



# Cross Disciplinary Informatics: A Future Look

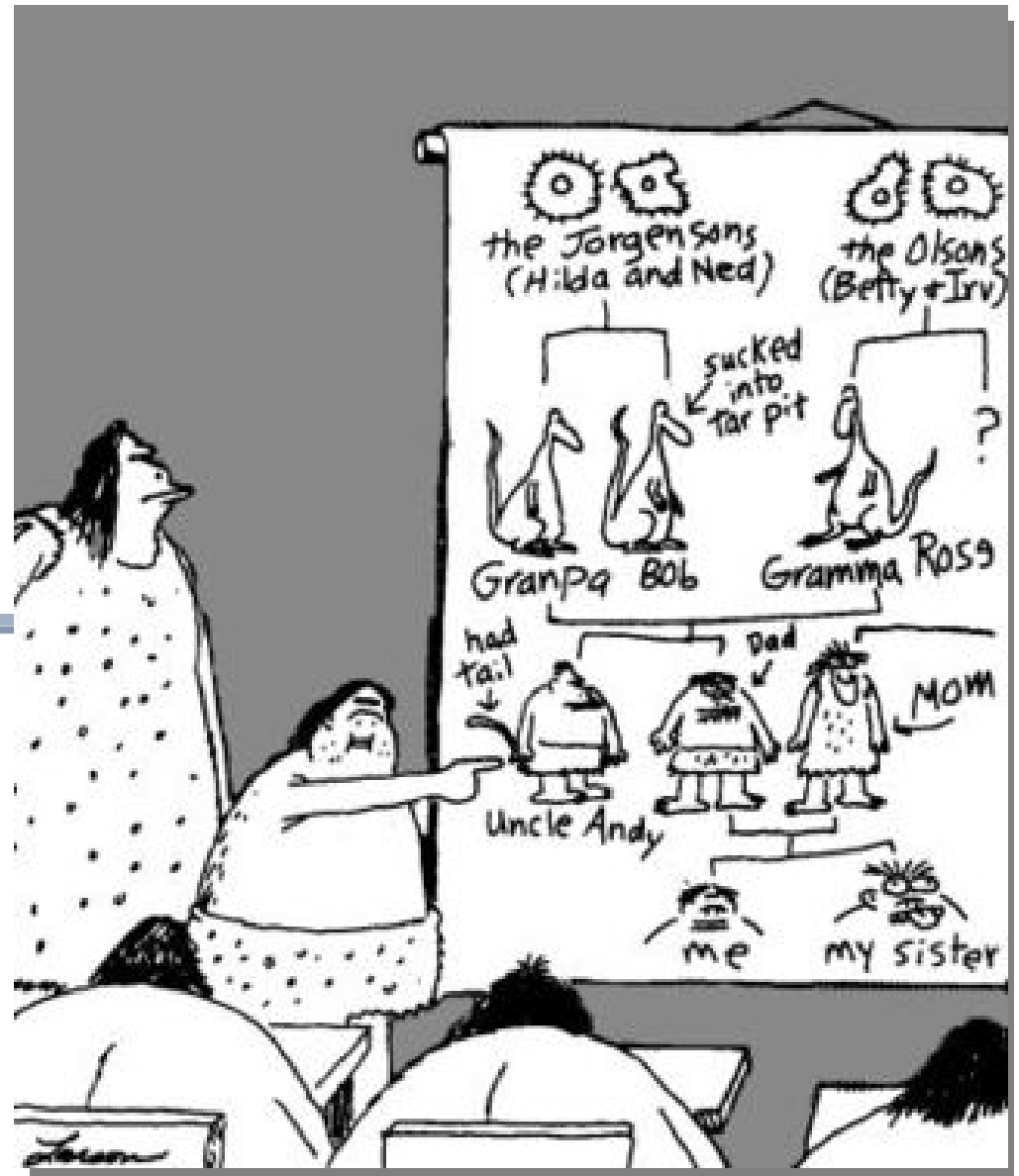
*Evolving Beyond the "Paperless Lab"*

*Michael H Elliott*

*CEO*

*Atrium Research & Consulting*

*[www.atriumresearch.com](http://www.atriumresearch.com)*



# Agenda

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- ▶ Introduction

- ▶ Trends

- *Convergence and Modularity of Informatics*
- *Data convergence and master data management*
- *External Technologies Impacting the Future: The Next "Wave"*

- ▶ Q&A



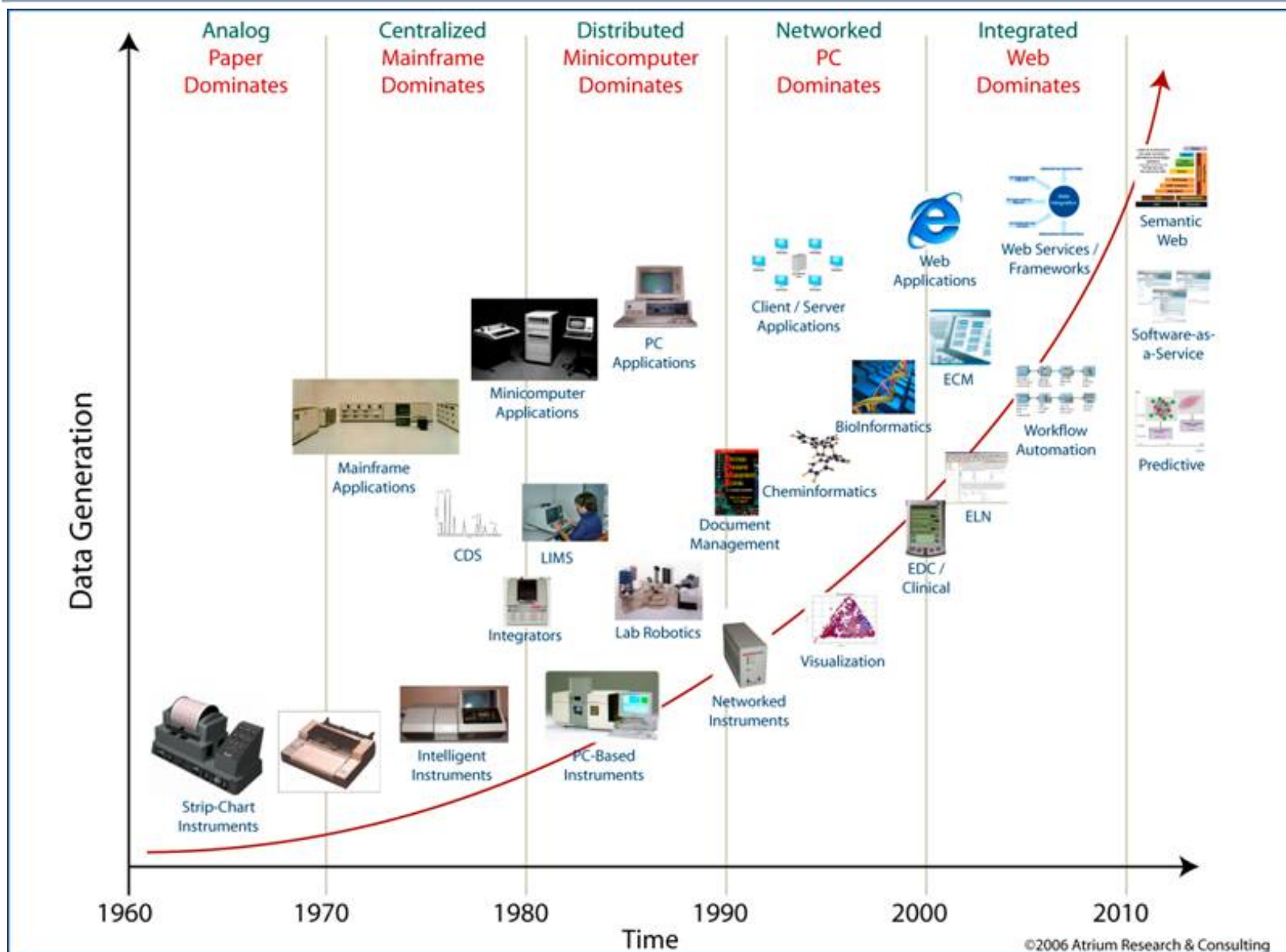
# About Atrium Research

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Atrium Research is an independent,  
vendor-agnostic market research and  
strategy advisory practice specializing in  
scientific informatics



# We Have Thrown Out a Lot of Technology Over the Years...



# ...but, Data Management Challenges Persist in the Laboratory

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1. Finding what I need when I want it
2. Storing and organizing data and information
3. Sharing data and information
4. I have to use too many systems and databases
5. I have to consolidate data from multiple sources
6. Keeping up with all the data being generated



Source: Atrium Research 2006,07,08 Surveys

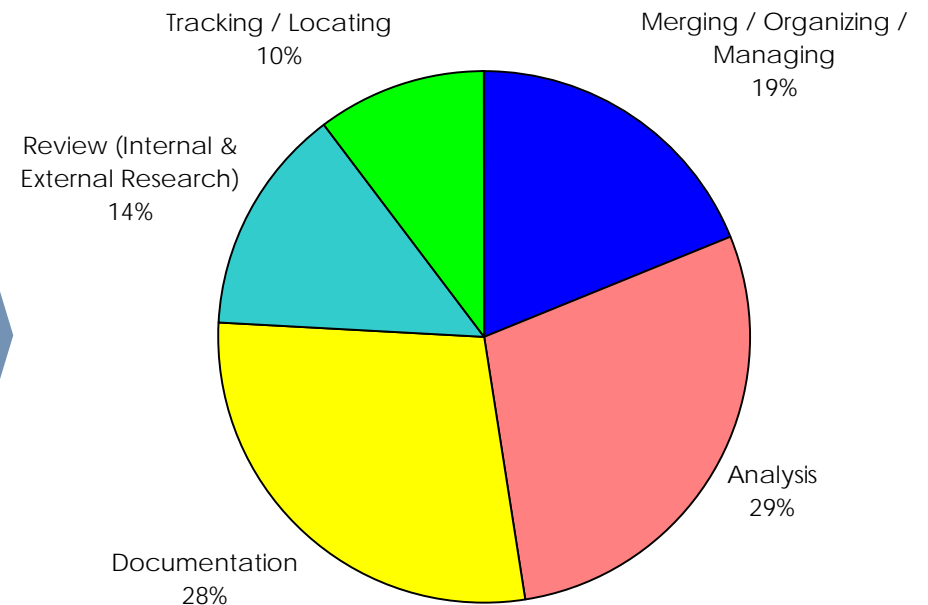
# Work Time Spent on Data Related Tasks is Approximately 50%

## Medicinal Chemist Study

Data and Information Tasks:	45%
Exp Design and Execution:	33%
Admin / Meetings / Other:	24%

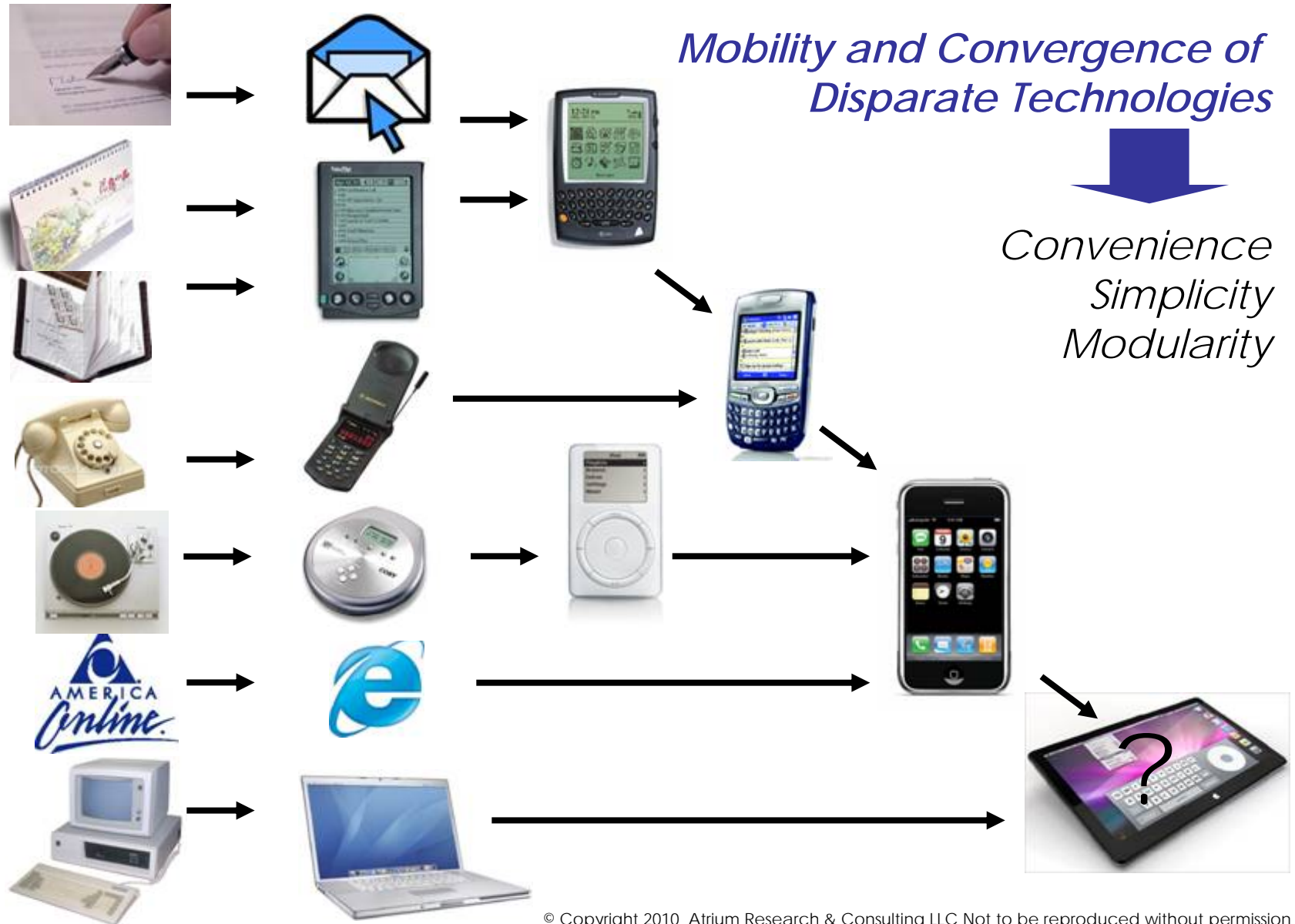
## Biologist Study

Data and Information Tasks:	48%
Exp Design and Execution:	36%
Admin/Meetings/Other:	16%



Source: Atrium Research Market Research

# External Factors are Shaping Customers' Expectations of Informatics in the Lab



# What is Informatics Convergence?

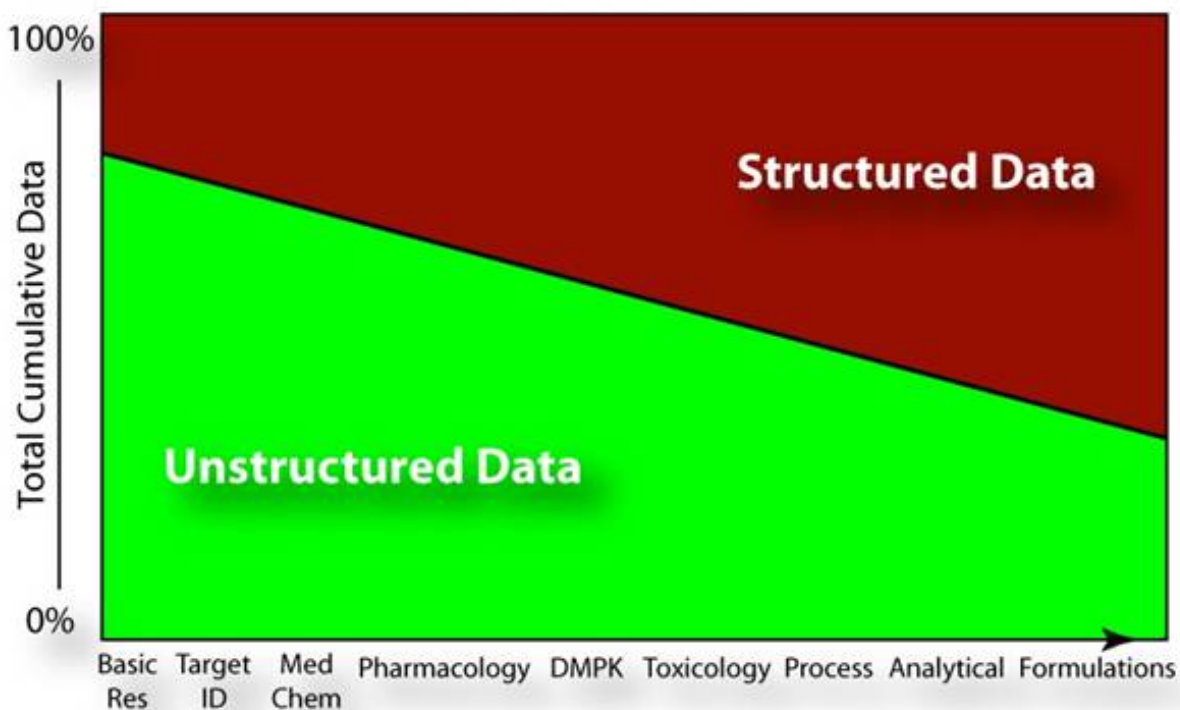
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(k n-vûr j ns)

*The evolution of informatics technologies that occupy a similar environment toward a holistic solution architecture with a common interface, eliminating overlapping functionality and independent integrations*



# There is a Reason for Convergence...



*...Customers expect holistic “whole product” solutions to their specific process, efficiency and data management challenges*

*... ELN is pushing farther downstream into areas of increasingly defined workflows and structured data*



# Vendors are Moving Away from Traditional Category Definitions

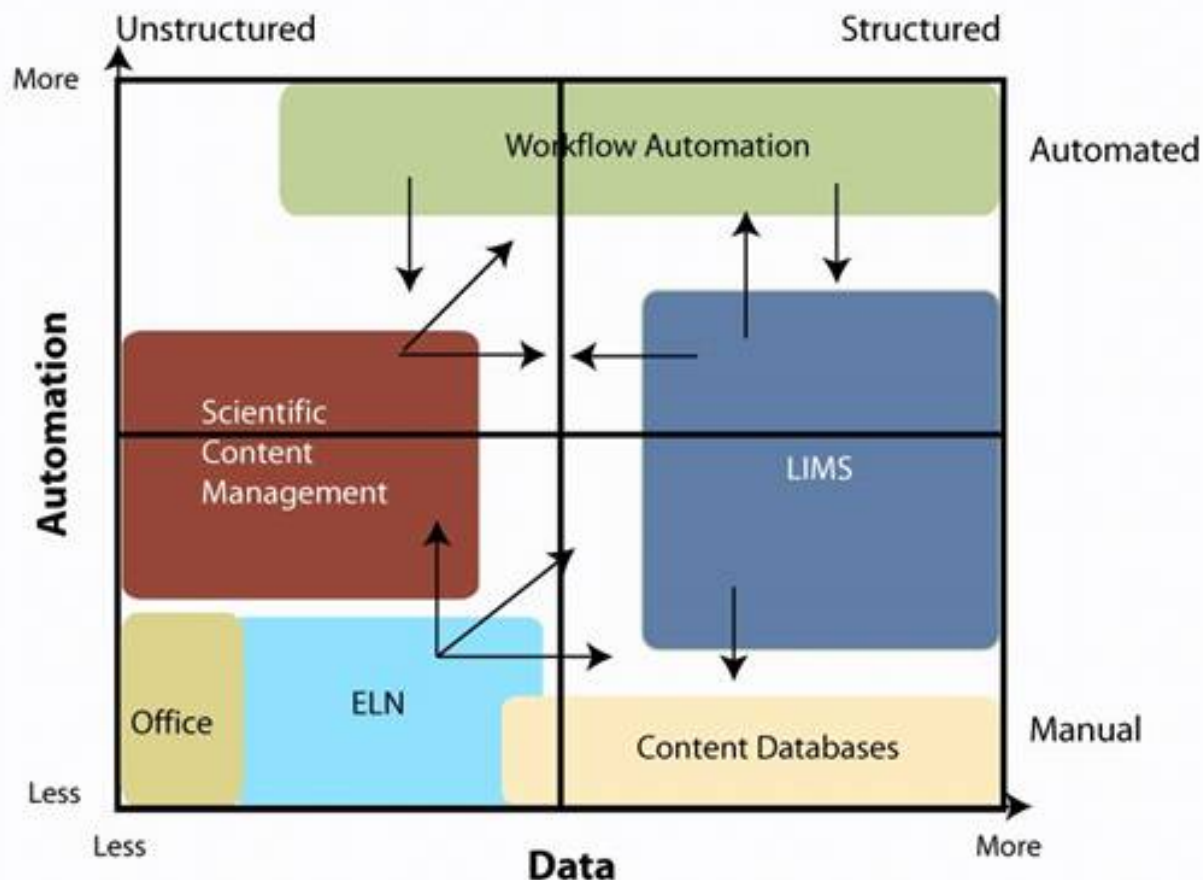
*LIMS companies are adding ELN components*

*ELN suppliers are improving structured data mgt and reporting*

*LIMS and ELN players are adding instrument data mgt capabilities*

*Consultants are adding ELN and SDMS capabilities to products like SharePoint*

*Workflow automation is moving quickly into ELN*

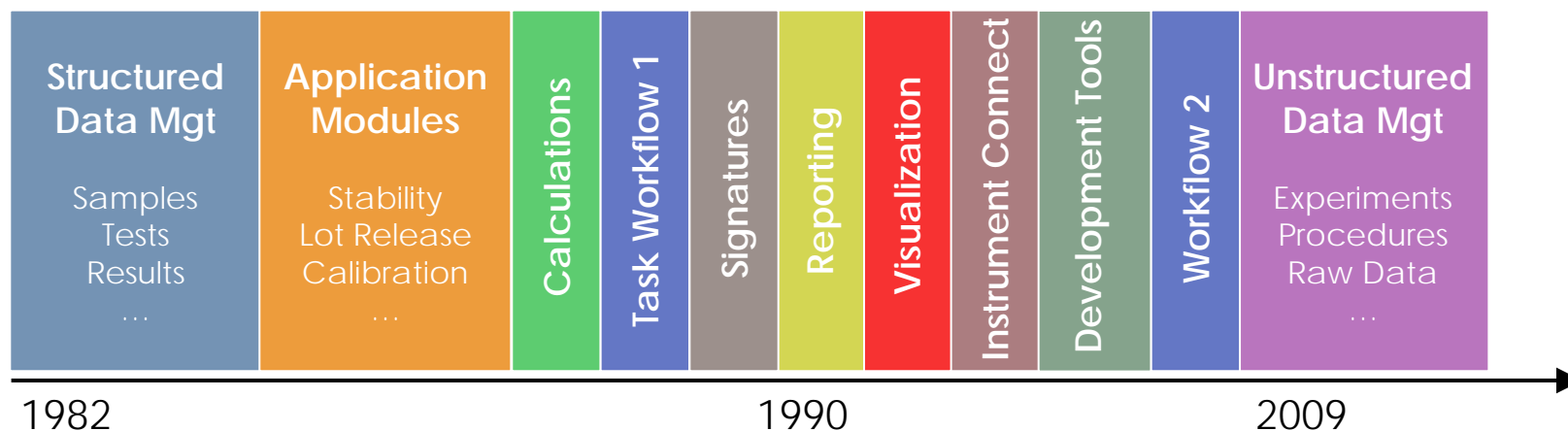


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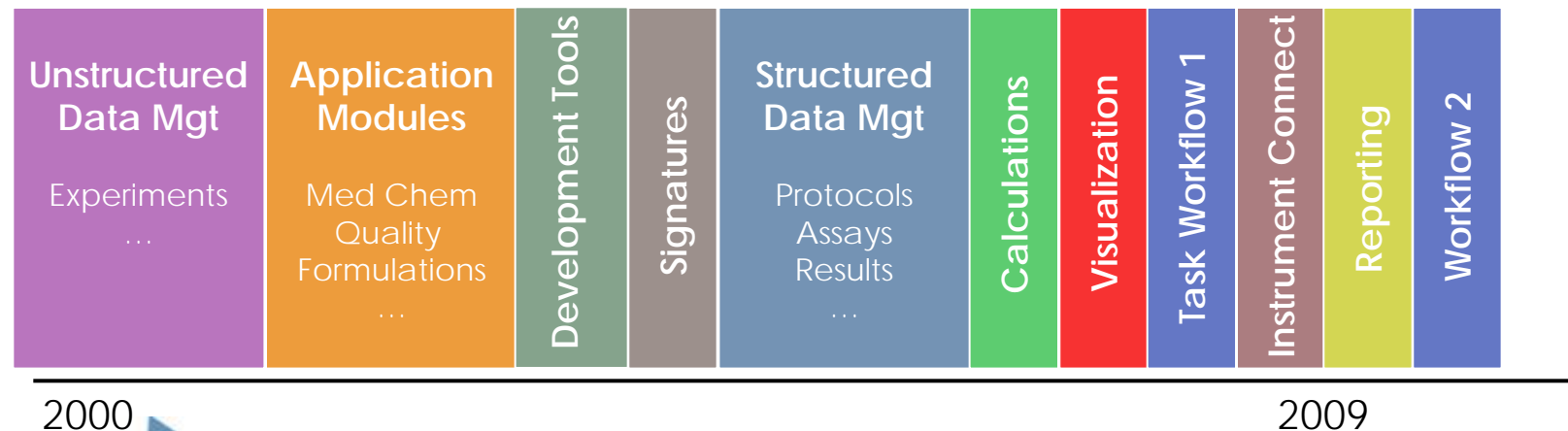


# ELN Evolution ... Look Familiar?

## LIMS



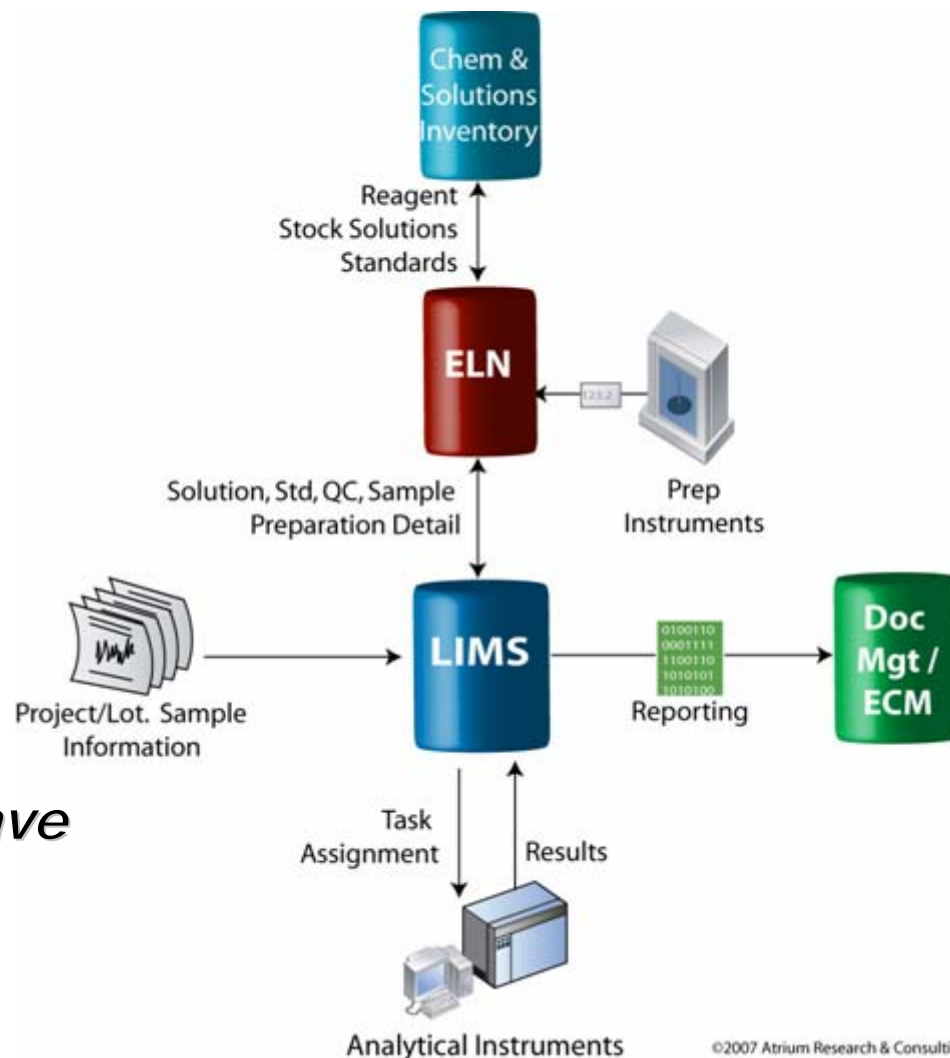
## ELN



# Thinking Holistically About Data Mgt

## Example: Analytical

- ▶ LIMS tracks samples, tests, tasks, and workflow
- ▶ ELN tracks sample, std, QC, and solution preparation details and other procedures

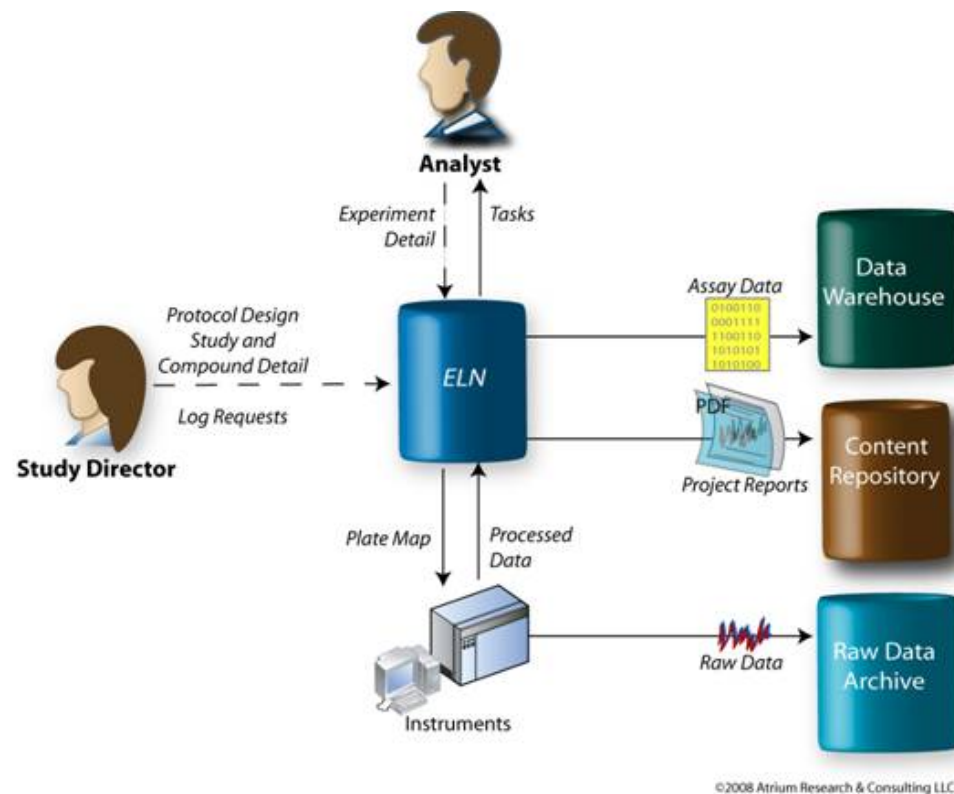


*People are asking: Why do I have to use two (or more) systems for information management in the lab?*



# Expanding Definitions: Generation 4 ELN

- Document experiment detail in the ELN
- Use ELN for study design, analysis, & visualization
- Enact lab work processes using ELN technology
- Collaborate with others via ELN
- Signature routing via ELN
- Integrate instrument data directly
- ELN contains structured data for re-purposing
- Report project data from ELN directly



*A modular architecture adapting to the needs of multiple domains*



# Gen 4 ELN: Expanding Capabilities far Beyond "Replacing Paper"

## Changing the Perception of ELN

**Protocol / Study / Experiment Design**

**Process / Workflow Automation**

**Data Analysis / Statistics / Calculations**

Phase	Time	Temp. %	Temp. %	Phase %	Phase %	Temperature (°C)	Temperature (°C)
1	0.00	100.00	100.00	100.00	100.00	37.00	37.00
2	0.00	100.00	100.00	100.00	100.00	37.00	37.00
3	0.00	100.00	100.00	100.00	100.00	37.00	37.00
4	0.00	100.00	100.00	100.00	100.00	37.00	37.00
5	0.00	100.00	100.00	100.00	100.00	37.00	37.00
6	0.00	100.00	100.00	100.00	100.00	37.00	37.00
7	0.00	100.00	100.00	100.00	100.00	37.00	37.00
8	0.00	100.00	100.00	100.00	100.00	37.00	37.00
9	0.00	100.00	100.00	100.00	100.00	37.00	37.00
10	0.00	100.00	100.00	100.00	100.00	37.00	37.00
11	0.00	100.00	100.00	100.00	100.00	37.00	37.00
12	0.00	100.00	100.00	100.00	100.00	37.00	37.00
13	0.00	100.00	100.00	100.00	100.00	37.00	37.00
14	0.00	100.00	100.00	100.00	100.00	37.00	37.00
15	0.00	100.00	100.00	100.00	100.00	37.00	37.00
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19	0.00	100.00	100.00	100.00	100.00	37.00	37.00
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42	0.00	100.00	100.00	100.00	100.00	37.00	37.00
43	0.00	100.00	100.00	100.00	100.00	37.00	37.00
44	0.00	100.00	100.00	100.00	100.00	37.00	37.00
45	0.00	100.00	100.00	100.00	100.00	37.00	37.00
46	0.00	100.00	100.00	100.00	100.00	37.00	37.00
47	0.00	100.00	100.00	100.00	100.00	37.00	37.00
48	0.00	100.00	100.00	100.00	100.00	37.00	37.00
49	0.00	100.00	100.00	100.00	100.00	37.00	37.00
50	0.00	100.00	100.00	100.00	100.00	37.00	37.00

**Data Visualization / Graphics**

**Chemical Inhibition of L23211 metabolism**

**Objective:**  
The objective of this experiment is to determine the percent involvement of the CYP450 isoforms responsible for the metabolism of X44343 in human liver microsomes via chemical inhibition with a known inhibitor at its approximate concentration. Since the CYP profiling experiment (XSDW121) indicated that 2D6, 1A2, and 3A4 have the potential for metabolizing X44343, three chemical inhibitors will be individually incubated with the substrate to....

**Documentation / Annotation**

**Collaboration**

**E-Signatures and Routing**

**Searching and Reporting**

**DM / Organization / Taxonomy**

- Study 1234
  - Chemistry
    - Exp123
    - Exp124
    - Exp125
  - DMPK
    - CYP 123
    - Microsomes123
    - PK123
  - Pharmacology
    - Locomotor
    - PK
    - Biomarkers
    - Exp R-001

**Security / Protection / Management**

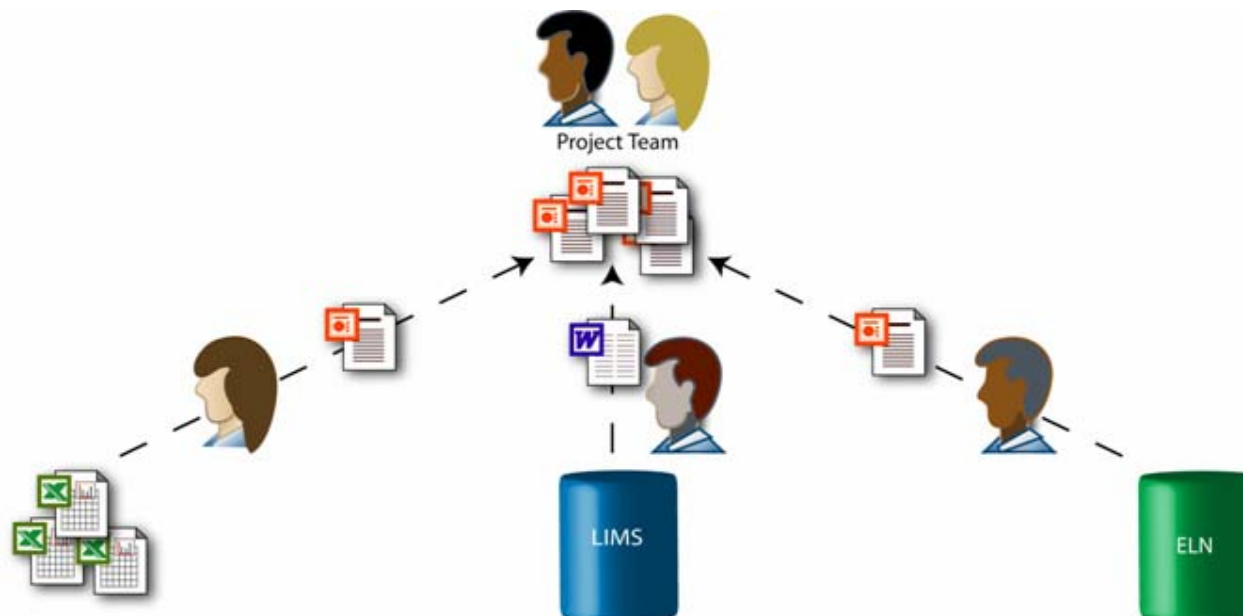
**Development / Configuration**

**Integration**

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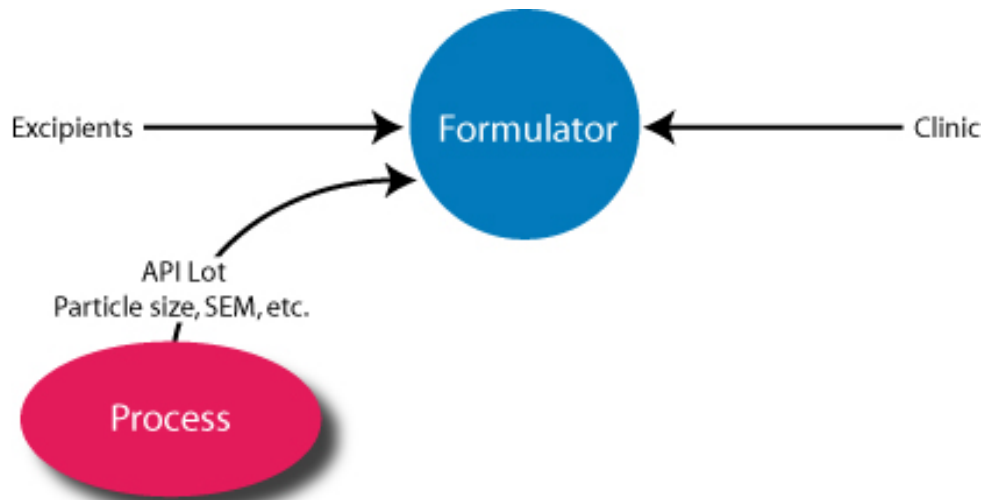
# Technology Aggregation is Not the Only Answer...

- ▶ R&D Projects are increasingly being managed based on uncontrolled PowerPoint files
  - Files are not accessible to the enterprise
  - Data are not codified, requiring manual interventions
  - Knowledge and IP are not captured
  - Decisions are based on incomplete data sets

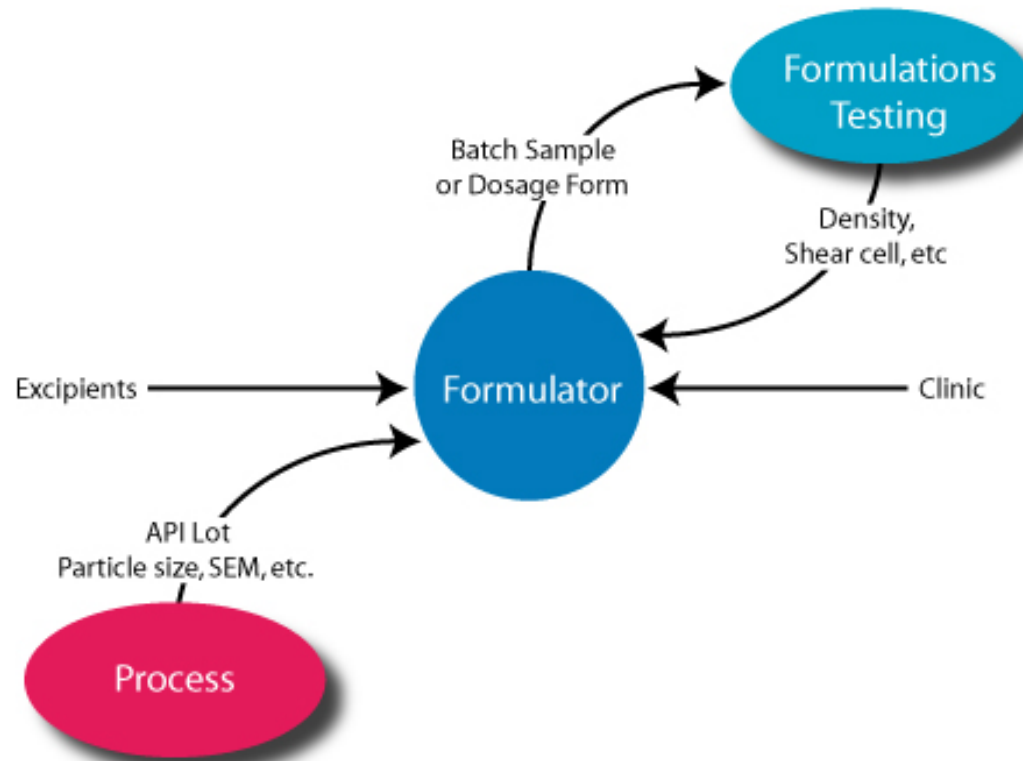


# Example: Consider a Formulation Data Integration Challenge...

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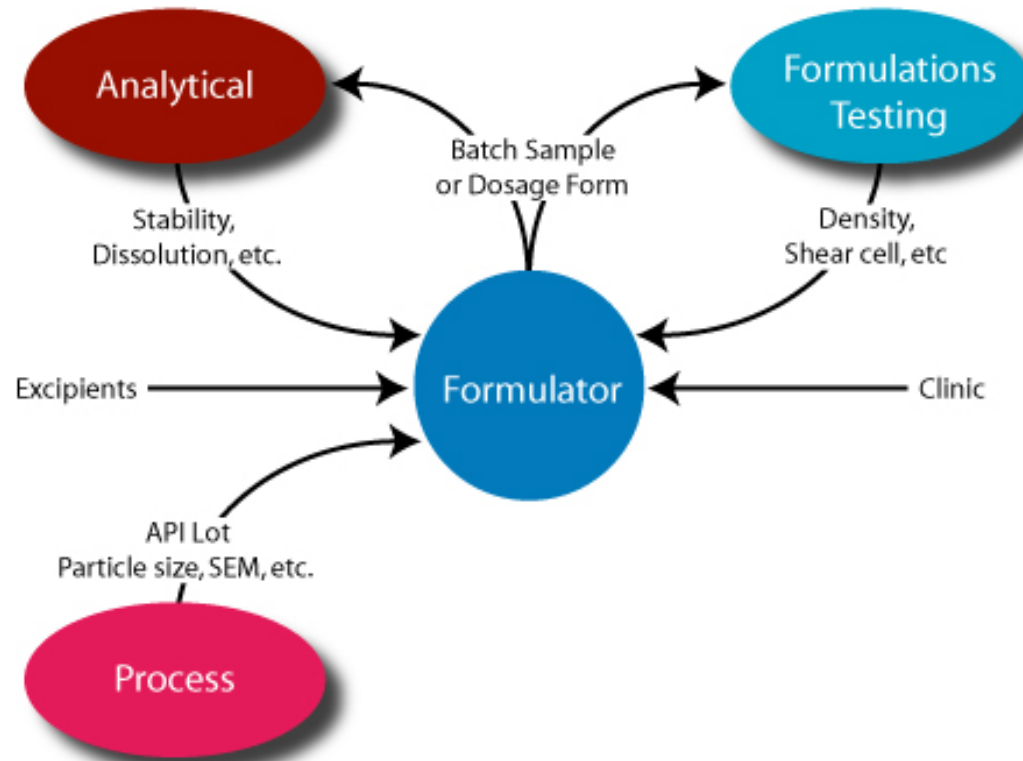
# The Formulator's ELN is Tuned to the Creation of Formulation Batches and Dosage Forms



## Formulation ELN

- ▶ Formulation Composition
- ▶ Creation of formulation batches and dosage forms
- ▶ Procedure documentation
- ▶ Managing materials
- ▶ Formulation calculations
- ▶ In-process testing
- ▶ Batch record generation
- ▶ ...

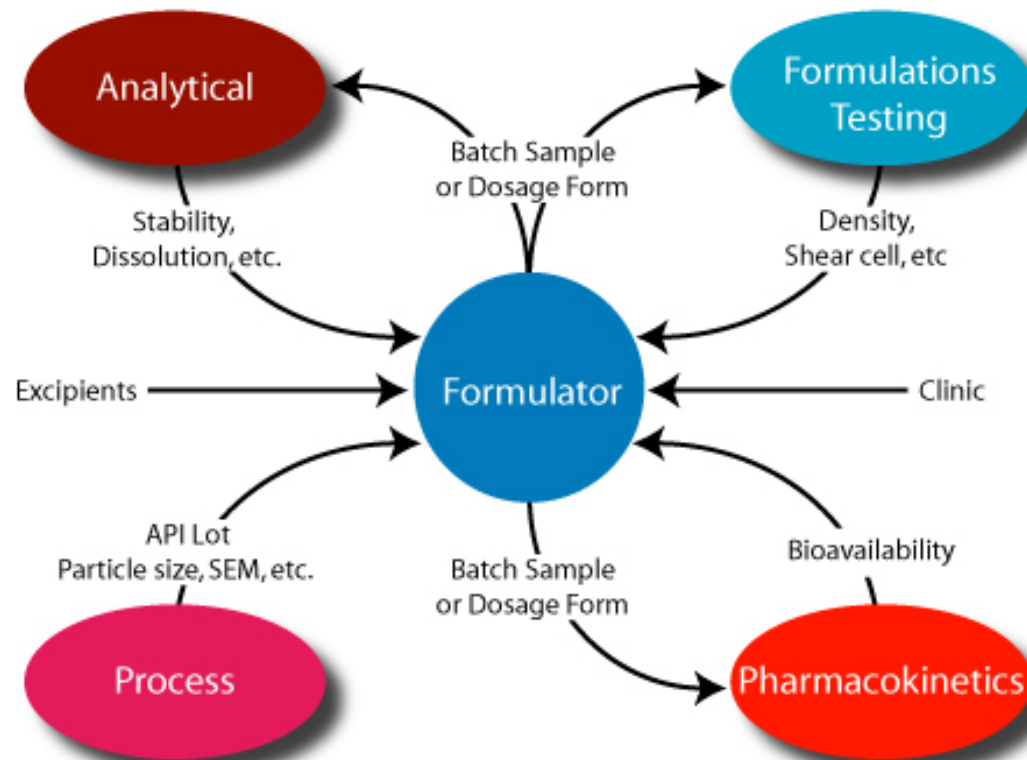
# Analytical Primarily Distributes Results Through LIMS Reporting



## Analytical LIMS

- ▶ Sample management
- ▶ Results management
- ▶ Work assignment
- ▶ CDS integration
- ▶ Stability management
- ▶ Reporting

# PK's ELN is Tailored to Management of their *in vivo* Studies and Data Analysis

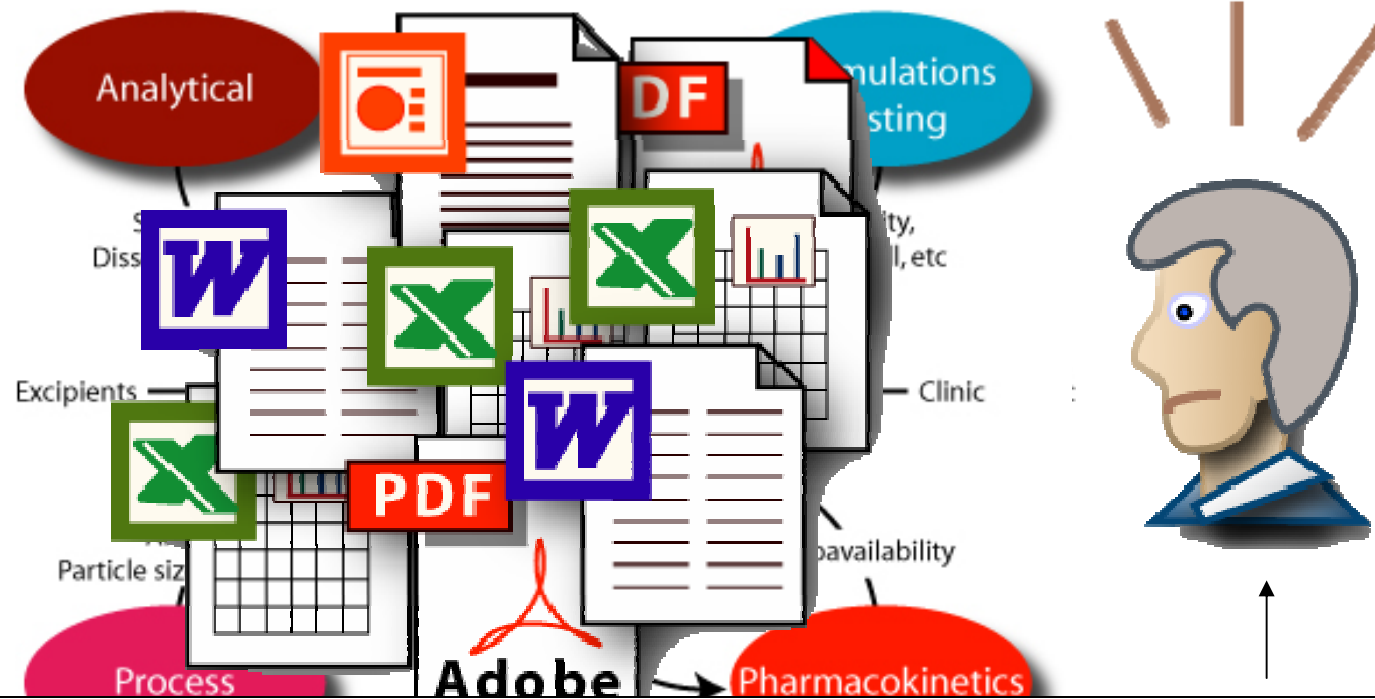


## Pharmacokinetics ELN

- ▶ Protocol/Study design
- ▶ Subjects, treatment groups, dose plan
- ▶ Work scheduling
- ▶ Animal weights
- ▶ Dose schedules
- ▶ LC-MS plate creation
- ▶ LC-MS data import
- ▶ Data analysis
- ▶ Data visualization
- ▶ Reporting
- ▶ ...

*... each group focused on their own departmental workflow requirements*

# Poor Bob, the Formulation Scientist

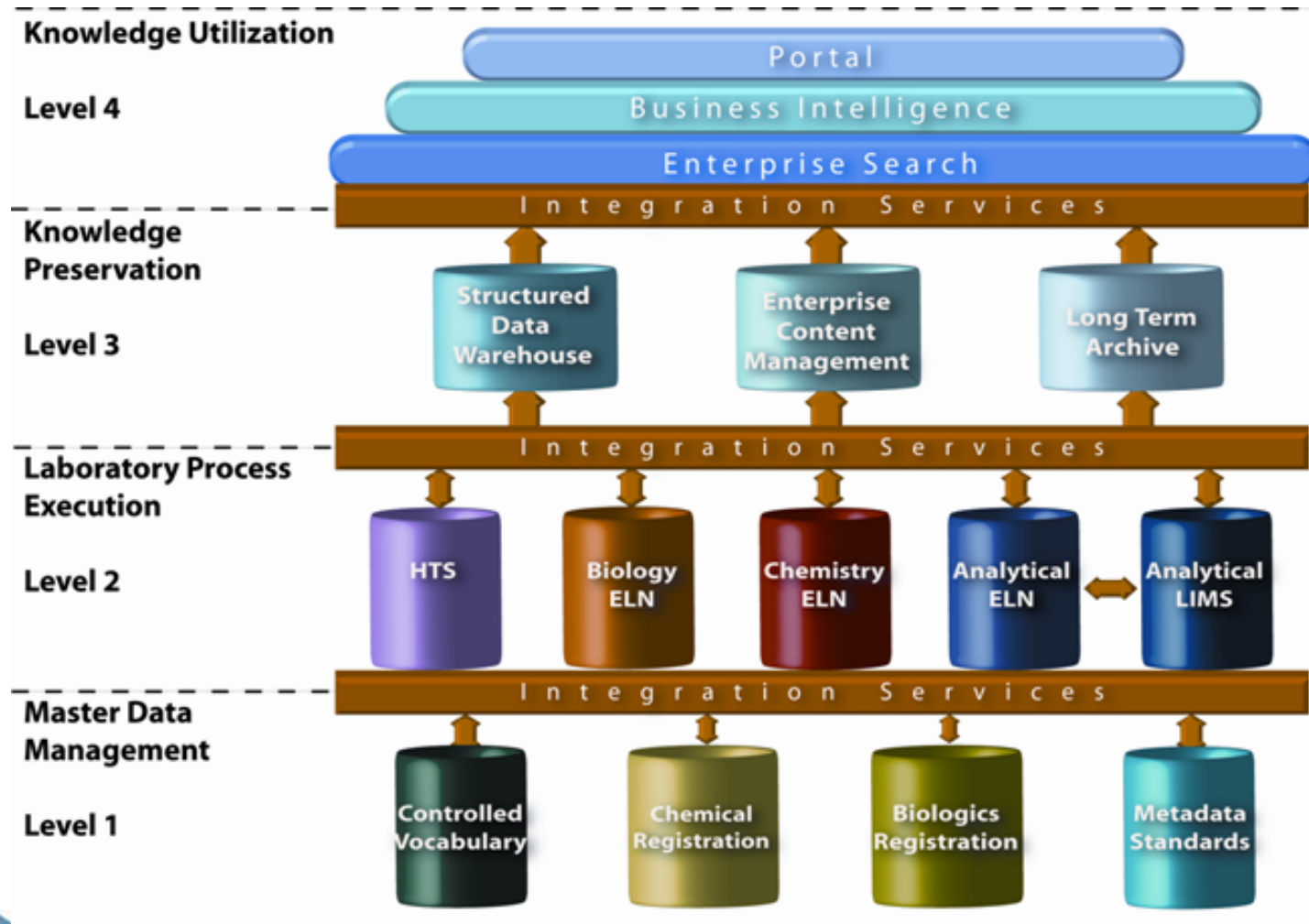


Bob has to manually aggregate data for analysis of dissolution v. bioavailability, particle size v. BA, stability v. particle size, ...

*Different formats and descriptors from each department*

***“PAPERLESS LAB” IS NOT GOOD ENOUGH!***

# The Future State will Require Data Architecture Systemic Thinking



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*Master Data Management impacts macro-level benefits*



# External Technologies Shaping the Future of Informatics

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*Catching the Wave*

# Scorecard of a Few Technologies Impacting R&D Informatics

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## ▶ Technologies

### – **Semantic Web**

- In holding pattern (visionary stage) waiting for a problem to the solution

### – **R&D “Cloud” Computing**

- So far, high in the “hype” cycle – very low adoption for IP mgt
- Academic and Government accounts show primary interest as a cross-site collaboration platform

## ▶ Products

### – **Microsoft SharePoint**

- Quickly gaining traction as a collaboration tool
- Visionaries are leveraging for ELN and project team spaces

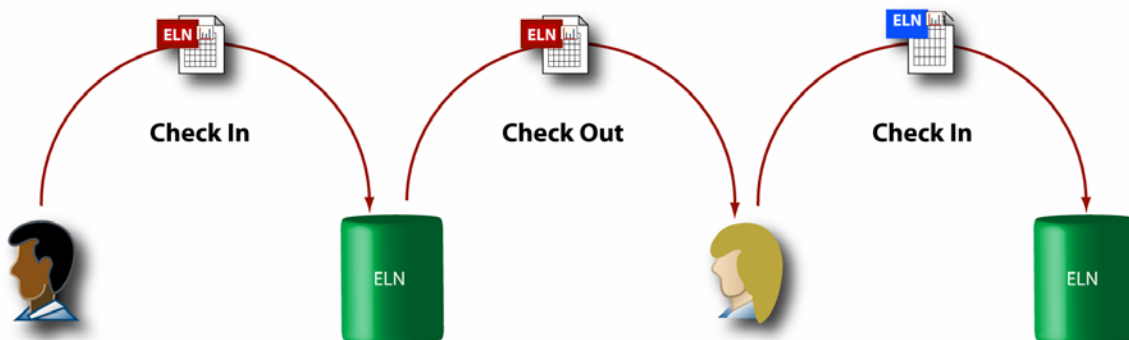
### – **Google Wave**

- Not yet delivered, but could solve many of the collaborative challenges not addressed by current technologies



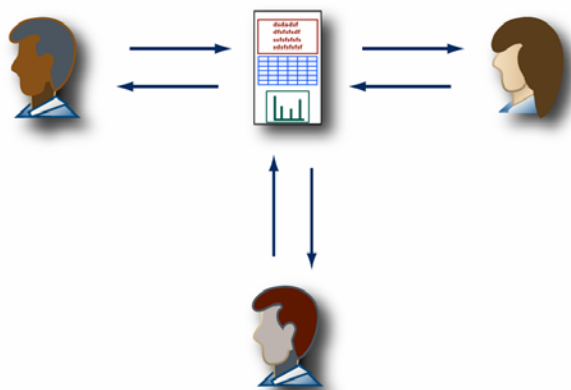
# Research in the "Wave"

## Traditional Document Mgt, E-Mail AND ELN!!



*Rethinking  
Information Flows*

## Collaboration in the "Wave"



*Contemporaneous  
collaboration  
without the  
Traditional "Paper"  
mindset!*



# Summary

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- ▶ The traditional lines between informatics categories is blurring
  - Focus on a “whole product” solution
  - Must understand complete workflow, not just a segment
- ▶ In cross-functional informatics, consideration of data suppliers and consumers and the information value chain is essential for macro-level benefits
  - Master data management plays an important part to ensure long-term integration
- ▶ New technologies are emerging to move lab informatics away from a paper-metaphor





Questions?

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