

Does a Laboratory Information Management System (LIMS) for Proteomics Laboratories Need to Be Customized?

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INTRODUCTION

Although there are many Laboratory Information Management Systems (LIMS) commercially available, their applications to proteomics facilities are currently limited. These limitations include: the lack of a web interface for interacting with collaborators and customers, the need for instrument interfaces for equipment from different manufacturers, the desirability of a graphical layout of 1D and 2D gels, and the need for tracking of sample containers and plates. For these reasons, it was proposed that we purchase and subsequently customize a LIMS.

METHODS

In order to address the deficiencies of the standard LIMS, a multifaceted approach was proposed. The biggest challenge in adding additional parts or modules to a LIMS is to create seamless connections between these external "pieces" and the main database and interface. The following modules were created and integrated into the LIMS:

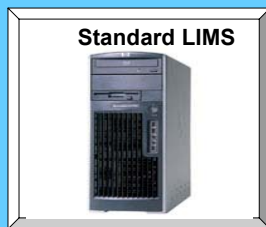
- Instrument parsers capable of automated sample data collection
- A web-based sample information submission and retrieval system
- Graphical 1-D and 2-D gel and sample container visualization system for relating gel bands or plugs to results data
- Protein database search results parsers
- Financial module to automatically link samples to charges in fee for service facilities.

ACKNOWLEDGEMENTS

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RESULTS AND DISCUSSION

This is the standard off-the-shelf LIMS. It is basically designed to track inventory, lot number information and other descriptors that relate to quality control in the manufacturing world. It does not have a web-enabled interface. It has no graphical sample visualization module or financial package for creation of customer invoices. It also does not have any type of instrument interface or database parsers.



CONCLUSIONS

Upon completion of the customized LIMS, we have reached several conclusions. There are many positives in the customization of a LIMS. The add-on modules of the customized LIMS have addressed the needs of the proteomics and mass spectrometry laboratory. Even when some instruments were replaced, the modules could be upgraded or replaced for compatibility, without forcing major changes to the overall LIMS workflow. The web-enabled portion performs well, allowing collaborators to submit 1-D and 2-D gels as well as individual non-gel-separated samples. The graphical interface also allows the collaborator to select spots for cutting and processing. The web submission tool is also very helpful in the collection of sample metadata which, in turn, can be used for data mining and trend analysis. The instrument and database parsers have worked quite well, capturing sample information already input into the mass spectrometers (spot sets, sample lists, etc.), as well as providing automated sample retrieval and LIMS database entry of processed sample data and results.

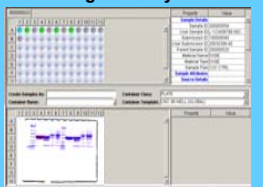
On the downside, all of the customizations have involved countless man-hours of meetings and flowcharting, since many LIMS programmers who create the customizations are unfamiliar with the workflow of a proteomics research facility. These customizations also raised the final cost of the LIMS to approximately 400% of the originally-quoted price, and the build time increased by over 200%.

After considering all of the effort that went into the design of the customized LIMS and the resulting product, it is our conclusion that LIMS customizations are necessary and worth the added cost, due to the specialized needs of most mass spectrometry facilities.

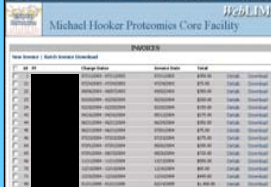
RESULTS AND DISCUSSION

Customized LIMS

Graphical Sample Container Management System



Financial Package



Mass Spectrometric Instrument Parsers



Sample positioning information

Processed Mass Spectrum Data

Peak Data



Protein Database Search Engine Results Parser



Accession	Score	Probability	Sequence
Q99686	100.0	100.0	...K
P01307	99.9	99.9	...K
P01308	99.8	99.8	...K
P01309	99.7	99.7	...K
P01310	99.6	99.6	...K
P01311	99.5	99.5	...K
P01312	99.4	99.4	...K
P01313	99.3	99.3	...K
P01314	99.2	99.2	...K
P01315	99.1	99.1	...K
P01316	99.0	99.0	...K
P01317	98.9	98.9	...K
P01318	98.8	98.8	...K
P01319	98.7	98.7	...K
P01320	98.6	98.6	...K
P01321	98.5	98.5	...K
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