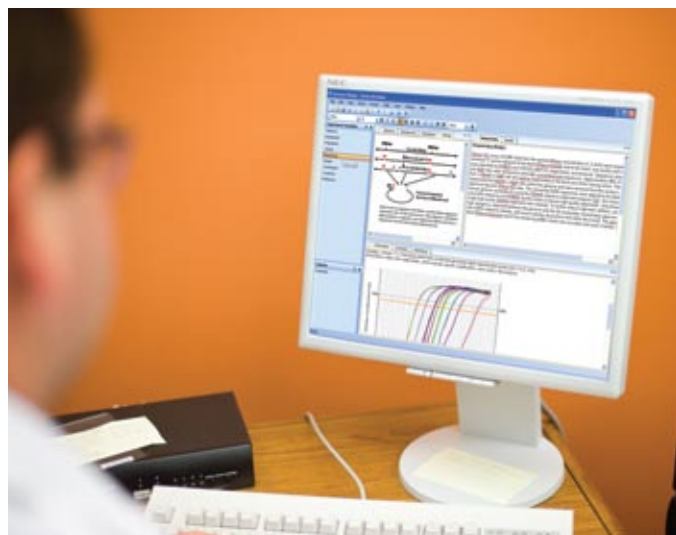
With the acquisition of MDL, IntelliChem, and Synthematix, Symyx's experience in delivering scientific Notebooks extends over 15 years with some of our earliest notebooks delivered using ISIS technology (formerly owned by MDL). In the last few years there has been a shift in our customers' notebook goals. Where individual disciplines previously had independent notebook strategies, these are now consolidating into a single, multi-disciplinary, enterprise notebook approach. Benefits realized by a unified notebook include:

- Consistent and comparable processes
- Centralized and accessible data
- Improved data consistency
- Agility for scientists to move between projects
- Lower cost of ownership
- Streamlined regulatory compliance
- Configurability to support the diverse needs of different domains without requiring extensive customizations with long-term cost of ownership implications
- Ability to deploy in regulated and non-regulated environments without requiring non-regulated departments to bear regulated compliance burdens
- Straightforward extensibility of core functionality using modern architectures and programming languages that foster easy integration
- Global deployment with a centralized data repository and infrastructure where all data can be readily accessed and shared

Furthermore, investments in global enterprises and contract research organizations are calling for added support of a single notebook that can be used worldwide across business ventures. Working with customers, Symyx has been quick to respond to the new strategies, releasing Symyx Notebook in 2008 to address the following core challenges faced by traditional electronic notebooks:

- Customizable workflows complimented with fine-grained security enabling individual parts of an experiment to be carried out by many individuals across different organizations

With the deployment of our enterprise notebook, Symyx is seeing a shift in the way scientists interact with their traditional desktop software and laboratory equipment. The notebook is becoming the hub of the scientist's day, the place where one orchestrates the design, execution, analysis, and reporting of experiments. Driving research



**An enterprise electronic lab notebook streamlines the capture of chemical and biological information in regulated and non-regulated environments.**

from the notebook makes it a priority to also integrate best-of-breed tools, information, and software into the notebook.

### Accessing content in context

The electronic notebook changes the way scientists interact with information. Not only is the data captured by the notebook fully searchable within and across experiments but third-party information is automatically built into the scientist's workflow. Without leaving their notebook, for example, scientists can look for commercial compounds or known synthesis pathways and populate the experiment details. As scientists enter molecules they are automatically informed about in-house and commercial availability.

### Integrating with other workflow/ lab automation solutions

The electronic notebook is ideally positioned to facilitate integration with existing workflows, apparatus, software, and colleagues. Common integration points include:

- Mettler-Toledo and Sartorius balances, enabling scientists to retrieve calibration information and record actual amounts directly from balances
- Chromatography Data Software (CDS) such as Waters Empower
- Data repositories such as Waters NuGenesis Scientific Data Management System (SDMS)
- Microsoft Excel spreadsheets
- Statistical analysis software such as SAS JMP
- Kinetic modeling software such as Pharsight WinNonlin

### Enhancing the value of notebook information

Sir Isaac Newton said “If I have seen farther than others, it is because I was standing on the shoulders of giants.” The ability to use and re-use the knowledge of others is critical in improving experimental success. A key focus of the Symyx notebook strategy is addressing existing notebook shortfalls for accessing notebook data. As well as supporting full text searching within and across experiments, including searching image annotations, it is also important to offer scientists extensive molecule and reaction searching techniques that include the ability to search reaction centers for transformations.

### Chemistry excellence

A key request from customers has been to integrate Symyx chemistry into the notebook, enabling both scalability and comprehensive searching. Symyx chemistry is the most widely adopted and proven chemistry in the industry. Symyx’s online DiscoveryGate application is powered by Symyx chemistry enabling thousands of researchers to query commercial bioavailability, synthesis, and sourcing databases containing over 30 million molecules and 17 million reactions. Taking the value of notebook information to a



**An enterprise electronic lab notebook fosters improved collaboration and decision making within and across project teams.**

new level, Symyx Isentris® decision support software enables scientists to search over both in-house data and commercially available data. For example, the Symyx reaction databases provide access to over 7 million chemical reactions. These reactions can be combined with in-house reactions captured through the notebook and accessed through a single search in Isentris.

To summarize, the electronic notebook is entering a new era. R&D organizations are looking for improved productivity and greater operational agility—the ability to do more with less. Today’s enterprise notebook strategies are raising the bar for notebook vendors, driving us to deliver software that streamlines scientific workflows and fully leverages our customers’ valuable intellectual property across disciplines, departments, and collaborating organizations.



**For more information on Symyx notebooks, visit [www.symyx.com/notebook6](http://www.symyx.com/notebook6)**

**“Customers are realizing significant efficiency improvements and cost reductions by cloning experiments, using pre-defined data entry forms, and storing frequently used procedures electronically. Scientists using our notebook have estimated a 20% increase in productivity simply by streamlining data input.”**

— Cheryl Lund Ph.D.,  
analytical notebook  
product manager at Symyx

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## GENOLOGICS

# LIMS to Enable Translational Research

### Q: What are the major challenges faced in translational research?

**JD:** Translational research holds huge promise to drive the advancement of molecular-based diagnostics, and enable early disease detection and personalized medicine. But, the very essence of translational research, being highly collaborative, multi-disciplinary, translating insights and results from one domain to another, creates many “systems” type challenges for research organizations. Many translational research efforts are taking scientific discoveries and applying them to a clinical context, for example, biomarker validation studies. This means higher specimen counts versus typical discovery experiments. It means clinical data must be integrated from many sources and marshaled into the research domain. It often involves many collection sites, biorepositories, core technology labs and instruments generating large data sets across sciences and institutions.

For example, it's becoming more common for large pharmaceutical companies to collaborate with academic medical centers for specimen, expertise and technology access, as well as for institutes working together in a highly collaborative manner such as under the CTSA program. All the people, expertise, specimens and instruments are available, but there are enormous logistical challenges of study and specimen management across an enterprise and challenges with data integration – both clinical and research data – and integrating data from different technology systems. Really, the missing component is integrative translational research informatics.

### Q: So how would you define translational research informatics?

**JD:** It took GenoLogics a while to define



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and figure out the bounds of Translational Research Informatics (TRI), as it fills the gap between patient care and clinical trial systems, and what many are now calling translational bioinformatics. Translational Research Informatics is the integrated end-to-end solution that provides: study management; electronic patient questionnaires; clinical information aggregation for research purposes; federated biorepository management; LIMS purposed for analytical and core technology labs; genomics, proteomics and other sciences data management; and traceability, data integration and marshalling for analytics.

### Q: What are the trends for LIMS within translational research?

**JD:** The requirements for LIMS in the translational research and systems biology

space are fairly different from laboratories in other domains. LIMS have been utilized for process chemical, petrochemical, food and beverage, materials testing, and many other procedural oriented areas for many years. But it's only been since roughly 2000 that life sciences research laboratories have been at sufficient scale to require LIMS solutions.

LIMS for translational research require something quite unique and different than traditional LIMS. A successful life sciences research LIMS requires a far higher degree of flexibility, configurability, deep instrument integration, science data integration, bioinformatics tools and algorithm automation, collaboration, and open data access. Only by focusing exclusively on life sciences and translational research, by providing a highly flexible, configurable and usable LIMS platform, by forming tight business and technical relationships with leading instrumentation providers and by building seamless integrations to genomics, proteomics, and other instrumentation, can a LIMS provide real value for life scientists.

### Q: What are the trends for data integration within translational research?

**JD:** To flourish, translational research requires a knowledge-driven ecosystem, in which constituents generate, contribute, manage and analyze data available from all parts of the landscape. The goal is a continuous feedback loop to accelerate the translation of data into knowledge. Collaboration, data sharing, data integration and standards are integral. Only by seamlessly structuring and integrating these data types will the complex and underlying causes and outcomes of diseases be revealed, and effective prevention, early detection and personalized treatments be realized.





More specifically, translational research requires investigators to have ready access to two critical types of data: (1) clinical information, including data contained in hospital systems and medical records, pathology reports and diagnostic labs, clinical trials systems, study participant questionnaires, etc. and (2) biomolecular information, including genomics, proteomics, imaging and other high-throughput molecular and cellular research data.

There are many clinical systems capturing information, many instruments generating ever increasing data volumes, and many statistical tools and algorithms available for analyzing the data, but the key bottleneck is contextual data integration from both the clinical and science domains, fused together and structured to be marshaled into analytical packages.

**Q: Can you provide some examples of organizations deploying translational research informatics?**

**JD:** Over the last couple years, we have seen a tremendous growth in the number of organizations struggling to integrate their informatics systems to achieve translational research outcomes.

We have a number of CTSA customers such as the University of Texas Health

Sciences Center-Houston that have implemented our research informatics platform to manage multiple genomics, proteomics, and other core technology laboratories. The primary focus has been on integrated data management to provision analytics, but also specimen traceability across their organization. As part of our work with the University of Texas Medical Branch on our biomedical informatics systems, we are discussing how our informatics solutions can enable translational research collaboration between both institutions.

Another example is Pfizer. As part of our global agreement to provide informatics solutions to their research groups, we are supporting Pfizer's investment in systems biology and biotherapeutics. The combination of our platform and collaborative methodology ensure we design and deploy an informatics solution that will enable their translational research and systems biology initiatives.

To connect the clinical and discovery research processes, the Fred Hutchinson Cancer Research Center pursues translational research under its Translational and Outcomes Research Group. We are provisioning the Center with a study management, clinical information integration database and biorepository management solution to sup-

## Solutions for Translational Research Informatics

GenoLogics believes informatics is the key enabler for translational research. Many of our customers have brought challenging requirements to us and overall we have been successful in providing valuable solutions for translational research informatics.

We work very closely with our customers, both with pharmaceutical and biotech companies and with academic medical centers and research universities. Many of our customers' informatics groups consider us to be an extension of their team, and we work together on an integrated solution to solve their challenges and provide value to principal investigators, study and lab managers, technicians and biostatisticians.

GenoLogics is taking an integrated and collaborative approach to solving the informatics challenges of translational research. Contact us to learn more about how our solutions for Translational Research Informatics can help your organization.

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port their translational research efforts.

There are many more groups we are working with that are conducting translational research, but they each have their own unique challenges, which is why an informatics solution must be highly flexible and configurable to seamlessly fit with each client's situation.