If The Shoe Fits: Adapting LabKey for Novel Applications

Quinton Dowling

IDRI is a Seattle-based not-for-profit committed to applying innovative science to the research and development of products to prevent, detect and treat infectious diseases of poverty. By integrating capabilities, we strive to create an efficient pathway to bring scientific innovation from the lab to the people who need it most.
Overview

Adapting LabKey Steps

• **Develop schema of real world process to model**
  • Interviewing
  • Developing Process Understanding

• **Review of LabKey Structure**
  • Sample Sets, Assays, and Studies

• **Harmonizing real world with LabKey**
  • Identifying analogous structure
  • When and where to customize
Goal of Project

*Being able to clearly define goal is critical to an efficient process*

- **Is the goal:**
  - To store data, relationships
  - Manage a large, complicated process
  - Collaborate
  - Regulatory purposes
  - Meta-analysis
Process Development

- Disease
- Antigen
- Lot
- Purification

- QC/QA
- Characterization
- Internal Studies
- External Collaboration
Understanding the System

Collecting Data

• **Understand processes**
  • Steps
  • Variability
  • Data collected, observations made

• **Understand data**
  • Meaning of data
  • Relationship between data and steps/objects
Broad Overview of Steps

1. Antigen Expression
2. Purification
3. QC/QA
4. Characterize
5. Release
Detailed Understanding of Processes

This scheme is applied to each antigen lot.

1. Cell Paste
2. Inclusion Bodies
3. Anion Exchange
4. Cation Exchange
5. SEC
6. TFF

Methods
Understanding the Data

**Metacontent**
- Lot number
- Antigen Name
- Production Date
- Volume Produced
- Buffer type, concentration, pH
- Host
- Processing Method
- Produced By, Purified By, Checked By

**Analytical Methods (data)**
- pH
- Protein Concentration
- Endotoxin Level
- Fluorescence
- Far UV CD
- SDS-PAGE
- Nanoparticle Tracking Analysis
Users, Users, Users

*Identify users, interview them, categorize them*

• **Who works on the project**
  • Scientists, technicians, admin, management, etc.
  • What role do they play?

• **Think: How will a user interact with LabKey**
  • Data entry/manipulation
  • View reports
  • QA/QC
  • Admin
## Identified Users

<table>
<thead>
<tr>
<th>User</th>
<th>Task</th>
</tr>
</thead>
<tbody>
<tr>
<td>Produced by</td>
<td>Enter data</td>
</tr>
<tr>
<td>Purified by</td>
<td>Enter data</td>
</tr>
<tr>
<td>Checked by</td>
<td>Review and enter data</td>
</tr>
<tr>
<td>Analytics performed by</td>
<td>Enter data</td>
</tr>
<tr>
<td>Internal Collaborators</td>
<td>View reports, request samples</td>
</tr>
<tr>
<td>External Collaborators</td>
<td>View reports, request samples</td>
</tr>
</tbody>
</table>
Simplifying Schema

Define the basic object(s)
- Participant, Formulation, Material Lot, etc.
- Determine relationships between data and object
- Characterize relationships between objects.

Group users
- Users needs can direct development work
  - Data IO
  - View customization
Simplified Schema

Antigen Expression/Purification

QC/QA

Characterize

Release

Purification Schemes

QC/QA Data

Bulk Lot

Characterization Data

Users
# User Groups and Needs

## Data Entry Group
- Produced by
- Purified by
- Analytics performed by

## Needs
- Ease of data entry
- Data entry history
- Access to analytical tools

## Data Viewer Group
- Internal Collaborators
- External Collaborators
- Checked by

## Needs
- Searching
- Print-ready forms/views
- Locked down permissions
LabKey Abstraction

Data Types

• **Data Sets**
  • Data about an object (often “participant”)

• **Assays**
  • More complex data generated that relates to an object

• **Lists**
  • Generic lists of data that can be linked to an object or other lists
Lot = Object

**Mapping to LabKey**

- **Lot dataset**
  - Metacontent: Lot name, antigen, date, etc.
  - Simple assay information: pH, Endotoxin, Concentration, etc.

- **Assays**
  - Complex data: Fluorescence, FTIR, Nanoparticle Tracking Analysis

- **Lists**
  - Useful for grouping data, limiting user input
Mapping to LabKey

LabKey Study Module

- Dataset
- Assays
- Lists

Process Development

- Lots
- Far-UV CD
- Purification Scheme
- Protein Descriptions
To Study or Not to Study

Select which modules to use by identifying analogous structure:

• Basic “unit” of module
• Relationships between data types/tables in module
• Tools available
• Customizability of Module

The Study Module is well developed
Advantages of using Study Module

Groups!

- Study module understands grouping relationships
- Easy development of views/analysis
Keeping the user in mind when doing custom development

Data entry
• **Consider how data is generated**
  • Output from instrument
  • Sample replicates, standards
  • Metacontent

Data display
• **Who is viewing the data**
  • Types of displays
  • Content in display
  • Exploration of data
Custom Development

Data entry

• **Minimize Error**
  • Select from
  • Data constraints

• **Ease of use**
  • Simple
  • Intuitive
Custom Development

**Data Views**

- **What views will users want?**
  - Data Reports
  - Figures: Historic...
  - Searchability
  - Further Analysis Tools
Acknowledgements

IDRI

• Lucien Barnes
• Traci Mikasa
• Richard Cabullos
• Ayesha Misquith
• Susan Lin
• Sandra Sivananthan
• Sarah Parker
• Millie Fung
• Chris Fox
• Tom Vedvick
• Darrick Carter
• Steve Reed

LabKey

• Nick Arnold
• Peter Hussey
• Brian Connolly

Funding

• Bill and Melinda Gates Foundation