Managing data

LIMS implementation in drug discovery

It is estimated that it takes approximately $1.25 billion[1] and more than 10 years for the drug discovery and development process to be completed and a new drug to be brought to market. During all of this long process, from pre-clinical testing to product development and approval from the FDA (Federal Drug Administration), a wealth of data from a wide variety of bioinformatic tools are collected, integrated and analysed in order to lead to the next big discovery. This is why there are many analysts who believe that an effective Laboratory Information Management System (LIMS) to collect and manage laboratory data can save millions of dollars from the overall associated costs.

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When referring to commercial LIMS, one typically means some form of computer software application that stores and manages laboratory-specific information[2]. Because it is developed to make the most of its available storage space, a LIMS does not store every piece of raw data from every analytical run. It stores only critical decision-making and process information, which it then links back to the original data, whether it's stored on the network, an SDMS (Scientific Data Management System) or a storage system. This is mainly because a LIMS is not intended to take the place of instrument analytical software and bioinformatic systems.

LIMS types

A LIMS can vary from self-built to bought, and from application-specific to generic, the suitability of each depending on the particular application it is intended to serve.

When deciding whether to buy a LIMS or develop it in-house, there are many important factors to consider, apart from total development or buying costs: time to market, inte-

gration costs, intellectual property, competitive advantage and ongoing support. In addition, companies need to take into account their core objectives and balance them with their need for software applications. For example, a pharmaceutical company's core business remains drug discovery and not internal software development. What is more, developing a LIMS is less than half of the battle; some estimates claim that nearly 80% of software costs are incurred while maintaining the system[3].

The most encouraging factor towards the development of a home-grown solution is that the system can

be designed to perform exactly the operations required by the specific application. So, pharmaceutical companies that have adequate resources, a team of dedicated scientists and enough time to employ in-house IT experts or consultants, can develop software for their research needs. This is the case especially when the particular requirements are considerably out of line with the capabilities of existing commercial systems.

Meeting user needs, though, is not an easy task and it can be made more difficult by many factors, such as vague or evolving requirements, limited developer's skills, developer

turnover and the restricted capabilities of the development tools. Moreover, there is seldom agreement among groups of users. Finally, as hardware and software are continuously upgraded and changed, and methods and processes are constantly evolving, continuity of development staff is absolutely necessary. Even the most skilled IT developer can have trouble deciphering and fixing another programmer's code.

Using an external software supplier, on the other hand, allows customers to benefit from a vendor's long-established experience and its valuable resources. LIMS vendors employ and train highly qualified development teams that integrate intellectual property acquired over many years of practice. And they do that on behalf of many different customers across diverse disciplines in order to meet the market's varying needs. In some instances, these needs are met via application-specific LIMS, while in others they are met using generic LIMS.

Application-specific or vertical solutions are systems that are purpose-built to meet the needs of a specific laboratory segment or process. These Commercial-Off-The-Shelf (COTS) LIMS are designed to offer the benefits of collaboration, standardization, productivity and data management at early discovery stages. Out-of-the-box COTS solutions also offer regulatory compliance with much less effort than generic solutions because of their refined nature. Indeed, the amount of validation effort demanded in a certain implementation is proportional to the amount of customization and configuration of the system in question. The closer the system is to the laboratory's specific requirements out-of-the-box, the less validation effort required.

Inflexibility is a criticism of purpose-built solutions since such systems are configured to perform certain tasks only in a certain way. Researchers, though, need an information management solution that is flexible enough to meet the dynamic needs of the research and development laboratory and responsive enough to keep up with the speed at which the laboratory evolves. Consequently, application specific systems are not always suitable for laboratory segments that are constantly changing their business processes and therefore need a LIMS capable of adapting to these changes without much need for extra validation effort, development time and cost. In this light, generic LIMS have been designed, providing research laboratories with the desired flexibility to pursue knowledge in many directions.

Generic LIMS do not serve a specific purpose and are intended to be customized or configured to meet differing laboratories' needs. A configurable LIMS solution enables researchers to totally control the LIMS and also ensure that the LIMS evolves as laboratory needs evolve with little reliance on IT organizations. This does not mean that a generic LIMS lacks functionality. On the contrary, functionality is present as a standard feature of the system. The term 'generic' simply implies that the workflows are not strictly defined in the system. In fact, the system is equipped with a built-in mechanism to allow the workflow to be changed, preferably without the need for writing a custom code.

The major downside of a generic LIMS is that it often uses modules to serve specific applications. Many times these modules are simply custom-code hacked together for demonstration purposes and they lack proper documentation and support, making it difficult to implement, validate and upgrade.

The benefits offered by LIMS

The benefits offered by an information management solution vary by laboratory type. In the case of quality assurance environments, the benefits are substantial allowing products to be developed in a more efficient, effective and accurate way, while adhering to regulatory compliance. This is mainly because the process in such environments does not change frequently.

In research and discovery environments, on the other hand, this is not always the case. While there are certain processes that are consistent, such as bioanalytical and *in vitro* studies, other areas of research are rapidly evolving and require that data and experimental conditions change from experiment to experiment or even during the experiment itself. Data from these laboratories may or may not need to be validated. Decisions are made at critical points throughout various processes and it is highly beneficial to store all of the data collected and document the decisions made in the process. Traditionally, these data are captured using incompetent methods such as notebooks, spreadsheets and disparate software systems. Collaboration is dependent upon frequent meetings and phone conversations. In many cases, there is no access to previous data resulting in repetition of the same mistakes. The benefits of LIMS in the case of research and discovery environments

are significant: equipment integration, reagent, inventory management, automation, high-throughput data management, data organization, collaboration and data security.

Workshop environments

Workshops are intended to promote user involvement in the configuration process of a LIMS, thereby resulting in prototypes, which can be used in the final implementation stages. This greater involvement of clients during the implementation of an information management solution has been triggered by the increasing trend towards an intuitive and configurable software design. Integrated groups of IT experts and scientists work in a workshop environment to make the best use of standard LIMS functionality, keeping the configuration as simple and minimal as possible.

Being a flexible, easy-to-use system, a LIMS is easily configurable by researchers with only limited training. As a consequence, IT experts are less troubled with the more routine LIMS administration tasks and are free to pursue tasks that truly benefit the business. Internal resources of the organization are maximized and individual resources are allowed to focus on their distinctive talents. LIMS companies are spending more time preparing training solutions, documenting systems and developing graphical interfaces, wizards and intuitive property sheets. Proprietary languages are being replaced by, or enhanced with, configuration options within the system.

Other LIMS capabilities

In order to co-operate efficiently with other applications as part of an integrated approach, information management solutions need to be open, flexible and able communicate with these other applications. Communication is accomplished through an import/export file transfer protocol, application programming interfaces (APIs) or other services type architecture.

There are certain web services that have led specific LIMS functionality, such as sample login, update and reporting, to become more secure and easier than ever before. Reporting is now allowed to gather data horizontally across disparate databases and datasets. By allowing the integration of web services, functionality can be embedded into the customer's own existing web architecture. Clients now have the choice to integrate common user functionality in a zero-footprint architecture without abandoning the previous client–server applications and having to create a new web client with proprietary Java functionality.

Summary

Drug discovery and development industries are increasingly relying on an efficient information management system to cut costs, decrease the duration of the drug development process and consequently increase productivity. Samples in research discovery laboratories can be very complex, dynamic and integrated. What's more, they are often split, diluted and multiplexed. But no matter how complex the workflow becomes for any given set of samples, the data needs to be readily available since future actions and decisions are based on the results of the previous test or assay. Although there is no single software solution to meet the needs of every laboratory, a LIMS holds a critical role in storing, organizing and managing data.

A LIMS is either built in-house or bought from long-established LIMS vendors depending on the specific application they are destined to serve. In addition, a LIMS can be application-specific, designed for a particular laboratory niche and workflow, whereas other systems are more generic in nature and designed to be configured and/or customized to meet varying laboratory needs.

Quality-assurance environments and research and discovery laboratories have much to gain from storing and managing laboratory data within a LIMS. Increased focus on out-of-the-box functionality and intuitive applications allows systems to be implemented with integrated groups of IT experts and scientists in a workshop environment. The end result is a consistent solution integrating all of the data collected across the drug discovery process.

References

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