Working on AnIML - A View from a Vendor's Representative

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Overview

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- History + Involvement
- Why standard formats?
- Challenges
- Benefits

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History

- September 2002: exploratory meeting
- March 2003: E13.15 set up
- April 2003: First AnIML working group meeting
- Workshops at PittCon
  - 2006 through 2013
- Expedited Project Proposal and gathering of funds – late 2010
  - Agilent Technologies
  - Amgen
  - Glaxo SmithKline
  - PerkinElmer
  - Waters Corporation
- Documentation contract awarded late 2012

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Who is involved?

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gsk GlaxoSmithKline

Agilent Technologies

NIST National Institute of Standards and Technology

ASTM INTERNATIONAL Standards Worldwide

SCIMATIC SOFTWARE

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bssn software

ACS

XML in Chemistry

PerkinElmer precisely.

JASCO

and more...

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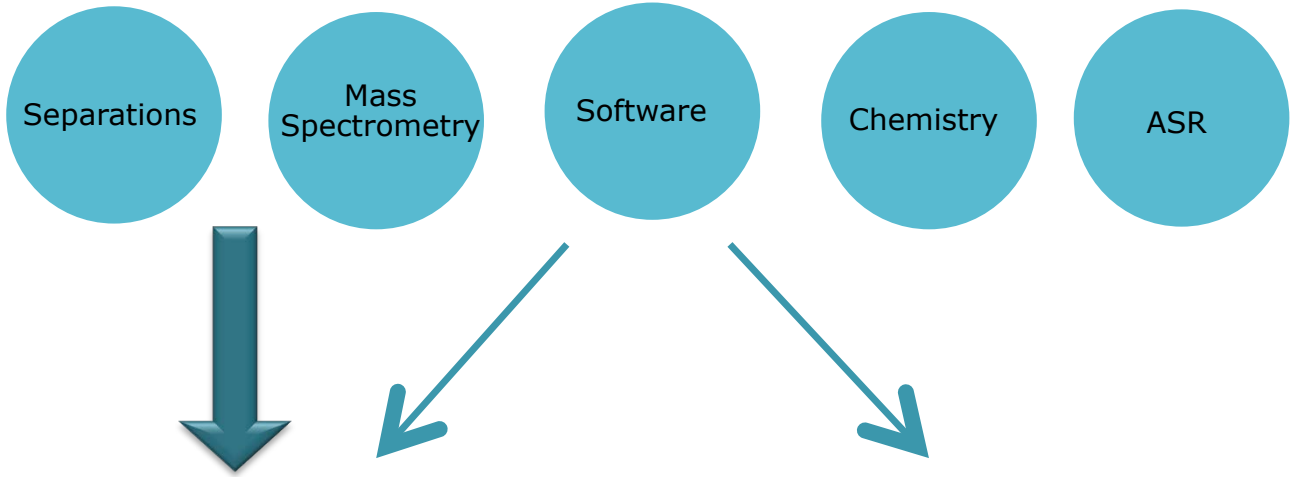
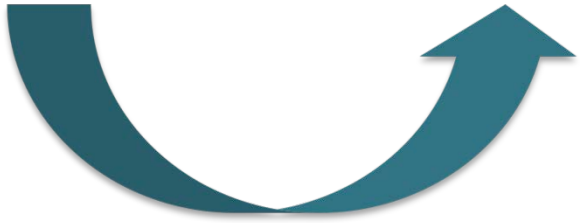
Core Competencies



- Software
  - Chromatography Data System
  - Mass Spectrometry Systems
  - Scientific Data Management System
  - Electronic Lab Notebook
  - Workflow Management and Lab Execution
  - etc.



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Why standard formats?

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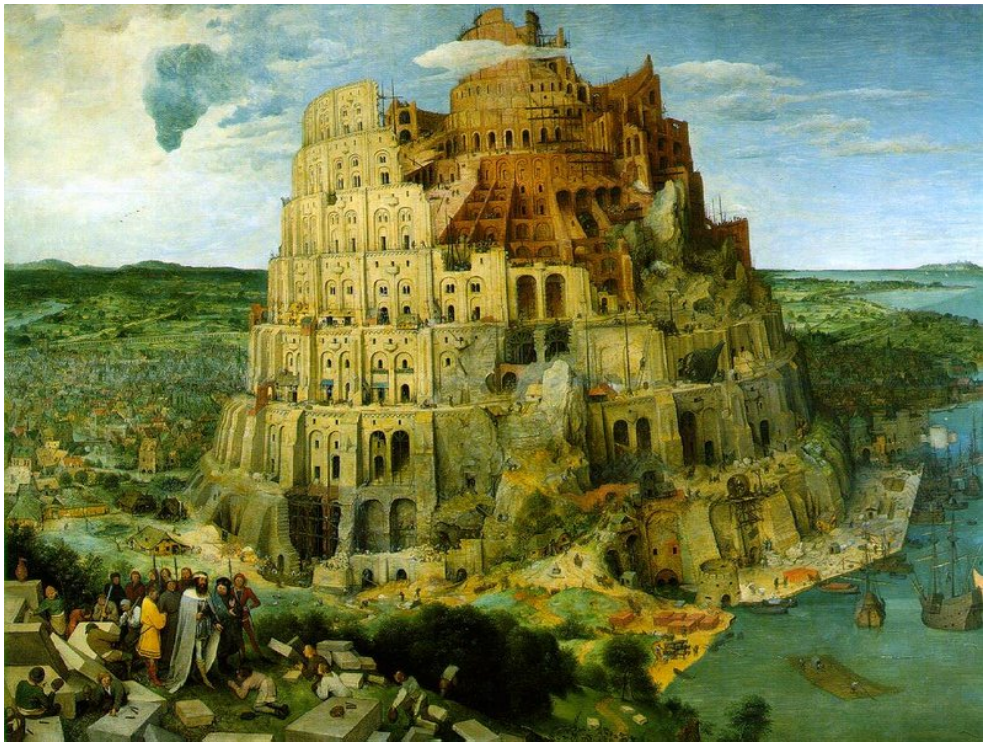

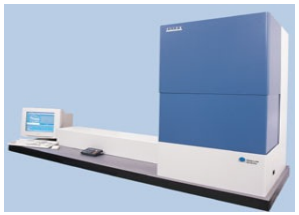

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Why standard formats?

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- Goals
  - Simple
    - Intra-organization data exchange
    - Inter-organization data exchange
    - Data storage and retrieval
    - Long term archiving
  - Additional goals
    - Platform independence
    - Free flow of information

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Regulatory Requirements

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- Copies of Electronic Records for Inspection
  - Accessibility for Inspection
  - Integrity of Content and Meaning
  - Human Readable Form
  - Standard Portable Formats
- Retention and Maintenance of Records
  - GxP demands Archival of Records for Extended Time
  - Requirement to keep the Raw Data
  - Ability to Reprocess

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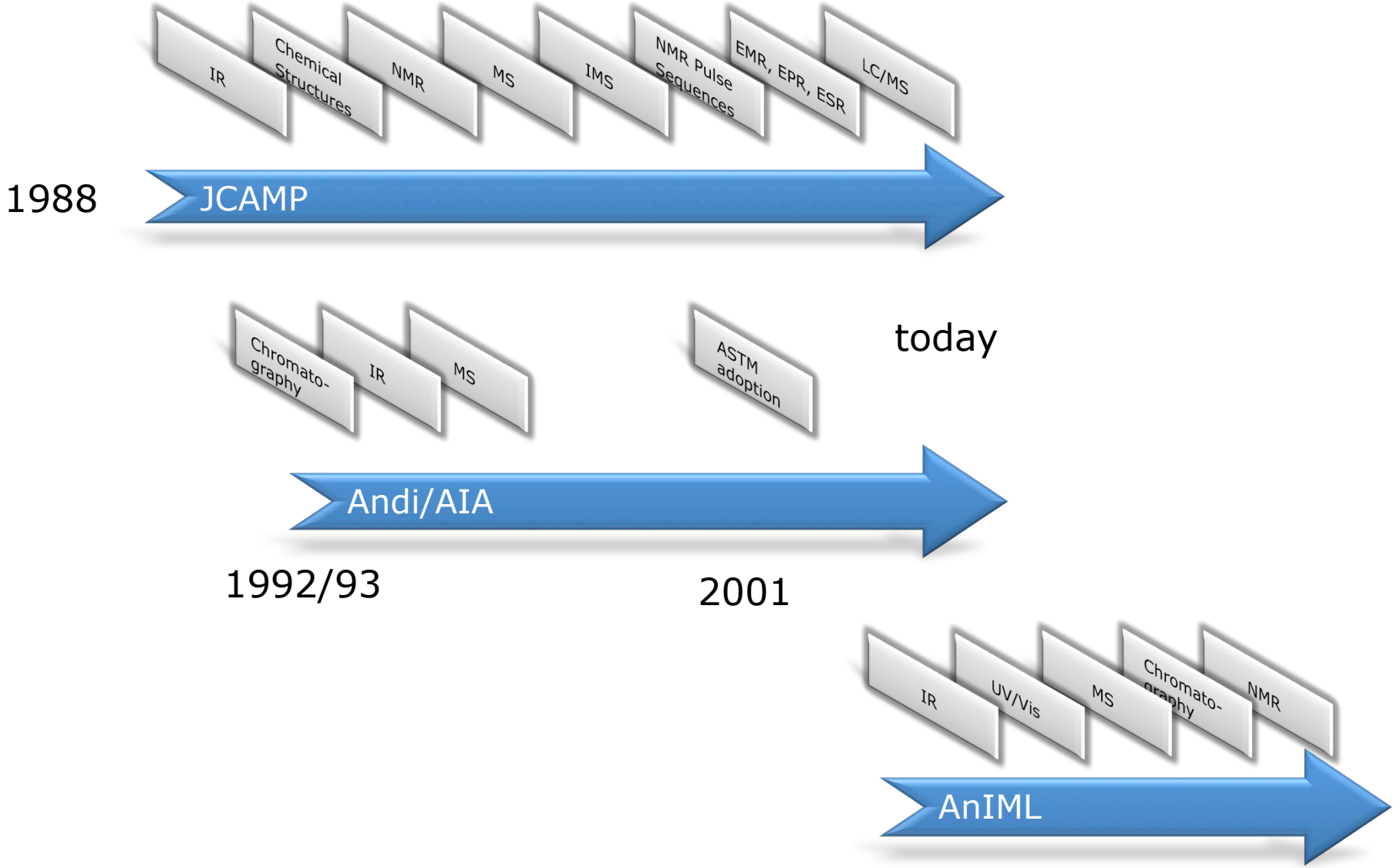
Current Data Standards



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Data Standard Support in Waters Informatics

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- Waters software supports
  - JCAMP
  - ANDI/netCDF used in
  - mzXML
  - mzData
- Read/Write/View
- AnIML will be supported once it becomes a public standard

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Challenges in developing a new standard

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- Agree on technology and structure
- Agree on data dictionaries
- Compatibility with previous standards
  - Faithful representation - Integrity of Content and Meaning
  - Allowed values
- Compatibility with proprietary formats
- Update to reflect current technology
  - Additions only!

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Challenges in developing a new standard

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- Management buy-in
- Participation
- Conflicts of interest
  - Proprietary vs. open
  - Inter-vendor politics
  - Vendors vs. customers
- Resist the urge to sell

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Why AnIML?

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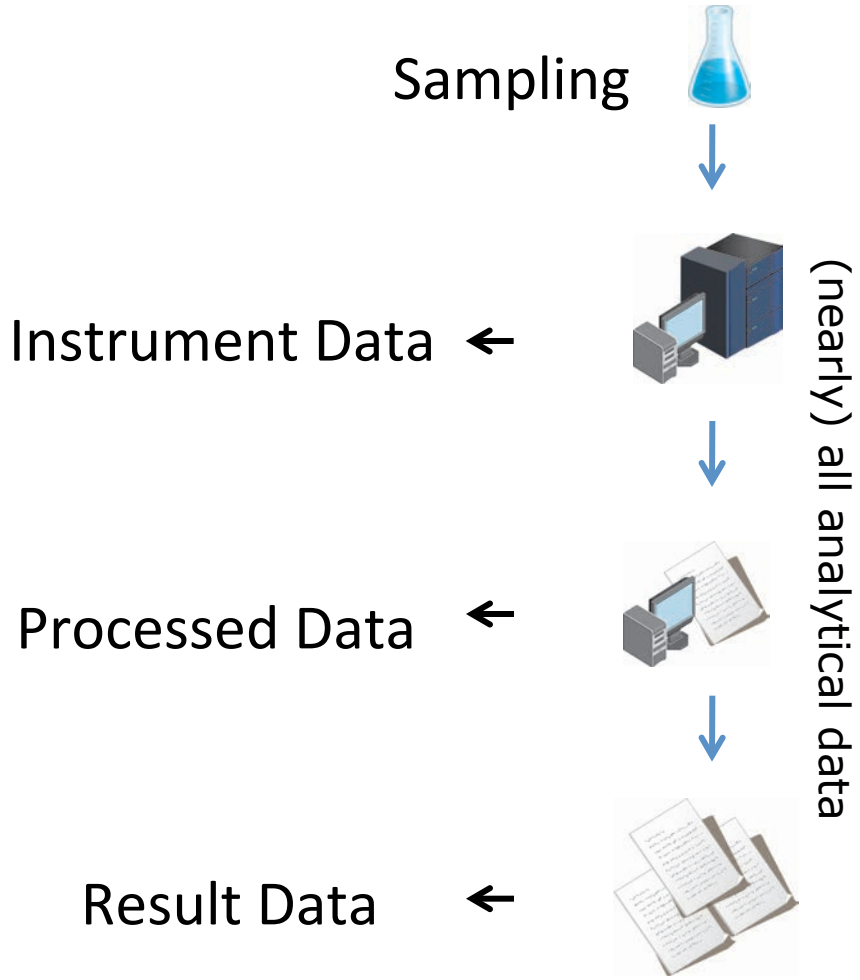
AnIML Data Set

- Workflow Information
- Metadata
- Instrument Data
- Processed Data
- Result Data
- Audit Trail, Signatures



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Proprietary vs. Standard Formats

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- Why don't vendors use Standard Formats internally?

Proprietary Formats	Standard Formats
Binary	ASCII-based (e.g. XML)
Compact	Verbose
Fast to Read/Write	Slow to Read/Write
Data Acquisition and Processing	Data Sharing and Long Term Stability

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Conversion

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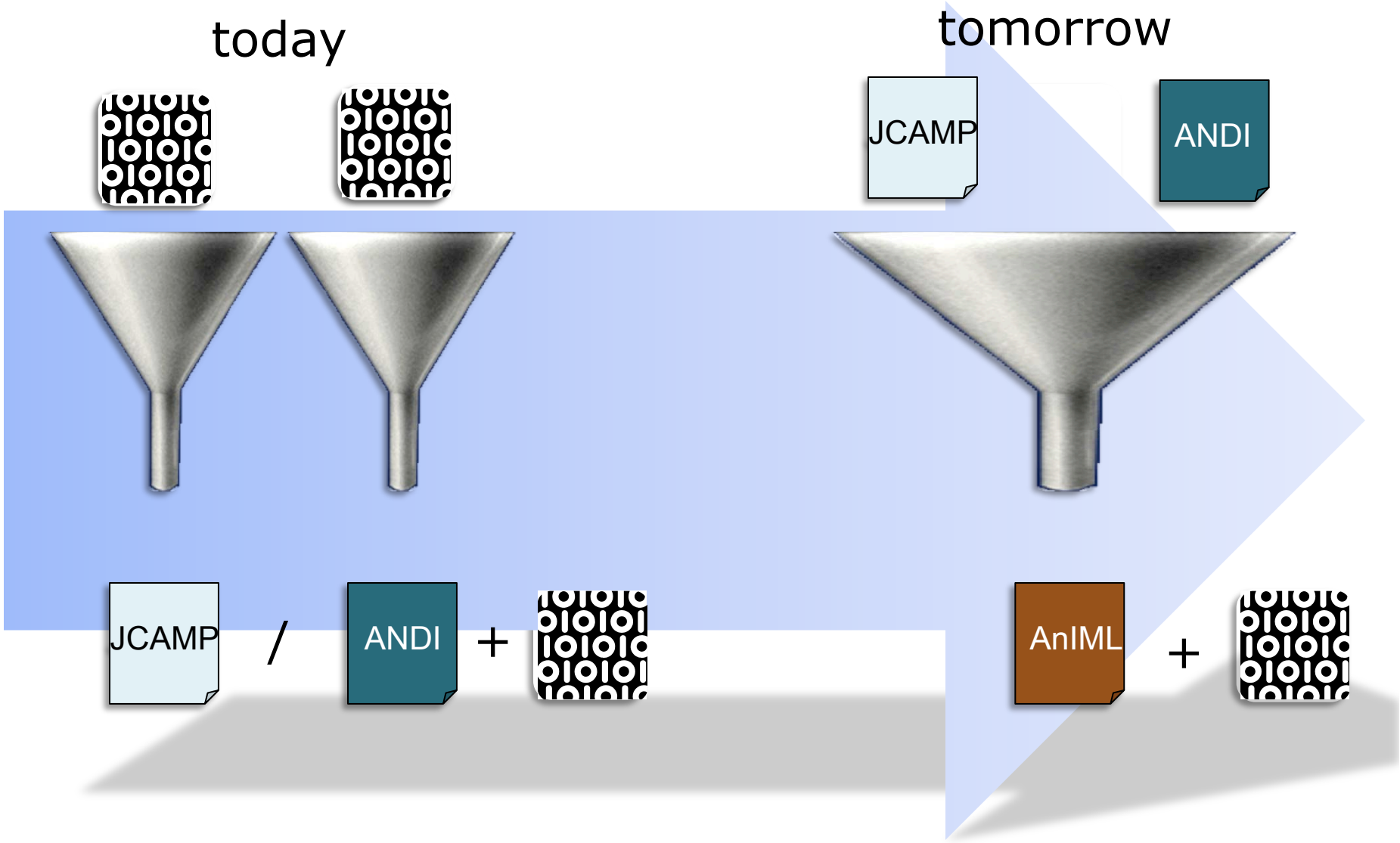

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Vendors' Benefits

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- Competitive
  - Influence on an emerging standard
  - Access to latest information
- Relationships
- Intangible Value
  - Marketing
- Expertise

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Sources of Information

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- The AnIML Web Site
  - http://www.animl.org
- The SourceForge Analytical Information Markup Language Project: Summary Page
  - http://sourceforge.net/projects/animl

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Q&A

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