Data Management Challenges for Academic Laboratories

- Multiple Users Sharing Systems (Open Access)
- Turnover in lab expertise
- Multiple Sources of Data and Instrumentation
- Record Keeping Paper
- Data Overload
- Access to Data – local or remote
- IP Protection, Regulatory Concerns
- Data Integrity
- Publication of Information
- Record Retention Policies
Agilent OpenLAB Laboratory Software Suite

**OpenLAB CDS**
Chromatography Data System
Workstation, Networked, Distributed
- ChemStation, EZChrom workflows
- OpenLAB ECM data integrity
- OpenLAB Reporting Module
- Scalable Architecture
- Regulatory compliance Features
- Regulated and non-regulated modes
- Web-based options – Smart Phone
- Lab at a Glance Mode
- LIMS / ELN integration

**OpenLAB ECM**
Enterprise Content Manager
Scientific Data Management System
- Data archiving
- Instrument vendor neutral
- Viewers, filters, converters
- Agilent workstation aware!
- Time stamp/audit trail
- Report capture
- E-signatures
- Regulatory compliance
- TNF conversion (LTDA)

**OpenLAB ELN**
Electronic Lab Notebook
Capture, Organize, Collaborate, Protect
- Smart, high productivity alternative to paper notebooks
- IP protection and compliance features
- Simplifies and accelerates lab work
- Smart data import and dynamic forms
- Simple web-based client
- Analytical request module

**OpenLAB Professional Services**
Integration of OpenLAB Solutions
- Speeds full utilization of OpenLAB software & instruments
- Maximizes the return on investment in OpenLAB
- Compliance Consulting and Execution
- Accelerates OpenLAB adaptation to existing workflows
Laboratory Data Management Solutions – Proposed

Data Management
OpenLAB ECM

- Data Archiving
  - Automatic or Manual Upload
  - Instrument Vendor Neutral
  - Time Stamp/AuditTrail
  - Report Capture
  - E Signatures

Electronic Note Book
OpenLAB ELN

  - Smart, high productivity alternative to paper notebooks
  - IP Protection
  - Linked to Raw Data (In ECM)
  - Simplifies and accelerates R&D
An Informed Way to Manage Information

Overview

Laboratory Data Collection, Analysis, Interpretation and Management
Agilent OpenLAB Laboratory Software Suite

**OpenLAB CDS**
Chromatography Data System
Workstation, Networked, Distributed
- ChemStation, EZChrom workflows
- Agilent and Non Agilent Instrument Control (Multi-vendor)
- OpenLAB ECM Intelligent Reporter
- Regulated and non-regulated modes
- Web-based options

**OpenLAB ECM**
Enterprise Content Manager
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What is OpenLAB ECM?

Enterprise Content Manager

A web-based electronic library that collects, organizes, indexes, stores, archives, and shares any electronic file.

- Archive
- Automate
- Retrieve
Managing Data in the Lab
How can OpenLAB help?

- Centralized data storage
- Minimize impact to existing workflows to reduce training costs
- Track and audit all data access / activities
- Protect data from unauthorized access
- Make data available to authorized users when and where they need it
- Search for all related data with a single query
- Allow users to more easily share data
- Remove bottlenecks in the review and approvals process
- Allow users to more easily use and re-use data in generating reports
- Manage data through its entire lifecycle
- Scalable to meet the needs of your environment
Minimize Impact to Existing Workflow
Automated Content Transfer

Automate file upload

- Scheduler monitors computers, drives, folders for files that meet user defined upload criteria
- Remove files from client locations automatically
- Specialized interfaces for analytical applications that generate groups of files or directory structure
- CyberPrinter XP manages electronic files printed from Windows based applications.
- MS Office integrated toolbars
Find All the Data You Need - FAST
3 Levels of Search Tools

The quick search tool is a web style search

- Web style search – just enter search text and go
- “Smart” search that guides users through query statements
- Advanced search for more extensive data mining
Keep Track of all Steps in Data Analysis
Version Control

A complete revision history of all files

- Users can review previous versions
- Users can compare file versions
- Users can roll back to previous versions if necessary

Every activity within the system is logged

- The audit trail is computer generated and time stamped with GMT based time line
Ensure Data is Available When and Where Needed

Collaboration Features

In addition to the web based access which enables document / file sharing:

- Users can check files out of the system
- Other users can still view files, but may not edit
- This prevents inadvertent overwriting of changes when 2 users are working on the same document
- When editing is complete, the new version of the file is checked in, releasing the file to other users
- Viewers available for Analytical data
Approve Results and Reports

Electronic Signatures

Any file within Content can be Electronically Signed

- PDF file signatures accomplished with plug-in for Adobe Acrobat
- This plug-in encrypts signature information within the document and displays a visible indication of signature on the file
- A generic signature tool is used to apply electronic signatures to any file type
- Each signature contains the date / time of the signing, the name of the signer, location that the signature took place and reason for the signature
Keep Data Useful and Available
Extracting searchable information in context

Metadata extraction from any instrument / any manufacturer

- User entered fields extracted from PDF forms
- Reports printed from any analytical instrumentation
- Metadata keys can be found and extracted from the PDF file content
- Extracted information can be searched in context

For example:
Find file where Project Name = XYZ
Tag Stored Files with Important Information

User Defined Metadata

Associate user defined metadata to files

- Users can add this type information to the file’s metadata with User Defined Keys
- These values can be automatically assigned, entered by users, selected from defined pick lists, or entered programmatically
- This information is also fully searchable with any of OpenLAB’s search mechanisms
Electronic record life cycle

**Agilent OpenLAB ECM supports hierarchical storage management and multiple retention policies**

With the record retention features, each step in a file’s lifecycle can be automated

0  10  20  Time

**Metadata**

**Database**

**Retention Policy**
Business Process Management

• Business Process Management helps to streamline and automate the flow of information throughout your enterprise.

• Within a process information can be collected from instrumentation or client computers, evaluated without user interaction for metadata content, routed for review with time limits, signed electronically, moved within the Content repository based on file or process metadata cues and much more…

• SOP management
• Compliance lifecycle
• Results checking
• Automated routing of results
• More…..
Summary

Helping you work Smarter with less effort...

• Complete Web Based Information Management System
• Secure Data storage and monitoring capabilities
• Built in Record Retention
• Modules for ELN, BPM in an integrated system
• Scalable Web-based, n-tier architecture
• Integration with 3rd party systems
Agilent OpenLAB Questions?
OpenLAB
UNLOCKS YOUR LAB’S POTENTIAL
CAPTURE ANALYZE SHARE
Agilent Technologies
Agilent OpenLAB Laboratory Software Suite

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- Agilent workstation aware!
- Regulatory compliance
- Report capture
- Technology-neutral data conversion

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- Maximizes the return on investment

Agilent Technologies
Have you ever tried to find the one buffer recipe that produced the best assay results for today’s experiment?

From chaos…

To a single search in seconds…
Paper based processes with hand written notes…

- What was the best method used?
- Has anyone done this before?
- How did I do this?
- How did someone else do this?
- Where are my results?
- Where are their results?
- What does that say?
- Who signed this?
With OpenLAB ELN

- Search across the organization
- Share methods and results
- Report experiment details
- Secure IP and protect results
- Store Excel, Word documents
- Import ChemStation, MassHunter

Spend less time documenting in your paper notebook and more time in the lab…
What is an ELN?

- **www.censa.org definition** "An Electronic Notebook is a system to create, store, retrieve and share fully electronic records in ways that meet all legal, regulatory, technical and scientific requirements."

- Basically; an ELN is a replacement for the Paper Laboratory Notebook

- Adding new dimensions in terms of knowledge management and collaborative work it is becoming much more: the everyday principal workspace of the R&D scientist
OpenLAB ELN Building Principles

• Gather & Secure the Intellectual Property
• Compliance in regulated environments (CFR 21 part 11, CLIA)
• Provide each scientist and researcher with a dedicated workspace with features that streamline data entry
• Provide an efficient information sharing & collaborative environment
• Provide the ability to configure workflow and experimental layout without custom code
• Develop enterprise-wide and open architecture in order to interface with the existing or third party specialized modules
OpenLAB ELN – Top three benefits

1. Expedite decision making
   • Smart Import: Automatically import data from ChemStation and OpenLab ECM for further calculations
   • Integration with OpenLab ECM: Access documents in ECM and link to experiments in ELN.
     – Increase productivity: Reduce cycle time from experiment to result

2. Decrease cycle time
   • Analytical Request Workflow: Manage electronic requests, create sample lists and queue work for analytical chemists
     – Increase efficiency: Reduce time from analysis request to result and final insight

3. Increase collaboration
   • Dynamic Forms: Flexible environment where users can design their own data entry templates
     – Increase efficiency: Capture all results in context of the experiment for easy searching and traceability.
Organizations spend thousands of dollars buying, moving, and storing paper each year. What is the impact of a paper based system on productivity and budget?
How much time is spent….?

- Printing paper based test requests, work lists
- Making copies
- Transferring (walking) paper based notes to the lab
- Distributing (walking) requests to individuals
- Printing reports, analytical data, conclusions
- Cutting and pasting data into a notebook
- Walking a notebook through the review process
- Waiting for the review to continue other experimental work
- Issuing, delivering, retrieving, and storing paper notebooks
- Looking through volumes of paper based records to find past work
The benefits and cost savings of a paperless system are clear. OpenLAB ELN can help transform your paper based processes into a paperless lab.
Working with the OpenLAB Products

**OpenLAB CDS**  
Chromatography Data System  
- Instrument Control  
- Data Collection  
- Data processing  
- Results generation

**OpenLAB ECN**  
Enterprise Content Manager  
Scientific Data Management System  
- Manage analytical data  
- Manage report data  
- Centralized, secure storage  
- Minimal impact to end user

**OpenLAB ELN**  
Electronic Lab Notebook  
- Log samples  
- Document sample prep  
- Interpret results  
- Review and witness
Sample ELN – ECM Integration Workflow

- Create Experiment
  - Document samples, preparation protocols, methods used, etc
- Run Chromatography
- Data is added to ECM
  - Metadata is extracted
  - XML
  - PDF
  - hyperlink
  - Experiment is reviewed
- OpenLAB CDS
- OpenLAB ELN
- OpenLAB ECM
- Data reviewed
  - Experiment is signed and counter signed
  - Experiment is published
OpenLAB’s ECM component can automate the centralized storage all electronic data within your laboratory – both raw analytical and report data.
Experiments have chapters. Chapters can be shown or hidden as needed.
Within each Chapter are paragraphs. Paragraphs are rich text boxes in which users describe their work using text, graphics, links to analytical data, chemical structures / reactions, calculations, etc…
Both the chapters and the paragraphs can be customized to better fit the way you work.
Configuring the Experiments to Your Workflow

Customize the experiment chapters:
- Rename
- Add
- Remove
- Reorganize

Customize the Paragraph titles
The customized chapter names and paragraph names are saved as an experiment template. The experiment template can be private, or shared across the lab or across the organization.
The experiment templates can be further configured to include fields for users to enter routine or required information. When a field is used, the information becomes standardized across experiments making it specifically searchable.
Fields can be grouped together into forms. The forms can be designed to follow the workflow associated with an experiment, sample preparation, procedure, conclusion, etc…
An experiment template can be pre-populated with forms, or users can drag and drop them onto the experiment page.
Forms can be locked (they appear with a pink background) meaning users can only enter information into the available form fields.
When forms are unlocked users can edit the information they contain. For example, add a new test.
The Methanol used was from VWR; Lot No: 1234567890

Or add additional text as needed to further describe their work.
Attaching analytical data to experiments – whether that’s spreadsheets users for data processing, reports, raw data, or graphics – can be done in a variety of ways:

1.) IMPORTED / LINKED FROM OPENLAB ECM
2.) BROWSE YOUR LOCAL MACHINE OR NETWORK SHARE
3.) DRAG AND DROPPED ONTO THE EXPERIMENT PAGE
As data is automatically transferred to OpenLAB ECM, it is tagged with searchable metadata that allows a single search to return all of the analytical data associated with an experiment.
Adding Excel Spreadsheets

When spreadsheets are included in the experiment, users can add a cell range, a worksheet, or an entire workbook.
The contents of the spreadsheet appear inline in the experiment text. To edit the spreadsheet, double click. Excel is launched. Update any information and save directly to the experiment.
Adding Analytical Report Data

When PDF files are included in an experiment, the user has the option to have the entire contents of the document displayed inline with the other experimental text.
Adding Raw Analytical Data

When raw analytical data is included in an experiment, hyperlinks are inserted in the experiment text. If at a later date the raw files are needed – they can be retrieved using these hyperlinks.
Graphics files or graphics copied and pasted from reports or other documentation can be inserted into the experiment. These graphics can be annotated.
Not only can the fields, forms, and experiment templates be configured to fit your workflow, the process for witnessing, review and approval can be configured.
Single or multiple witness and validator steps can be configured.
At each step in the process a PDF copy of the experiment is published and can be reviewed and compared to previous versions at any time.
Reviewing Experiments
The ability to query past experimental data is a tremendous advantage over paper based systems. With a mouse click see all experiments that meet any search criteria: Positive results over the last year, relating to a specific sample type, run on a specific instrument.
“Send/Print To ELN”

1. Print from any application

2. Select OpenLAB ELN virtual printer
“Send/Print To ELN”

3. The output is converted to PDF, ready to be sent
4. Can be incorporated into any experiment later when the scientist is ready to report on his experiment
“Send/Print To ELN”

Similar to the print feature, it is possible to upload files directly to the Inbox through the Windows menu …
“Send/Print To ELN”

... and incorporate it into any experiment later when the scientist is ready to report on his experiment
Agilent Lab Informatics for Academics

Teaching Labs and Research Departments

Jon Welsh
April 2014
Large Diverse Labs

**Need:** A cost-effective solution for teaching labs to enable remote access for many students to data acquired on just a few instruments

**Current Situation:** Individual workstations are cost prohibitive and require software to be loaded on specific data analysis PCs

**Solution:** OpenLAB ChemLaunch
OpenLAB ChemLaunch

- Compatible with nearly all Agilent instrumentation
  - LC, GC, CE, Quad, QQQ, TOF, ICP-MS, Spec...
- Can be used with non-Agilent instrumentation
  - Protects current investment
- Requires only one copy of instrument software
  - Cost effective
- No software to load
  - Simple deployment & upgrades (Zero footprint)
- No limit on the number of users accessing data
  - Scalable
- Remote access from PCs, Macs, Tablets
  - Compatible with most devices (windows/mac/unix)
- Data is accessible but secure
  - Controls data access
- Flexible pricing model
  - Concurrent or site licensing
Why ChemLaunch?

- Full access to data analysis...without loading software
- Students can use their personal devices (Win PC, Mac, tablet)
- Data is stored centrally, controlled, and available from anywhere
- Deploy multiple software platforms (e.g. ChemStation & MassHunter)
- Access to software is controlled
- Central software deployment and management

**ChemLaunch:** A simple, cost-effective solution for teaching labs with IT support for Citrix