Trends in Laboratory Informatics

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About Atrium Research

Atrium Research is an independent, vendor-agnostic market research and management consulting practice specializing in scientific informatics.

We develop market research reports, supplier reviews, strategic planning, requirements definition, and process analysis services.
Trends in R&D Laboratory Informatics

Objectives

• Increase efficiency of operations
  – Eliminate information bottlenecks
  – Better tools for the scientist

• Increase knowledge sharing and collaboration

• Increase data quality and consistency of data capture

• Reduce downstream costs
  – Fail early, better upfront design

• Reduce information technology (IT) costs
  – Fewer software solutions to support and maintain
Trends in Laboratory Informatics

Meeting the Need

- Eliminate paper-based data capture
- Redesign processes and automate where possible
- New tools for simulation and prediction
- Integrate silo data sources
- Reduce vast array of software solutions to a manageable level
- Develop common ontologies, integrate data from multiple sources
- New methodologies for archiving and management of digital assets
BioPharma Discovery Integration

Meeting the Need

- Elimination of paper roadblocks
  - ELN, EDC
- New tools for automating workflows
- Common integration framework
- Modular software systems
- Data standards and common vocabulary
- Information Lifecycle Mgt (ILM)
Emerging Informatics Technologies

R&D Informatics Technology Adoption S-Curve

- Laggards
- Late Majority (Conservatives)
- Early Majority (Pragmatists)
- Visionaries
- Early Adopters
- "Chasm"
- Clinical EDC
- Scientific Data Mgt
- Cheminformatics
- Bioinformatics
- Image Mgt
- Bioassay
- Registration Inventory LIMS
- Document Mgt
- Electronic Laboratory Notebooks
- Workflow / Process Automation
- Simulation / Prediction

Time from Introduction

Source: Atrium Research

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Time for a Change?

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Students are getting high results for % in unadjusted samples. Sample studied to make sure mixed well to be 100% pure. Dried at 105°C for 30 min. Then dehydrated and dried.

Dried at 105°C with nitrogen. Directly to determine %.

Dried salt run by 2000 ppm. Student was optimal.

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Electronic Laboratory Notebook (ELN)

Eliminate the Roadblocks

“An ELN is a secure system that assembles content from multiple sources that are related to each other, allows for annotation, and packages it in a legally acceptable document which can be searched, mined and collaborated.”

- Technology for capturing and reusing experimental data and information lost to paper

- Two different categories
  - Non-specific (“generic”)
  - Specific

- Currently a visionary market making the leap to the pragmatic

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Laboratory Process Mgt (LPM)

Automate and Simulate

- New technologies for data pipelining, experiment design, simulation and integration
- Model-centric, not sample-centric
- Objects are created for specific functions
  - Can be for data processing, instrument control, step in a method, etc.
  - Can be for getting or posting data from another system
- Currently a visionary market
Web Services

Common Integration Framework

- A standard way of integrating applications using XML (eXtensible Markup Language) data

- Enables multiple applications from different sources to communicate without custom coding
  - Flexible, eliminates “one off” interfaces
  - Can “wrap” around a legacy application API
Service Oriented Architectures (SOA)

*Modular and expandable*

- Design of an application where the logic is organized into loosely coupled modules (services)
  - Services use an agreed message standard
- Uses XML for data and SOAP (Simple Object Access Protocol) for messaging
- Allows for “pull out and/or plug-in” configurability
- Web services and SOA are *not* the same thing
  - SOA is *architected* around Web Services
Ontologies

Common Vocabulary – Consistency of Approach

“Ontology is a set of concepts - such as things, events, and relations - that are specified in some way (such as specific natural language) in order to create an agreed-upon vocabulary for exchanging information.”

Source: Whatis.com

• Integration is difficult (if not impossible) to accomplish without an agreed vocabulary – i.e. “study” to one person could mean “project” to another. How is a computer to know this?

• The increased use of outside collaborators further necessitates an ontology

• There are emerging scientific ontology standards:
  – i.e. Gene Ontology, Plant Ontology, SNOMED
Semantic Web
*Integrating Data Across Sources*

- For integrating data from multiple sources and collaboration
- Designed for the application of *meaning* to data
- Will enable agents to crawl for data that has similar meaning
- Ontology is key for understanding relationships
- Currently an early adopter market

See: http://www.w3.org/2001/sw/

Source: W3C
Information Life Cycle Management (ILM)

Improve Management of Digital Assets

- “Monolithic” repository isn’t working due to exponential growth in data
  - Multiple repositories are needed managed by content management systems
  - Time based, size based, project based, etc. movement between media
  - There comes a time when data must be destroyed
  - Managed by data class

Source: Atrium Research
Informatics Convergence

Meeting the Need to Reduce Number of Applications
Summary

• Barriers must be eliminated to improve efficiency of R&D operations
  – More time for science!

• Processes must be simplified and automated where possible

• The market is trending toward integrated application suites using industry standard technologies
  – Web services, SOA, Semantic Web

• Information Lifecycle Management is critical for digital asset protection and record maintenance
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