



ACD/Labs

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Dealing with the Data Avalanche: A Knowledge Management System Designed Specifically for Your World of Metabolism & Impurities

Scott Lee
ACD/Labs
September 25th , 2007
NJ MS/Chrom Seminar

Advanced Chemistry Development, Inc. (ACD/Labs)

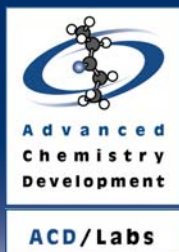
Visionary Software

Advancing Research

Analytical Data Challenge

Def. (n): Data are symbols, i.e., raw numbers, formula, text, etc.

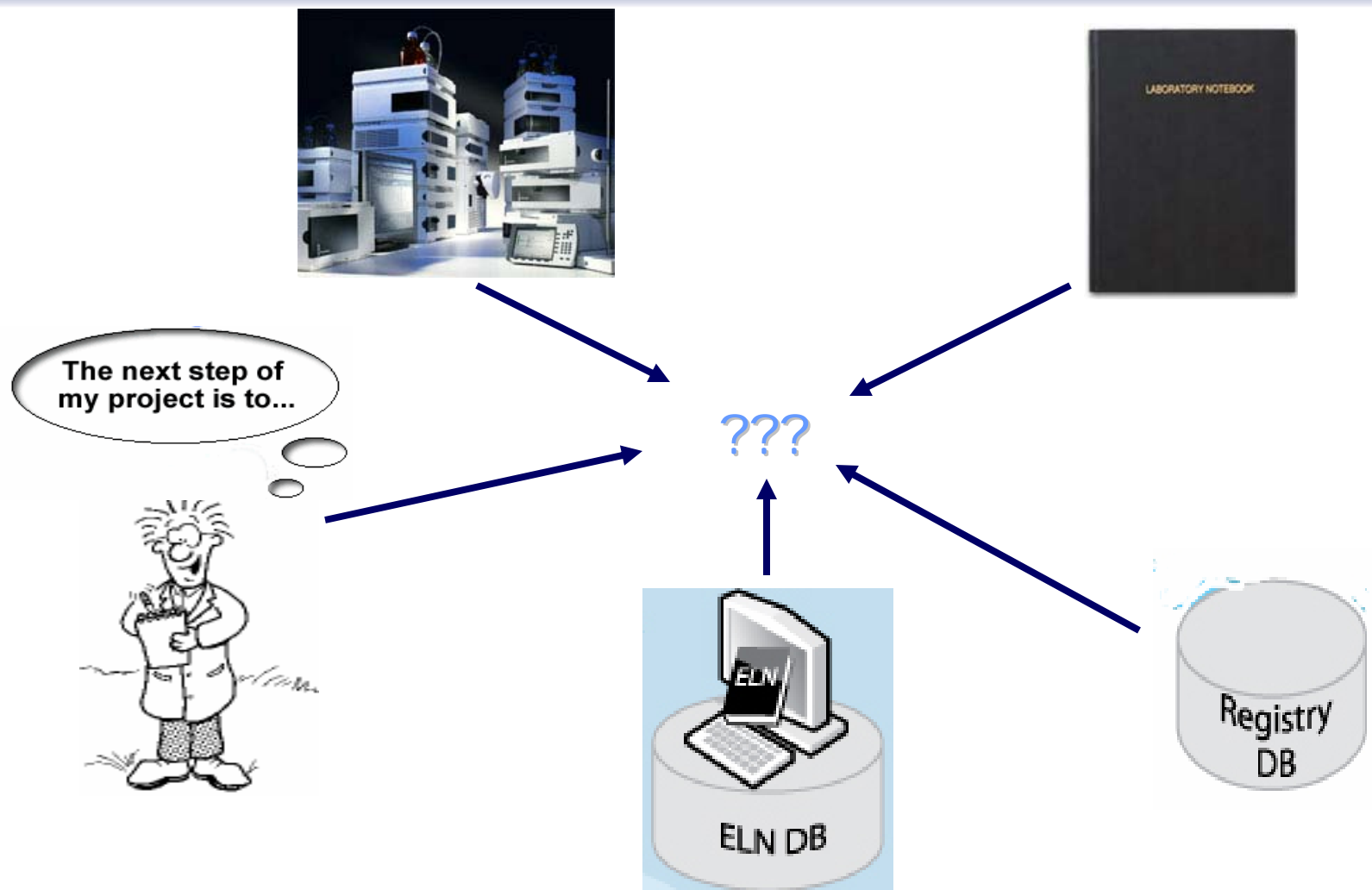
- ④ Primary Issues for Data
 - ④ Data overload
 - ④ Multiple disjointed data sources
 - No standard data formats
 - Complex multi-file arrays
 - ④ Low intrinsic significance
 - Useless until refined into meanings

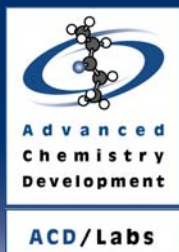


Common Pains

- ④ Many instruments and various manufacturers of instruments
- ④ Many different file formats
- ④ Many instrument vendor's processing software
- ④ Data not centrally located
- ④ Data not easily shared

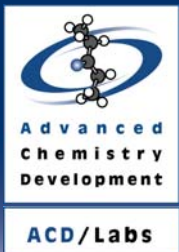
"Data Centers"



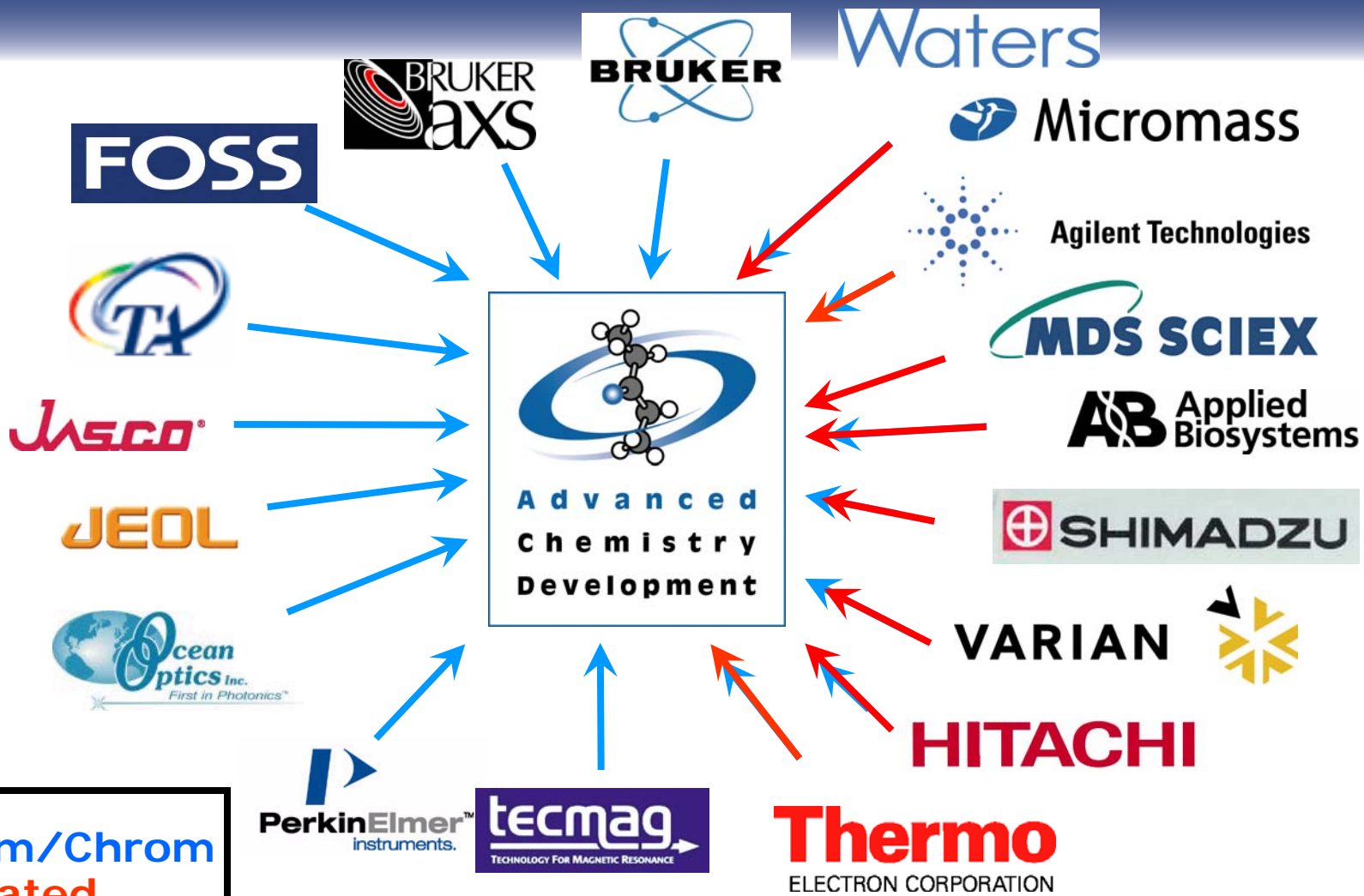


Enterprise Perspective

- ⦿ Generating Data Is Easy **BUT** Expensive:
 - ⦿ Instrument Market ~\$25B/year
 - ⦿ Lab infrastructure & technician salaries (>> \$25B ↑)
 - Data avalanche increasing(↑)
 - Cost of managing raw untreated data(↑)



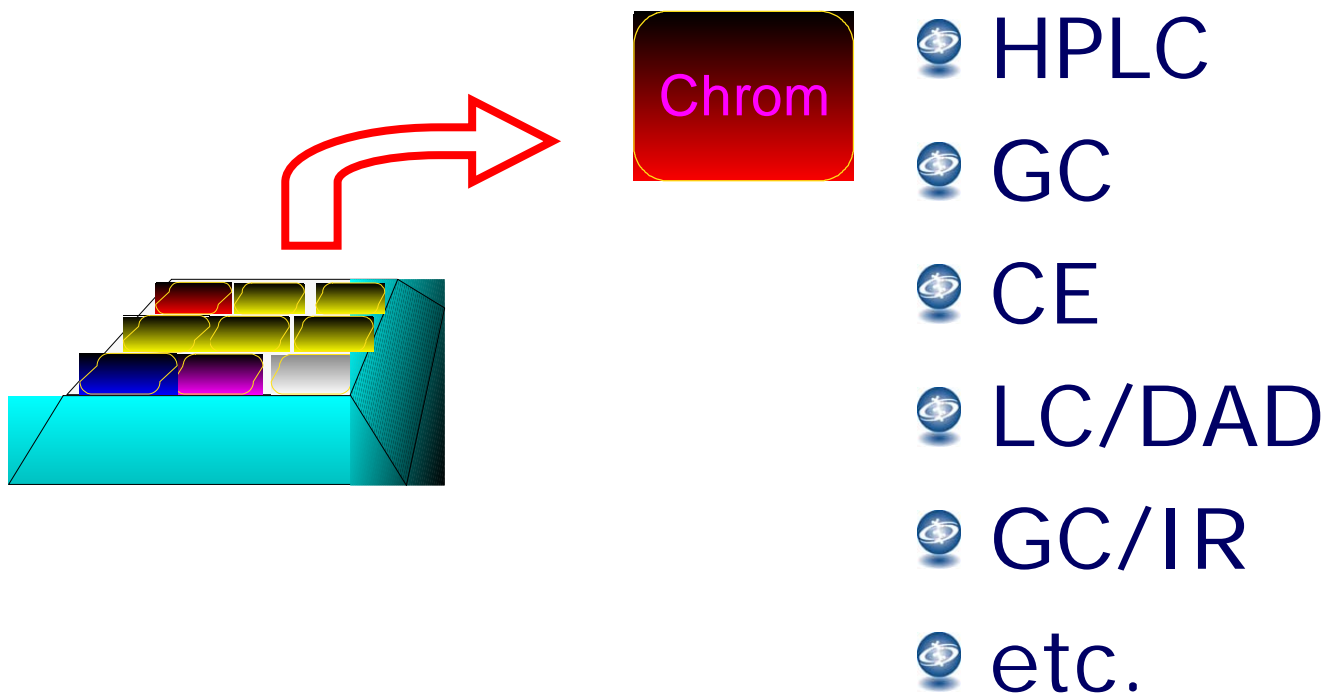
Import Instrumental Data Directly



Spectrum/Chrom
Hyphenated —

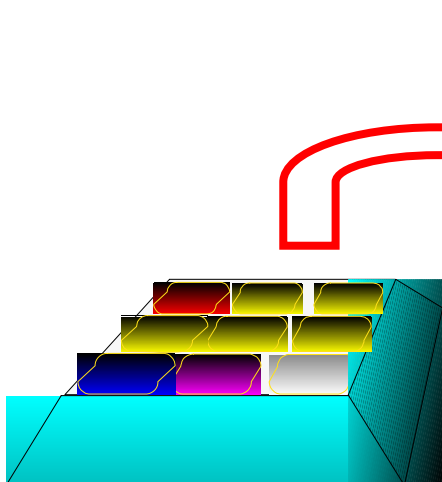
Simplifying Data Handling

One System to Support All Analytical Data
from **Different Techniques**



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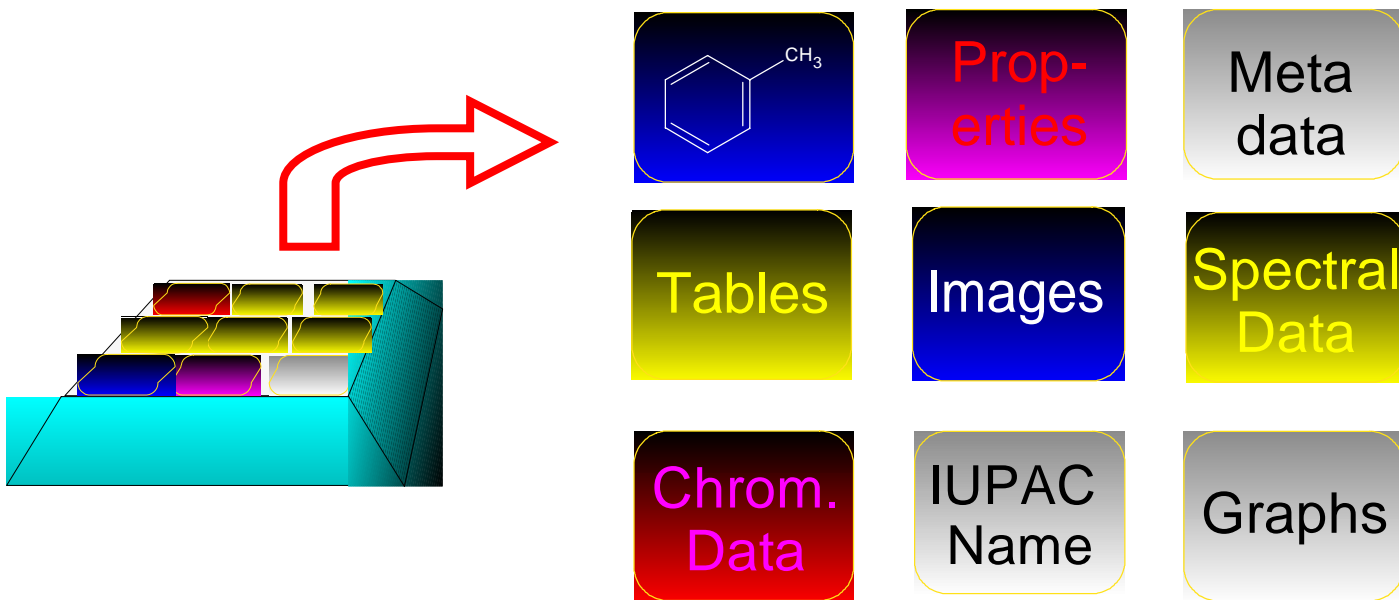
Mass
Spec.

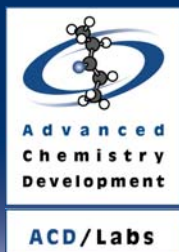
- ESI
- EI
- FAB
- LC/MS
- LC/DAD
- MS(n)
- etc.



Simplifying Data Handling

One System to Support **Different Types** of Analytical Data



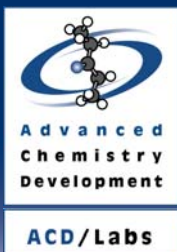


Beyond Information Collection and Generation

- According to an Outsell survey
 - 86% of scientists don't feel they know what information is available
 - 73% think it is too hard to find information
 - 73% find themselves unable to compare information alternatives
 - 71% complain of dubious information **quality, credibility, and accuracy**

What is Knowledge?

- Knowledge encompasses abstract concepts, so multiple definitions exist
 - Ideas, facts, truths, principles (rules), states of mind
- In practical terms, communication is the principal thread that connects information and knowledge



Knowledge Challenge

Def. (n): Application of information to produce scientific or business value

Primary Issues for Knowledge

Communication

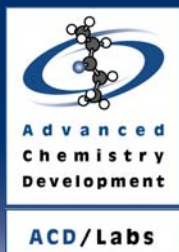
➤ Sharing data/information

Providing Insightful Perspectives

➤ Recognizing Patterns

➤ Recognizing Opportunities

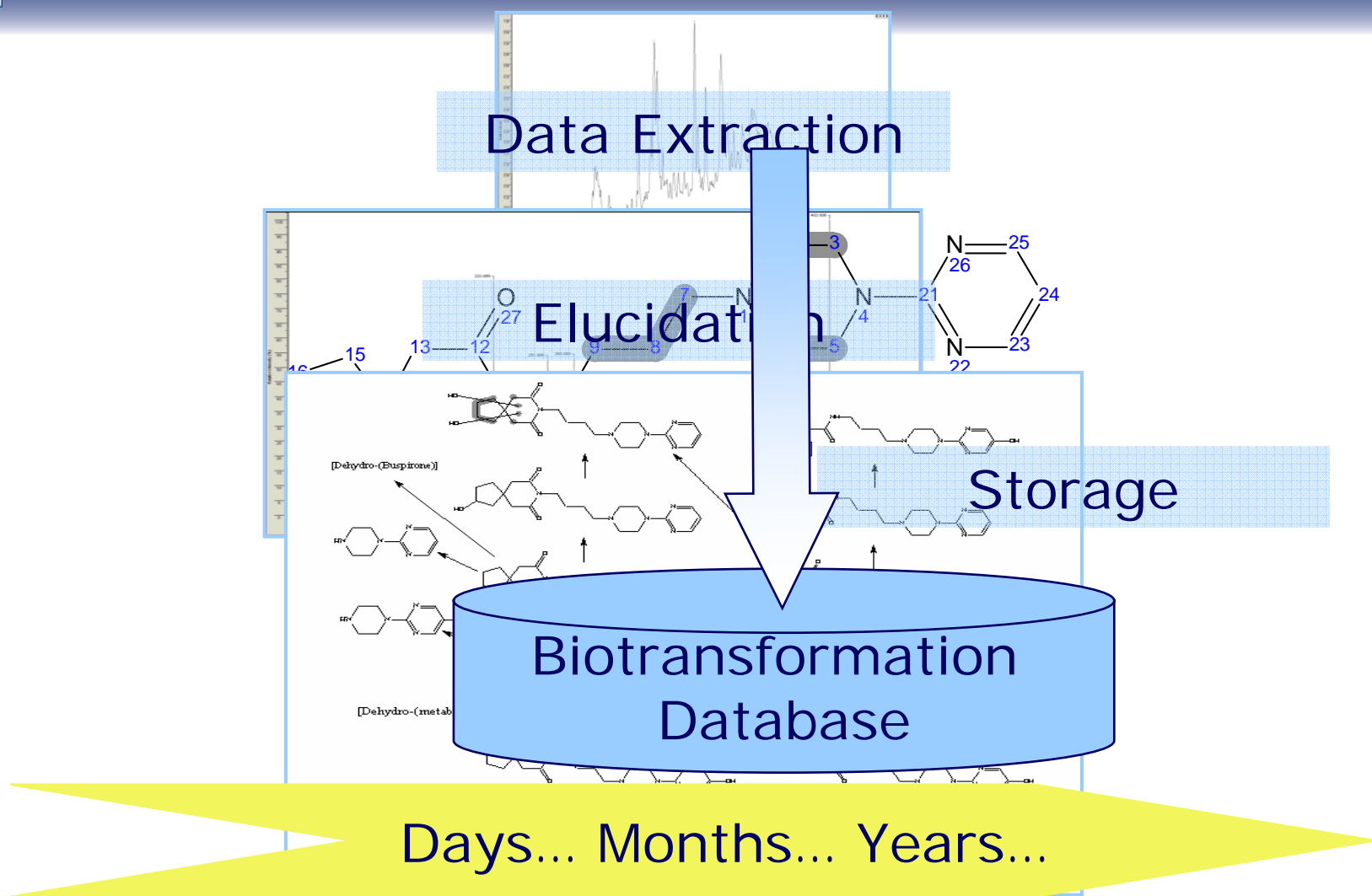




Benefits of Computer Assisted Information Extraction

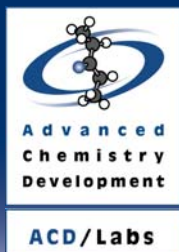
- With ACD/Labs software you can
 - Design better experiments with the insight of the property and spectral predictions (e.g. ACD/Method Development Suite)
 - Directly graph experimental or predicted responses which ties in analytical and property information

Application to the Metabolism World



Solution

- ④ Many Ways of Sharing Information
 - ④ On the desktop
 - ACD/SpecManager
 - ④ On the corporate intranet
 - ACD/WebLibrarian
 - ④ In conjunction with complementary third-party software vendors
 - ④ Structure searchable reports

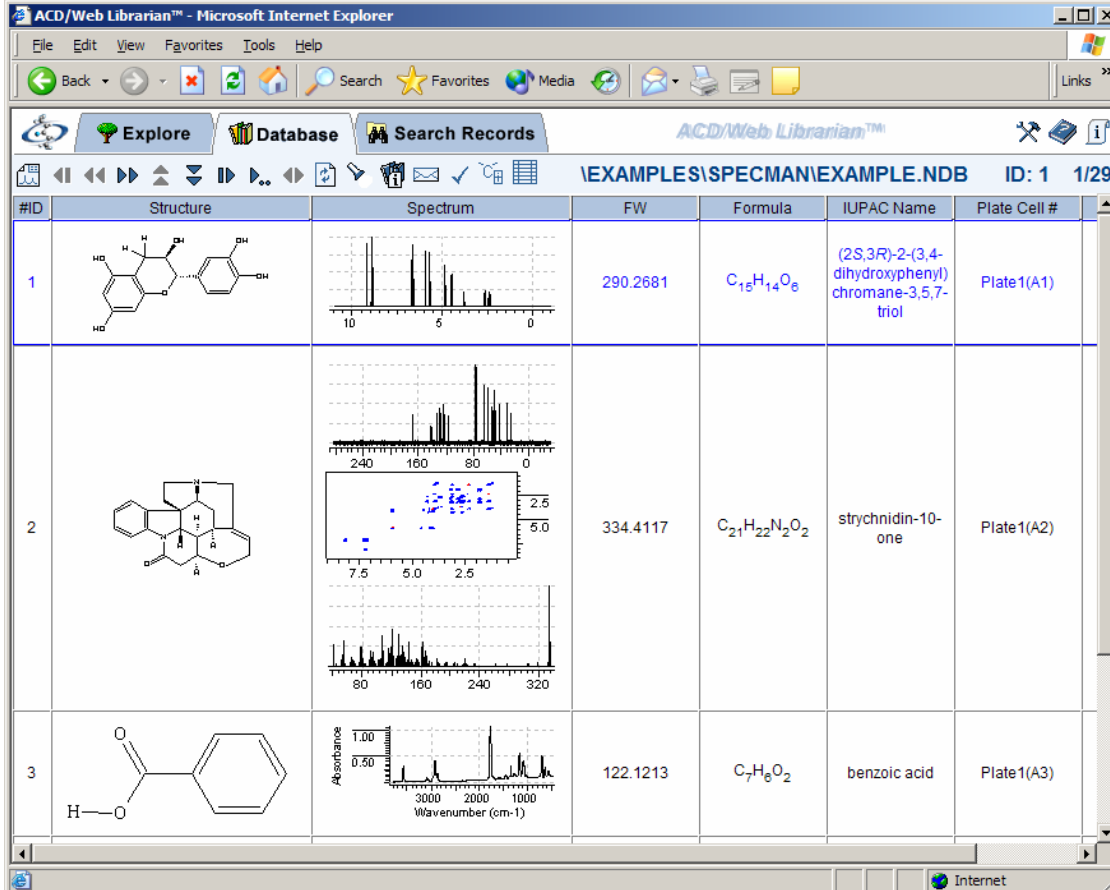


ACD/SpecManager

- ④ Automatically organize data streams with ACD/SpecManager
 - ④ Different data types and sources
 - ④ One integrated management system
 - ④ Automatically pass data to built-in analysis system
- ④ Manage Data generation workflow

ACD/WebLibrarian- Intranet Communication

View and search local and remote databases with ACD/Web Librarian



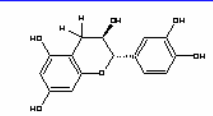
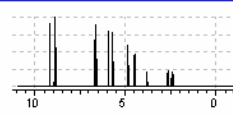
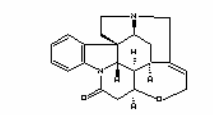
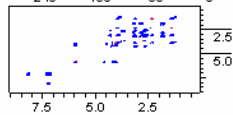
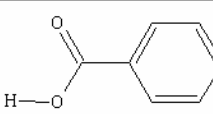
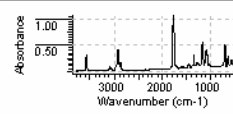
ACD/Web Librarian™ - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Forward Stop Home Search Favorites Media Mail Print

ACD/Web Librarian™

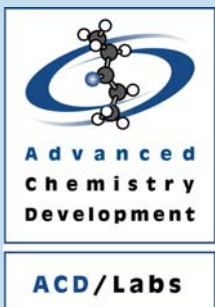
EXAMPLES\SPECMAN\EXAMPLE.NDB ID: 1 1/29

#ID	Structure	Spectrum	FW	Formula	IUPAC Name	Plate Cell #
1			290.2681	C ₁₅ H ₁₄ O ₆	(2S,3R)-2-(3,4-dihydroxyphenyl)chromane-3,5,7-triol	Plate1(A1)
2			334.4117	C ₂₁ H ₂₂ N ₂ O ₂	strychnidin-10-one	Plate1(A2)
3			122.1213	C ₇ H ₆ O ₂	benzoic acid	Plate1(A3)

Internet

Key Benefits

- Productivity
 - Saves time and reduces workload
- Improved Quality, Credibility, Accuracy
 - Increases decision making consistency
 - Enhances compliance with organizational standards



Processing Expert Tools



Files & Reports

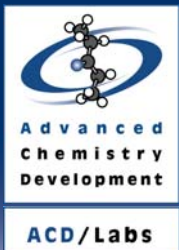


PhysChem
ACD/LogP, pK_a ,
LogD, Aq Sol,
Name
IUPAC, CAS Name



ACD/Labs' Software Solution for
Integrated Analytical and
Chemical Knowledge Management





Thank You

- 🌐 **Questions?**
- 🌐 **Comments?**