Your Electronic Laboratory Environment –It's a Holistic Journey

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EPA Quality Assurance Conference

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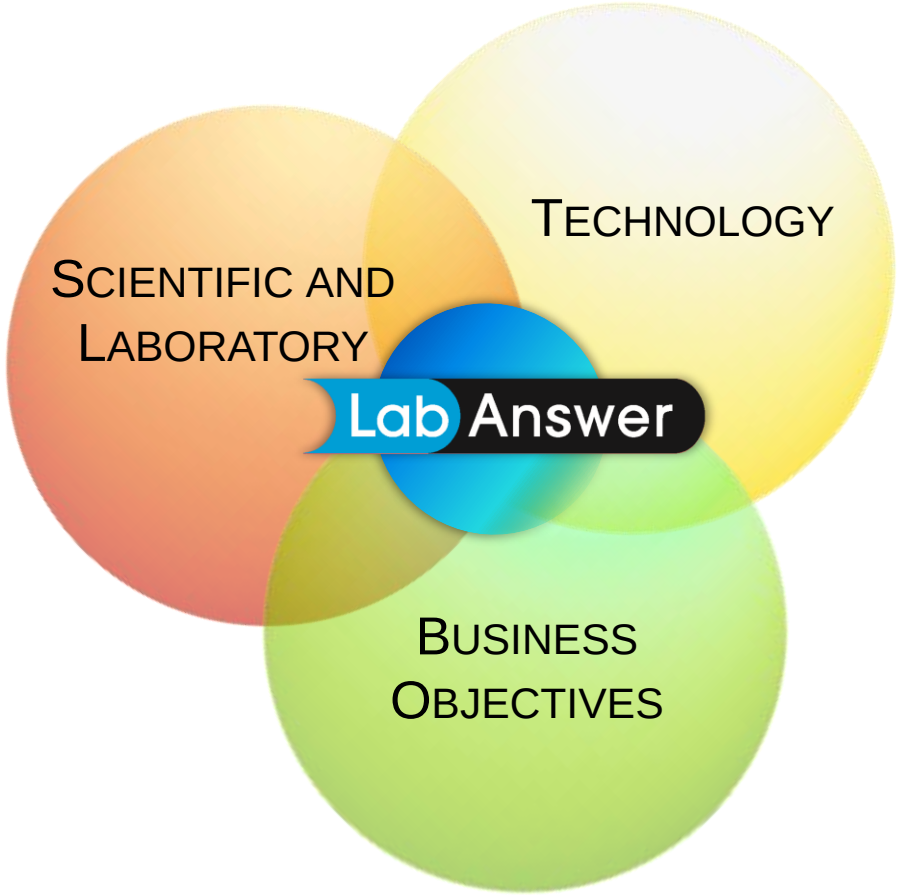
LabAnswer
LABORATORY INFORMATICS

About LabAnswer

Helping clients meet business objectives by leveraging informatics technology to accelerate science

- Founded in 1990; first Lab Informatics project done in 1993
- Vendor and technology-agnostic, consultancy that specializes exclusively in laboratory and scientific informatics (including LIMS, LES, ELN, CDS and SDMS)
- With over 250 full-time employees, we are clearly the largest lab informatics consultancy in North America
- Support wide range of industries and laboratory types with focus in Pharmaceutical, Life and Material Sciences and Government/Clinical Research Sectors



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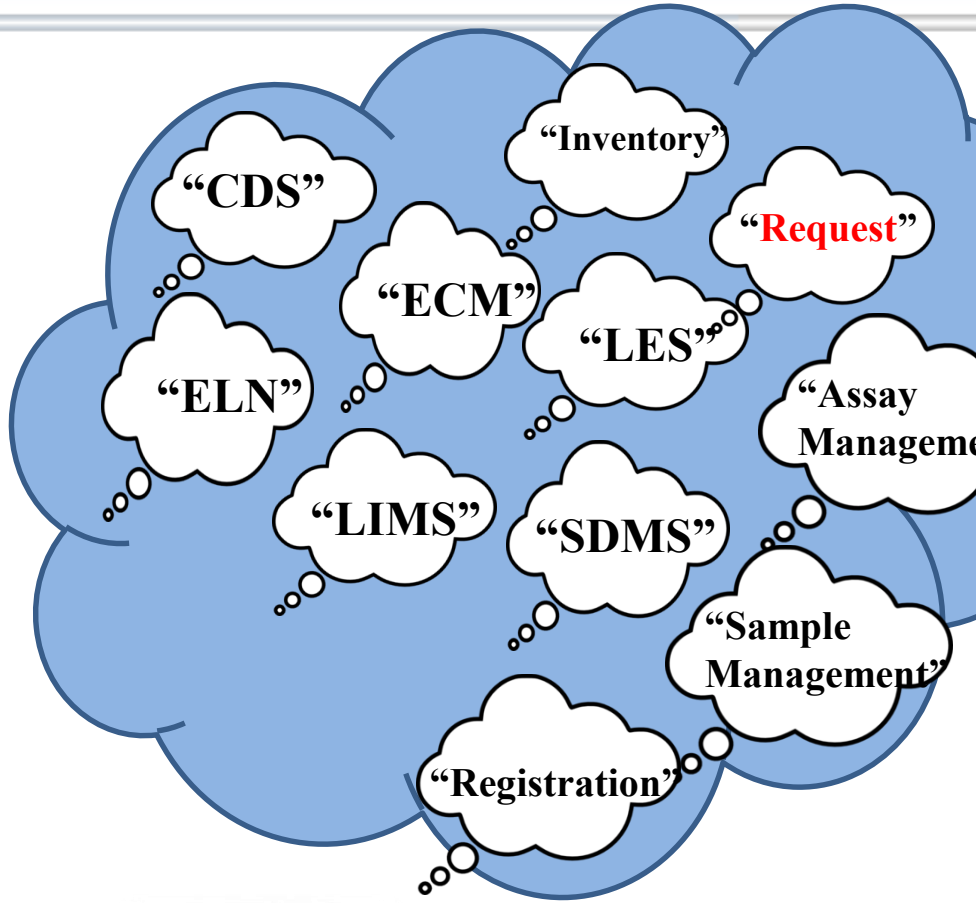
Agenda

- 20+ Years of Lessons Learned….
- Details
- Doing Your Due Diligence
- Value and Pros and Cons
- Prepare for the Data Lake Not the Pond

20+ Years of Lessons Learned

- Focus on functionality and requirements (FRS)
  - Good requirements = Good fit
  - With the future in mind = Best Fit
  - Research vs Quality vs Analytical vs Manufacturing (one size rarely fits all)
- Ensure best business practices are or will be in place
  - Solving cultural, people or data processes with technology change is a risky venture
  - COTS functionality was probably built and debugged for someone else...
- Harmonization before implementation
  - Taxonomies and ontologies
  - Manual business processes

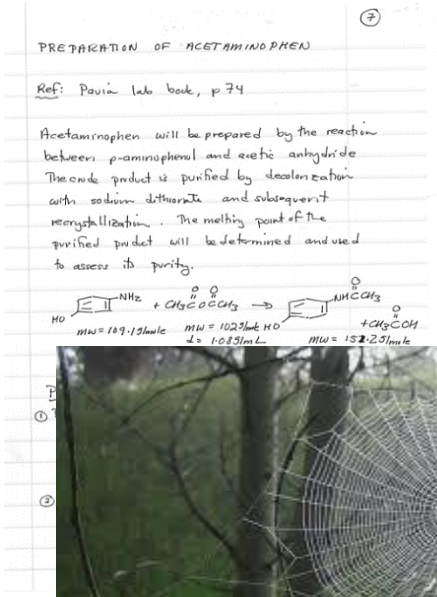


Lessons Learned Continued

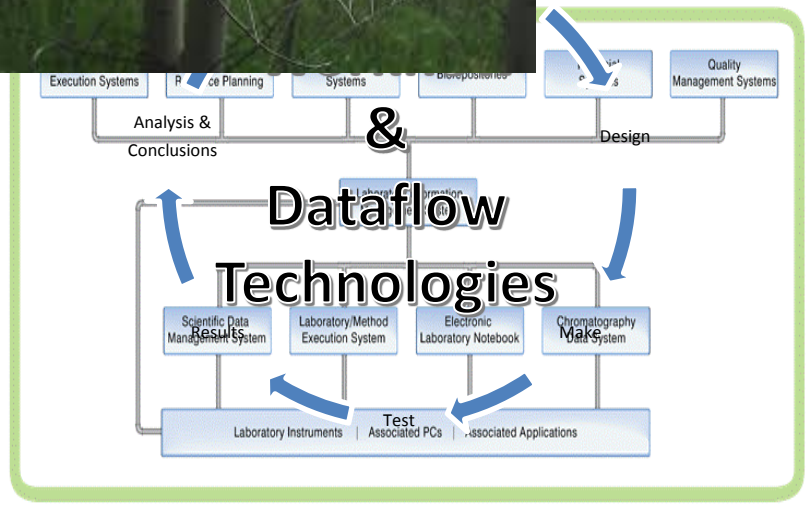
1. Move slow in the beginning in order to <u>manage change and complexity</u>….e.g.
   1. Paper on glass in R&D, Prioritized templates in QA/QC
   2. Phased deployments
   3. Proven value milestones
   4. Balance WIIFM vs Organizational Goals

2. ELNs for example, are very sticky solutions so think it through before it becomes a core of your laboratory informatics platform
   1. Prototype, prototype, prototype

3. ELNs can be a cornerstone in your scientific and laboratory informatics infrastructure
   1. Ideation (hypothesis, rationale) Capture
   2. Experimental design
   3. Tracking failure and success



- Hypothesis/Purpose
- Materials
- Procedure
- Observations/Data
- Results & Calculations
- Conclusions



One Size Doesn't Fit All

- R&D
  - Less Structured
  - Must accommodate Ad hoc
  - Mixed GXP
  - Scientifically aware
  - More Ad hoc reporting
- QA/QC
  - Structured
  - Method Driven
  - GXP
  - Scientifically Aware
  - More Structured reporting

Informatics System Characterization

	LIMS	Research ELN	Analytical ELN	SDMS
Focus	Storage & Reporting on Sample, Tests & Final Results; Lab Workflow	Organizing the Science: Chemistry & Biology	"Right First Time," Procedure Execution & Data Capture	Capturing and Controlling Instrument Output
Main Business Drivers	Final Results & Decision Making	IP & Knowledge Sharing	Compliance & Productivity	Knowledge Sharing & Compliance
Design Approach	Highly Structured	Free Form	Very Highly Structured	Semi-Structured
Data Focus	Sample Hierarchy Centric	Experiment Centric	Test Method Centric	Instrument Run Centric
Data Capture Drivers	Product Centric for Final Results	Research Data and Instruments	Raw Data for Preps, Calculation & Instrument Mgmt	Raw Instrument Data and Assoc. Metadata
Integration Approach	Up to Business Systems & Down To Instruments	Research Databases & Links to External Data	Direct Connections with Instruments	Connections with Instrument Software

ELN Focus Overview

	Research ELN	LES	LIMS
Where in use	Chemistry & Biology Research & Development	Analytical Testing laboratories	Analytical Testing laboratories
Main purpose	• IP Protection • Knowledge re-use • Research efficiency	• Electronic SOP's • Compliance • Error reduction	• Secured laboratory information hub • Compliance
Database focus	Document centric RDBMS	Transactional RDBMS	Transactional RDBMS
Typical IT infrastructure	• Windows workstation • Web client • Cloud • SaaS • SOA	• Windows workstation • web client • portable devices	• Windows workstation • Web client
Application behavior	Experiment centric	Sample/Process centric	Sample/Process centric
User Interface behavior	• User centric • Free form & Adaptable	• User centric • Procedural • Natural language	• Organizationally centric • Procedural • System defined
Related Applications	Scientific databases	LIMS, ERP, Instruments	LES, ERP, MES, CAPA
End user adoption	High	High	Mixed
Compliance support	+/-	++	++

Due Diligence-Off to the Races….

- A list of critical considerations:
  - System and architectural integration
  - Ease of use => End User/Administration
    - OOB configuration vs customization
    - Instrument & application integration lists
    - Support and maintenance
    - Search-ability
  - Data location and ultimate migration plan
  - How does it handle collaboration
  - Vendor Specific
    - Overall vendor score (services, quality, technology)
    - References

How will this Support Quality?

- Consistency
- Reproducibility
- Structured Reporting
- Searchable/Findable
- Documented workflow
- Method/SOP Execution
- Auditable
- Validation
- Calibration Verification

ELE: Pros and Cons

- Pros
  - Organization, efficiency gains, electronic archival
  - Traceability (Data, Processes and People)
  - Part of shareable “Information and Data” foundation

- Cons
  - Vendor dependent with possible technology mismatching
  - Functionality scope creep or solution bloat
  - Solutions become very sticky
  - Support and maintenance
  - Potential data silo
  - IP protection?

Making Better Choices and Decisions

Intelligent Decisions

Intelligence in the right situations drives better decisions

Knowledge plus foresight or intuition becomes intelligence

Information plus insight becomes knowledge

Data in context becomes information

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Best in Breed ELNs

- Cloud based
  - Biovia Science Cloud (MT)
  - IDBS
  - Arxspan (MT)
  - Core (MT)
  - Sapio Sciences (2 mode notebook) (MT)

- Client server (On Premise)
  - Perkin Elmer (CambridgeSoft)
  - Biovia (formerly Accelrys/Symyx)
  - IDBS
  - Waters

Laboratory Execution Systems

- Biovia- LES
- Perkin Elmer-iLAB
- Thermo Scientific- LES

Best In Breed LIMS

- Cloud
  - Sapio Sciences Exemplar
  - Core Informatics LIMS
  - Genologics (NGS orientied)

- Client Server
  - Thermo Scientific
  - Starlims
  - Labware
  - Waters' Nugenesis

Market Trends

- ELE and ELN are great opportunities to couple MDM (data standards and taxonomies) and governance/stewardship.
- Cloud….true multi-tenant ELN/LIMS etc.
  - Bundling of ELN, LIMS, SDMS
- 1 ELN per company/organization, worse case 2
- Holistic ELE… ELN, LES, LIMS and integration

Externalization-The Distributed Industrialized Science Business Model

- Many research and development organizations today have adopted a distributed business model.
- Our clients are both Industry, Government and Academia
- The challenges:
  - Data/information and knowledge exchange
  - Capturing data and process
  - Starting and ending new relationships
  - Technology mismatches
  - Being prepared for externalization
  - Managing the logistics
    - Request
    - Sample/Patient/Experiment tracking

Conclusion

- Organizations may need very specialized ELNs that have a plethora of supporting applications. This will be a key part of their ELE

- Task or method driven areas of research based companies may not need an traditional ELN but instead a laboratory design and execution solution that captures information and data.

- Keep the big picture in mind when choosing and implementing an ELN…
  - First to file not First to Invent (Research)
  - Knowledge management and Analytics
  - Distributed Research or Service Model
  - Request Management

Backup Slides and SMILES

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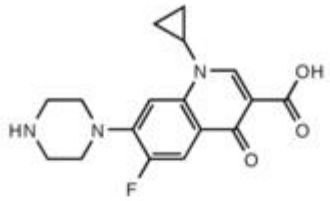

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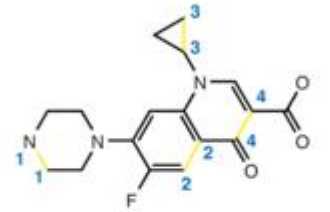

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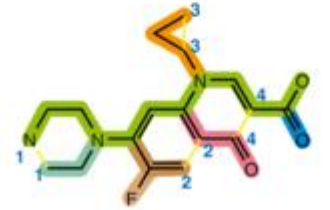


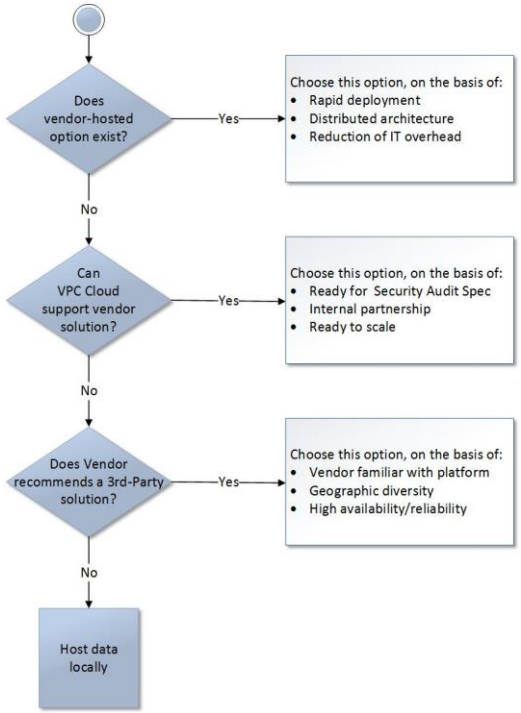
D

N1CCN(CC1)C(C(F)=C2)=CC(=C2C4=O)N(C3CC3)C=C4C(=O)O

The **simplified molecular-input line-entry system** (**SMILES**)

Example Decision Trees for Selection and Implementation of Solutions

- Data virtualization
- Security
- Latency
- Support burden
- Accessibility
- Ease of migration (solution and or data)
- Hosting Solution(s)
- Architecture (flexibility)



ELNs on the Market Today

Agaram	QA/QC ELN (LogiLab)
Agilab	Biology focused (ELN Biolab)
Agilent	Non-specific with add-on modules (OpenLAB ELN)
Amphora Research	Non-specific (PatentSafe)
Arxspan	Chem and Bio (ArxLab)
Axiope	Biology (e-Cat)
Benchling	Life science (Benchling)
BioData	Non-specific (Labguru)
Bio-ITech	Academic life science (eLabJournal)
Biovia (former Accelrys)	Multiple (Biovia Notebook, Biovia E Notebook, Biovia LES)
ChemBytes	Chemistry-specific (Espresso ELN)
Core Informatics	LIMS foundation, Cloud (Platform for Science)
DeltaSoft	Chemistry-specific (DeltaBook)
Docollab	Free, cloud-based (docollab)
Dotmatics	Multiple (Studies Notebook)
eNovalys	Chemistry specific (ePro)
Enso Software	Chemistry (Ensochemlab)
EZQuant	Biology (EZQuant)
Findings	Mac-based (Findings)