OpenLAB and Kalablie ELN
Overview

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### Agilent’s Software & Informatics

#### Data Systems Directions

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<th>Yesterday</th>
<th>Today</th>
<th>Tomorrow</th>
<th>Future</th>
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<td><strong>Shared Services</strong></td>
<td><strong>Web Services</strong></td>
<td><strong>Collaboration Services</strong></td>
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<td>Special Purpose</td>
<td>1:1 Instrument / data system relationship</td>
<td>Desktop - Workgroup - Enterprise scaling</td>
<td>Internet is UI</td>
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<td></td>
<td>Expensive ongoing administration</td>
<td>Content management (text / image / object)</td>
<td>Anywhere / anytime access</td>
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<td></td>
<td>Creates data islands</td>
<td>Reporting / Search</td>
<td>Integration by default</td>
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<td>Higher replacement costs</td>
<td>Instrument control</td>
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<td>Workflow automation</td>
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<td>Distributed workflows</td>
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<td>Extended shared services</td>
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<td><strong>Benefits</strong></td>
<td><strong>Infrastructure leverage</strong></td>
<td><strong>Pervasive (common) UI</strong></td>
<td><strong>Higher information utility</strong></td>
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<td>Lower initial deployment risk</td>
<td>Linked systems</td>
<td>Greater collaborative sharing</td>
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<td>Lower introduction fixed costs</td>
<td>Central administration</td>
<td>Improved information quality (contextual)</td>
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<td>Perhaps simpler deployment</td>
<td>Lower cost / seat than Special Purpose systems</td>
<td>Predictive analysis capability</td>
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<td>Operation without boundaries (disciplines, depts., locations, entities)</td>
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<td>Cross-entity outsourcing</td>
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**Increasing Value**

Help laboratory managers / directors reduce the time, effort & cost to go from raw data to final insight
Agilent Software & Informatics
Offering comprehensive software and services solutions for laboratories and enterprises

- ChemStation
- EZChrom Elite
- OpenLAB ICM
- MassHunter
- Feature Extraction
- GeneSpring
- CGH Analytics
- eArray
  - Partnering with Strand
- OpenLAB ECM
  - Partnering with PSI
- Kalabie ELN
  - Partnering with Accelrys
- Electronic Lab Notebook
- Kaland ELN
  - Partnering with Accelrys
- I & F
- IQ/OQ
- Consulting
- Customization
- SMA
- OpenLAB ECM
  - Partnering with Accelrys

Help laboratory managers and directors reduce the time, effort & cost to go from raw data to final insight
Levels of Information in an OpenLAB Enterprise System

ECM: Enterprise Content Management
• Data storage and management

ICM: Instrument Control Module
• Multivendor Instrument Control

BPM: Business Process Management
• Workflow Engine for OpenLAB

ELN: Electronic Laboratory Notebook
• Experiment design and IP protection

PP Accelrys PipeLine Pilot
• Scientific Business Intelligence
Centrally Manage and Protect All Your Data

Manage and organize ALL electronic content regardless of source

- Analytical Data
- Chromatography results
- Procedure Documents
- PDF files and forms
- Scanned paper files
- Training Records
- Microsoft Office files
- Electronic reports
- ANY electronic content
Tag 3rd Party Data With Ancillary Meta Data and Information

Associate LIMS or ELN defined metadata to files

- Information such as an ELN batch ID or LIMS ID can be added to the file’s metadata with User Defined Keys
- These values can be programmatically assigned, entered by users, or selected from defined pick lists
- This information is also fully searchable with any of OpenLAB’s search mechanisms
Automatic Meta Data Extraction and Agglomeration

Metadata extraction with filters
- Metadata associated with files can be searched and reported against
- Filters programmatically extract metadata from files as part of the upload process
- With no user interaction, metadata is extracted and stored with the file
- Filters are drop in, server modules that can be added to the system at any time with no application down time
Multi-Level Search Tools

3 Levels of Search Tools

Programmatically query the ECM system for files or file information

- Web style search – just enter search text and go
- Generate simple query statements using common metadata values
- Use the Advanced search for more extensive data mining
OpenLAB ICM
Centrally Manage Instruments

Organize all Laboratory Instrumentation

- Locations define the instrument topography
- Limit User access to instrumentation through the hierarchy
- Instrument portal give high level view into instruments current activities
- Launch instrument control window from the web portal
ChemStation Integration with OpenLAB ECM
LC/GC, GC/MS, ICP/MS...

Access common ECM functionality directly from the ChemStation UI

- Load and save methods, sequences, and data directly from ECM
- Access to files stored within ECM without leaving ChemStation.
- Access to all ECM search functionality is available inside ChemStation
OpenLAB BPM

Automate the Information Flow in your Lab

The process designer is Microsoft Visio

- The BPM stencil contains a variety of functions to be performed as part of a workflow
- The activities are dragged and dropped on the drawing surface, and joined together with logical connectors
- Each activity has an additional configuration step that defines that step in the workflow
- The completed process is saved within the content repository and registered with the process management engine.
What is Kalabie ELN?

Kalabie provides a robust platform that can be used to …

- Document and manage experiments and insights
- Protect Intellectual Property
- Facilitate collaboration by implementing transversal processes between users
- Support and bridge multiple R&D disciplines through adapted Activity Profiles
- Connect to the R&D IS system
- Accommodate for special requirements by extensibility at various levels
Product Features

User-centric feature set

– Simple and straightforward UI (focus on using not software training !)
– Multidiscipline, Chemistry or custom environment: adapted to your discipline

Knowledge Sharing & Mining

– Share, Find, Reuse and Report

Integration to the Lab Informatics System

– The all day every day window to your Lab informatics
– A true, highly scalable, enterprise solution with rapid deployment

IP Protection and compliance

– Includes mechanisms for IP protection
– 21 CFR part 11 compliant
Vision: The ELN is a focal point

Research Processes

Collaborate

Inform

Support - Share

Chemistry

Biology

Analytics

Research Activities
Application domains: Breadth and Depth

The scientist is selecting the experiment related to his specific scientific domain.
Kalabie multi-discipline environment

Meta data entry to facilitate information classification and searching
- System provided information (Author, Notebook reference, Date…)
- User selected information from Admin references (Project, sub-project…)

Rich Flexible entry/attachment of text, images, objects
- Insert and attach using Rich text Palette, Drag and drop and right click
- Sophisticated version management of attachments
- File size and types permitted are managed in Kalabie Admin
- Attached files are opened using the software choice of the user (application on client station)

Protocol Library
- Content managed through the Kalabie Administration module is available to all authorized users
- Cascading lists to fill protocol section with the appropriate library protocol content
- Possibility to append several entries from the library within the same protocol section in an experiment.
Kalabie for Chemical Synthesis

Follows chemist’s workflow (from design to results handling)
Contains contextual information (Project, Study, Lit. references …)

Advanced reaction design
  – Multi-role molecule entry (reactant, intermediate, product, impurity, solvent, reagent and catalyst)
  – Accepts copy/paste of a reaction from Drawing Tool
  – Connects on local or global repositories for molecule searches
  – Allows structure validation (when connected to Checker)
  – Computes atom-atom mapping (uses cartridge functions)

Complete set of calculation functions
  – Composition, expected results and results tables allow chemists to manipulate and convert quantities needed within their experiments

Structured but flexible interface
  – User interface is a mix of predefined, structured fields and rich text fields (like the protocol where lot of illustrations and attachments can be inserted)

Accurate batch management
  – Mixture definition (multi compounds and multi additives) and reuse in subsequent experiments
  – Ability to fill analytical properties form and to record analysis performed
Analytical Request Workflow

**Analysis Request**

1. Sample + Analytical Request (with context)
2. Analytical Request completed with results and conclusions

**Project analytical manager**

- Review, accept or update the Analytical Request
- Register Sample
- Store the sample + affect the AR to one lab
- Review AR
- If AR completed:
  1. Enter conclusion
  2. Generate the analytical report, signs it and send it to the submitter
- Execute the next requested analysis

**Analyst**

- Record result
- Print the analytical report (all available results) and attach it to the AR
- Transmit AR + sample to the next lab

**Instrument**

- Generate Raw Data
- Print the experimental run’s report

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*Agilent Technologies*
Knowledge Repository Mining

Various search modes
  - Keywords
  - Full text
  - Structure-driven
  - Fields
  - Advanced modes

Personal files
Permanent requests
Exports
  - Excel, RDF, SDF
Reporting

- The experiment PDF (IP document) is available for each Activity Profile
- Simple data export from Kalabie Explorer to Excel is always available
- Export to Word
- Standard 3rd party report tool against DB

![Kalabie Explorer](image)
Integration with the Lab Informatics System

Kalabie has been designed to integrate specialized modules in a seamless way.

Kalabie is a 3-tier architecture which allows integration to be done at each level:

- At the client level allowing the integration with desktop software e.g. Molecular Drawing tools.
- At the middle tier (the Application Server) e.g. access to information sources, ADMS.
- At the database level for data management e.g. archiving systems.

Examples of integration realized:

- MDL (MDLDraw, Isis Direct), Accelrys (Accord), Chemaxon (JChem), NuGenesis, LIMS, ChemBase, Inventory, Registration, Naming Tools (ACD).
- OpenLab ECM.
IP Protection

IP Protection is based on key internal mechanisms

– Electronic Signature
– Long term data format preservation by relying only on XML and PDF core formats
– Administration options allowing the user to manage the type of data that may be incorporated into the ELN
– Search capabilities to find out anteriority information
– 21 CFR part 11 conformity and particularly the audit trail mechanism
IP Protection: Signature Workflow

Signature workflow offers:

- Graphical status
- Notification of next signers

Configuration:

- Witness rules
- # level of validation

Agilent Technologies
OpenLAB

“The Operating System for the LAB”

Reduce training / documentation costs via standard interface regardless of vendor; define single workflow across multiple vendor products.

Set business rules & automate audits for workflow/protocol compliance (paperless).

Broader customer choice with largest library of instrument drivers.

Outstanding information asset leverage; ensures information is captured and shared in context; simplifies compliance reporting.

Avoid lock-in; retire the application and still view and repurpose the data.

OpenLAB, when combined with archival systems deliver business continuity (backup, recovery, and archiving) for high availability of laboratory information while meeting regulatory compliance.
Kalabie: Extending the OpenLAB Architecture

Agilent User Interface

Workflow / Business Logic (BPM) Layer

Instrument Layer

Reporting Layer

Content Management

Storage Management

Kalabie ELN plugs in at the workflow Layer & takes advantage of all Successive services

ELN enables researchers to capture, process, save, and search data in a completely digital, networked environment. It facilitates access to commonly-used software programs for scientific, statistical, visualization, MS tools, etc., while capturing all content electronically for collaboration, IP protection, etc.
A Winning Combination for Customers

“Pre-integration” Enables Customers to Achieve Objectives Faster

Customers currently piece together informatics products from different vendors, incurring costs in time, money and training.

Accelrys and Agilent will develop products that work seamlessly with each other, allowing customers to realize the benefits in combination.

Agilent’s strength in Laboratory Informatics, QA/QC and manufacturing are a natural complement to Accelrys’ expertise in research, early development and scientific data management.

Customers will enjoy unprecedented integration of laboratory data, experimental results and insights across the enterprise.
Data Pipelining

A powerful new paradigm for data processing

Pipelines guide the flow of data through a network of modular computational components
Administration Report
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Integrating Agilent Kalabie ELN with your analytical lab using the NEW Analytical Request Profile

August 27, 2008 – 1:00 pm EST

Integrating Agilent Kalabie ELN with Accelrys Pipeline Pilot to intelligently manage results

September 24, 2008 – 1:00 pm EST

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