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IMPROVING QUALITY OF EXPERIMENTATION PROCEDURE THROUGH ELECTRONIC NOTE BOOK (ELN): A QUALITATIVE STUDY

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ABSTRACT

There is a need for digital recording of experimentation in the already highly computerized scientific laboratory work. This is especially true for molecular biology and chemical biology where ELNs are still infrequently being used to record, store, and share experimental data electronically. In this research paper we justify the need for development of an ELN by presenting issues and best practices in scientific data record keeping. We feel that in spite of this challenging undertaking in terms of technological, integration, cultural and scope challenges investments in time and money will be returned many times over. The objectives of meeting the goals set by the best practices in record keeping through the usage of an ELN are also discussed.

Keywords: *Best practices, Collaborative research, Electronic Lab, IP issues, Quality Research, Record Keeping.*

INTRODUCTION

With an increased adoption of Informatics tools, web services, public databases and other computational methods and automation tools, there has been tremendous increase in volume of collaborative research and accompanying research and experimental data (Brody, 2007). ELN is one of the most important informatics tools which are being adapted by research organizations to cope and manage the challenges of data and knowledge management (Tabard, 2008). Owning to information intensive and collaborative nature of scientific domains more specifically of biomedical research, adaption of ELN also results in productivity boost and accelerated product development (Brody, 2007). In this paper, we have focused on the issues related to research intensive disciplines more specifically for biological and chemical research which are the largest global R&D sectors (Struss et.al, 2009). The impact of adaption of ELN is

even more significant as paper note books manifest the last non-digital components in many wet and dry labs (Elliot, 2004, Polonsky et, al, 2009). The importance of computerizing and automating the record keeping of experimental procedure and data can be further reiterated further as " Atrium Research suggests that a researcher spend more than half of the time on information-intensive tasks such as meetings, literature analysis, writing papers and reports, and less on conducting experiments " (Elliot, 2004).

NEED FOR AN ELN IN SCIENTIFIC RESEARCH

Considering the growth of biological and chemical research based multibillion dollar pharmaceutical and genetics industry, we feel that it is an appropriate time to propose development of ELN so that scientists and researchers become more productive (Scharge, 2005, Michael, 2004). With a proposed transparent and smooth interface to fully map paper laboratory notebooks, it will enable easy handling of disparate and heterogeneous data that is endemic to scientific and biomedical research and will strive to offer a configurable, secure, dependable and convenient information flow organization system. It will also enable cross-sectional view of data both horizontally and vertically across organization offering classification based on projects, assays, compounds, researcher, submitter or any other classification of interest. This will offer better flexibility than ELN systems that adapt traditional knowledge management approaches and either are too flexible without any real organization or worst still are too rigid thus sacrificing and meaningful organization (Michael, 2006, Butler, 2005). This is also one of the reasons that paper note books are still being used in research community resulting in problems of information retrieval, lost data and procedures, difficulty in useful interpretation of data and collaborative research (Knight, 2003). (Phillips, 2006, Sarini et. al, 2004). A semantic tagging approach towards development of ELN will allows sufficient flexibility of data entry and will also result in a thorough organization of the recorded information (Berners-Lee, 2001, Neuman, 2005). Also the following will give our product an added advantage over other available products (At present there are only two which care worth mentioning i.e. CambridgeSoft ELN and iPad ELN):

i) A competitive price (existing solutions cost USD 2000 (5 users) to USD 55 (single user iPad application))

ii) Focus on biological and pharmaceutical industry. This may be extended to a more general product catering sectors and domains.
iii) Availability as a web service.

ELN: BEYOND A LABORATORY TOOL

With the growth of bioinformatics as an industry and the resultant increase in collaborative and multidisciplinary focus, the domain of application of Electronic Laboratory Notebook (ELN) has broadened to cater for a broad spectrum of laboratory experimentation. This is especially true in case of pharmaceutical research relating to drug discovery. Although ELN is providing services for management of data and requests, services to automate workflows in assay development etc., it has still to completely overcome the challenge of offering transparency to the scientist through integrating information both horizontally and vertically across departments. Without overcoming this challenge, it would be difficult to remove the bottleneck of manual integration and manipulation.

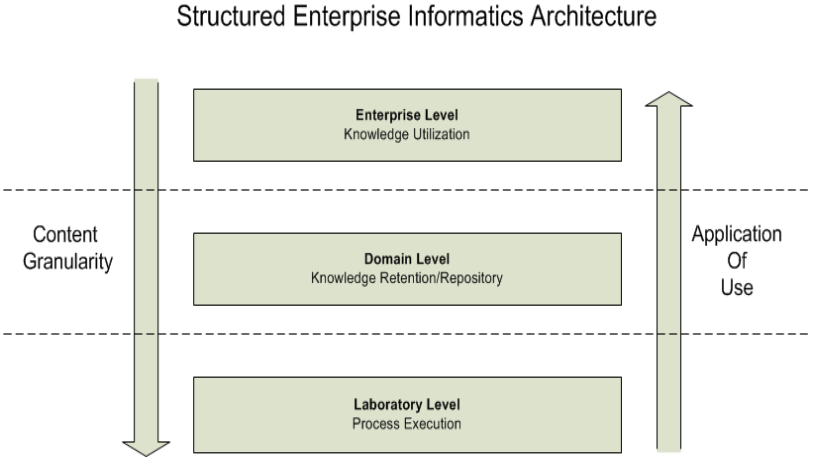

Figure 1: Structured Enterprise Informatics Model

To overcome this challenge, a Laboratory Informatics Architecture Model (Figure 1) has been suggested which may help to increase the scope of ELN from laboratory towards enterprise level, especially in R&D by accommodating the requirements of both data/information generators and consumers. Fine grained experimental data is to be maintained at laboratory level while coarse grained knowledge is provided to enterprise

level. In the proposed model, functionality is structures into three levels of granularity depending on application of use.

At the Enterprise Level, Knowledge Utilization is facilitated through the integrating middle ware. Integrating tools decipher such knowledge from the Domain Level repositories. Such tools may be data mining engines, ontological structures and tools etc. At Domain Level, project and assay centric information is integrated. This information may consist of molecular data, assay protocols and other structured or unstructured data. ELN tool at Laboratory Level facilitate experiment enactment from the stages of design to its execution.

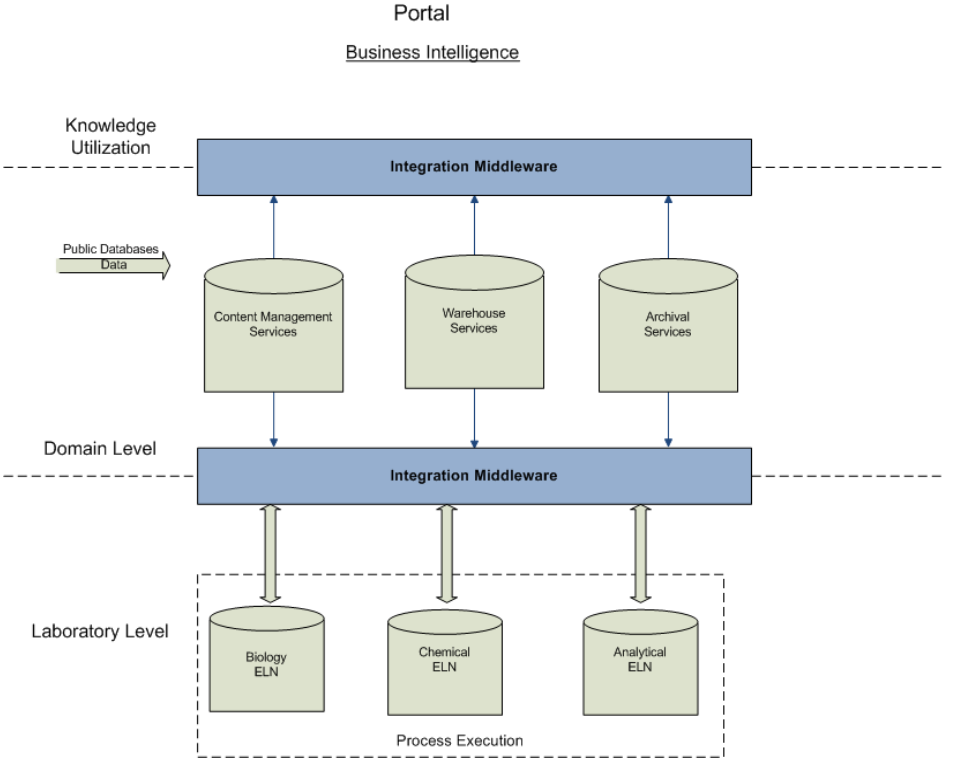

Figure 2: Drug Discovery ELN informatics Model

A specific example of drug discovery and pharmaceutical domain is shown in Figure 2. At the Laboratory Level, data is generated through various ELNs such as High Throughput Screening (HTS) data or Assay Compound Data. This data may be further tagged with project identifiers, scientist's ids, compound registries, and other such meta data that may

help in organizing it at the higher Domain Level. At Domain Level, this structured data is organized according to metatags and further enriched by annotating it with public data sources. This enriched content is then posted to Knowledge Utilization Level where it may be accessed through web portals.

ELN SUPPORT FOR RECORD KEEPING BEST PRACTICES

Successful adaption of ELN by any organization is dependent upon consideration and adaption of data management and record keeping best practices issues is bound to fail (Knight, 2003). In the next section, we describe various components of our proposed ELN, their benefits and how these components conform to the best practices.

Our proposed ELN system can meet the requirements of a research organization at various operational levels (scientific, managerial, legal etc) as described below.

i) One major goal of data management is to improve the search quality of the stored data. This includes data retrieval time and relevance of the retrieved data. A major problem is posed by retrieval of multimedia content such as pictures, graphs etc (Knight, 2003). Ease of sharing including that of experimental methods, data, analysis results and, resources used for conducting the experiment (Brody, 2007). Any data management and record keeping facility should accommodate various perspectives on the research findings thus enabling knowledge sharing across organizations. In case of an electronic lab notebook facility to store holistic experimental data which may include assay details, experimental lineage, false negatives, and results which are not of interest in immediate context along with replications and unfinished projects should be provided (Tabard, 2008). Our proposed ELN will achieve this by capturing experimental data and related information independent of data and format thus achieving transparency. This will also provide interoperability enabling collaborative research. Various data provenance methods will be employed to establish lineage and audit trail (Bondarenko, 2005).

ii) Our proposed ELN with provision of providing the facilities for both import and export of data and enabling access at multi

granular level will help achieve simplicity and straight-forwardness in data entry procedures thus reducing room for ambiguity and erroneous interpretation of results (Tabard, 2008).

iii) Owning to the evolutionary nature of scientific research and more specifically biological/chemical research, there is a need for long term archival of scientific information including research hypothesis, research papers, experimental procedures and methods and research and experimental results (Knight, 2003). This sharing of research data warrants some sort of policy to control sharing to guard against malicious and unwarranted use. This is especially true for domains such as pharmaceutical research where research results are directly transferable into monetary gains (Tabard, 2008). By supporting record retrieval and sharing over time, support for document life cycle, and by producing records that are neither delete-able nor editable our proposed ELN will contribute towards the above mentioned objectives.

iv) A collaborative research environment can only be realized if data integration across databases and public archives is achieved. These databases and archives may belong to bioinformatics, chemo informatics, clinical data repositories and other related disciplines. Various individuals and groups within an organization may also prefer an integrated environment in which they can share various applications and web services. However while achieving data integration some level of access rights may be enforced to protect personal and cooperate information. This information may include research notes, data files, and email or business processors (Struss et. al, 2009). Another problem with a departmental view is long-term records retention and management. An electronic lab notebook is also an aid to project management by ensuring quality of process and experimental design also work evaluation a task management is better performed through an up-to-date view of a project (Trigg, 2011).

By associating a record with the originator, oyr proposed ELN will provide lineage and audit trail to support scientists' working practices, including re-use of procedures, calculations, text, and data. From legal and regulatory perspective, the proposed ELN will provide IP protection through lineage and audit trail (Bondarenko, 2005).

Table 1: Major gains incurred by an ELN are when it is introduced in manual intensive operations.

Task	Hours/week	Man-Hours consumed (for a 4 member team) and incurring cost
Data Entry	8	32 x 30 USD = 960 USD
Patent Preparation	2	8 X30 USD = 240 USD
Record Keeping	2	8 X30 USD = 240 USD
Reporting	4	16X30 USD=480 USD
Collaboration and Sharing	4	16X30 USD=480 USD

The table above shows the direct ROI by adaption of an ELN. This mainly includes Data Entry, Record Keeping and Patent Preparation which are inherently static tasks. By using built-in templates of ELN, a researcher can increase his productivity by saving 30% to 40 % of non-productive efforts.

Indirect returns are even more significant which incur mainly through avoiding reenactment of experiments and protection of copyrights and IP. Besides, reenactment of experiments, experiments which have resulted in insignificant results may be avoided.

CONCLUSIONS

Scientific research is highly evolutionary and dynamic in nature. However, researchers spent most of their time doing static procedures and tasks. Although, most of scientific experimentation has been automated, record keeping and keeping track of experimental procedure is still manual. Adaption of an ELN will remove this last bottleneck in full automation of scientific research. IN this paper we provided justification of adaption of ELN in scientific research by arguing how ELN record keeping best practices for scientific research.

REFERENCES

Berners-Lee, T., Hendler, J.: Scientific publishing on the 'semantic web', Nature Web Debates (2001)

Bondarenko, O. & Janssen, R. (2005) Documents at Hand: Learning from Paper to Improve Digital Technologies, InProc. CHI'05 Human Factors in Computing Systems, ACM, pp. 121-130.

Brody, S. Data Management: Keeping a research notebook, files and related issues. Department of Internal Medicine. Washington University School of Medicine

Butler, D.: A new leaf. Nature Vol. 436 (2005)

Elliott, M. Thinking beyond ELN - The Informatics Architecture Model, Electronic Laboratory Notebook. Atrium Research & Consulting LLC "A Prism forum white paper.(2004)". Retrieved from http://www.pharmagrid.com/Default.aspx?pageId=683496

Knight, J.: Null and void. Nature Vol. 422 (2003)

Laidboeur, T. Sanofi-Synthelabo Chemical Development and the Development of an Electronic Laboratory Notebook: Inge ´nieur de Recherche et de De ´ eloppement, Sanofi-Chimie, 45 Chemin de Me ´te ´line -B. P. 15-04201 Sisteron Cedex, France

Michael, E.H.: It's Not About the Paper. Scientific Computing & Instrumentation (2004)

Michael, E.H.: Electronic Study Management. Scientific Computing (2006)

Neumann, E.: A Life Science Semantic Web: Are We There Yet? Science Vol. 2005, Issue 283 (2005)

Phillips, M.L.: Do you need an electronic lab notebook. The Scientist (2006)

Polonsky, P, A. Kotelnikov, M. Polonsky,V Polly, R. Brey, P. Semantic Laboratory Notebook: Managing Biomedical Research Notes and Experimental Data

Strauss, R. ChemBioNews.com: E-Notebook Cloud Economics. Strong Science, Lower Cost.

Schrage, M.: For innovation success, do not follow where the money goes. Financial Times (2005)

Sarini, M., Blanzieri, E., Giorgini, P., Moser, C.: From actions to suggestions: supporting the work of biologists through laboratory notebooks. Proceedings of the 6th International Conference on the Design of Cooperative Systems (2004)

Tabard, A. Eastmond, E. Machey, W. From Individual to Collaborative: The Evolution of Prism, a Hybrid Laboratory Notebook. CSCW'08, November 8–12, 2008, San Diego, California, USA. Copyright 2008 ACM 978-1-60558-007-4/08/11...$5.00

Trigg, J. Getting started with an electronic notebook.(2011)