

If The Shoe Fits: Adapting LabKey for Novel Applications

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WHO WE ARE

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

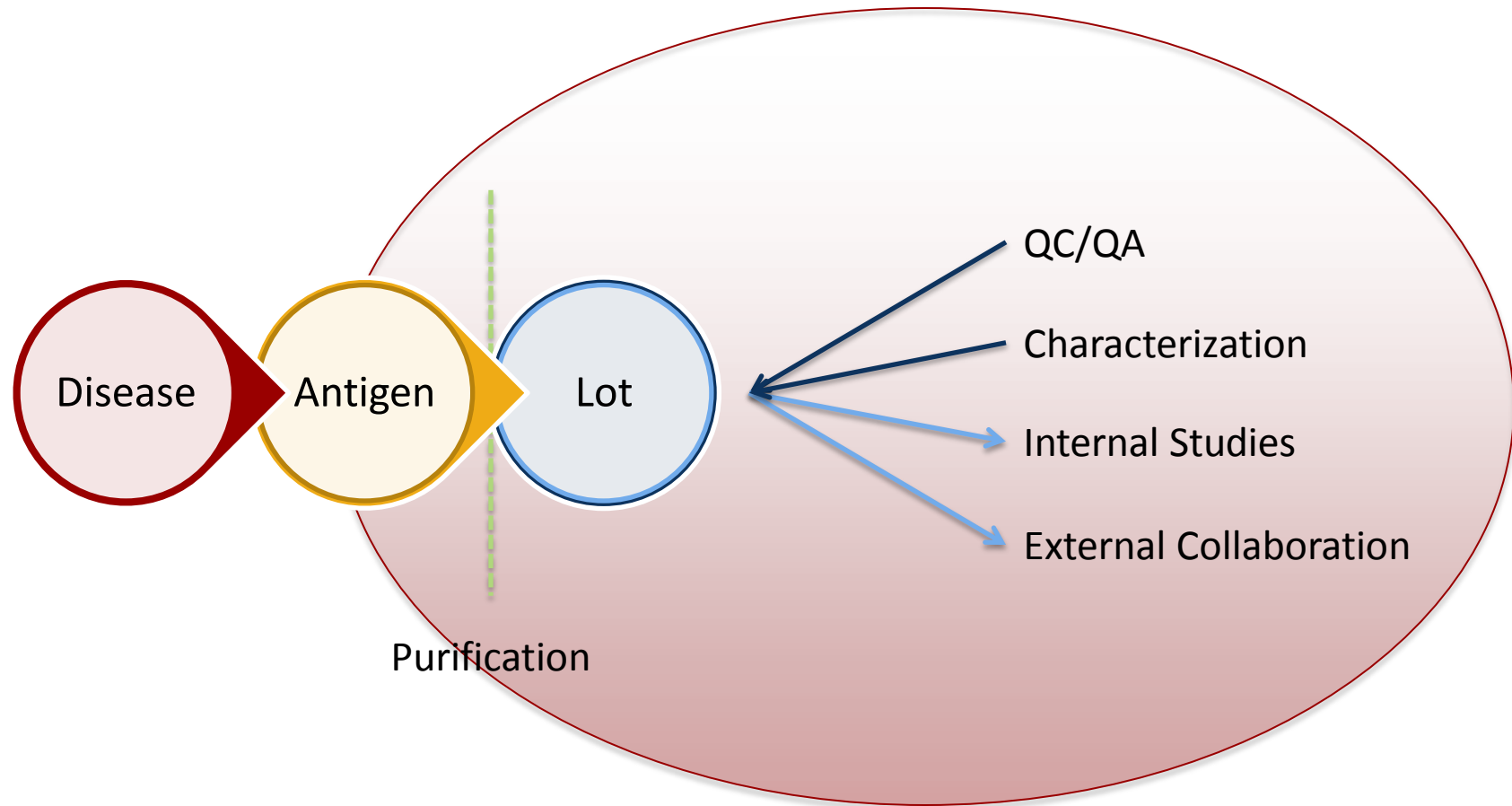
- *Develop schema of real world process to model*
 - Interviewing
 - Developing Process Understanding
- *Review of LabKey Structure*
 - Sample Sets, Assays, and Studies
- *Harmonizing real world with LabKey*
 - Identifying analogous structure
 - When and where to customize

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

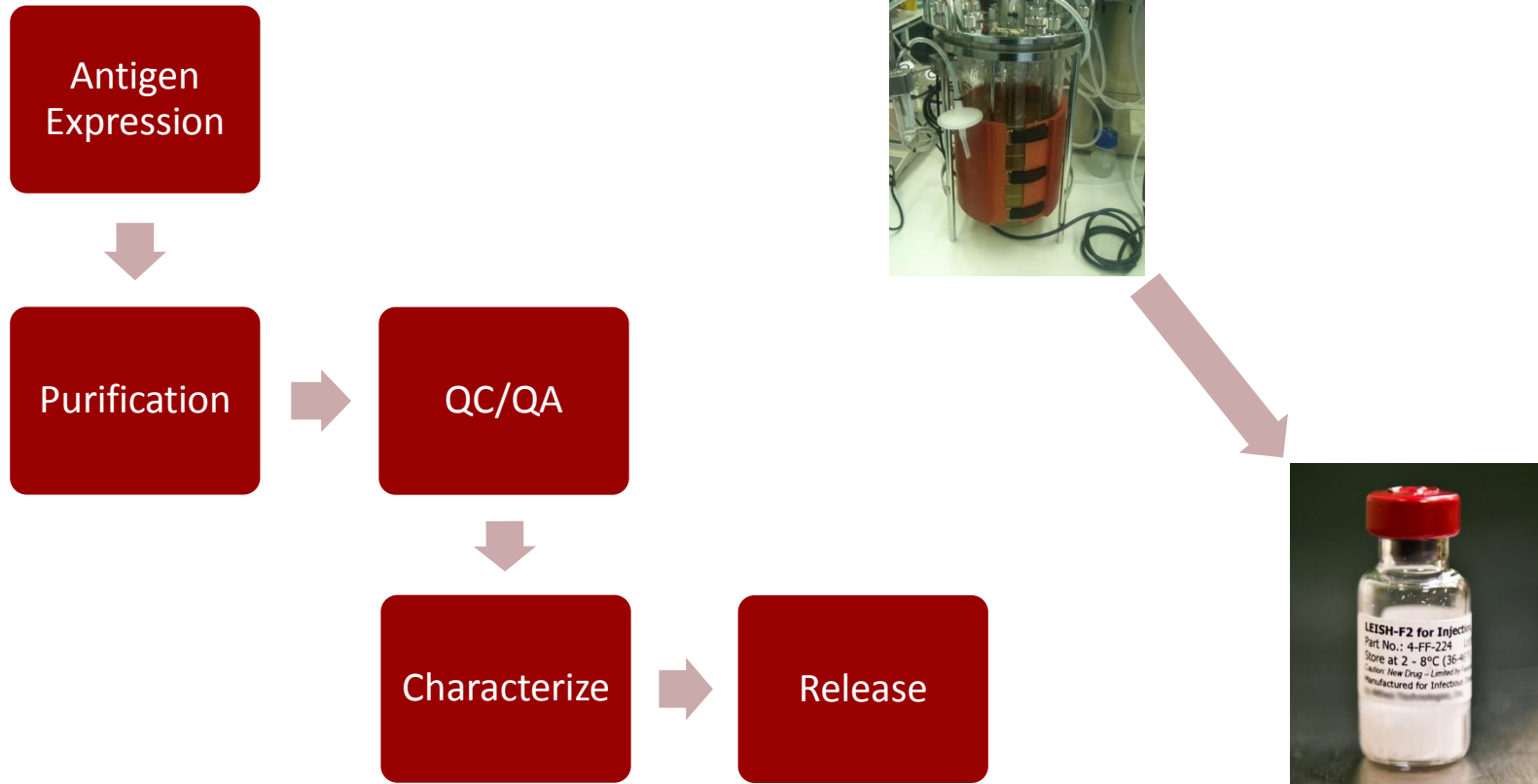


Understanding the System

Collecting Data

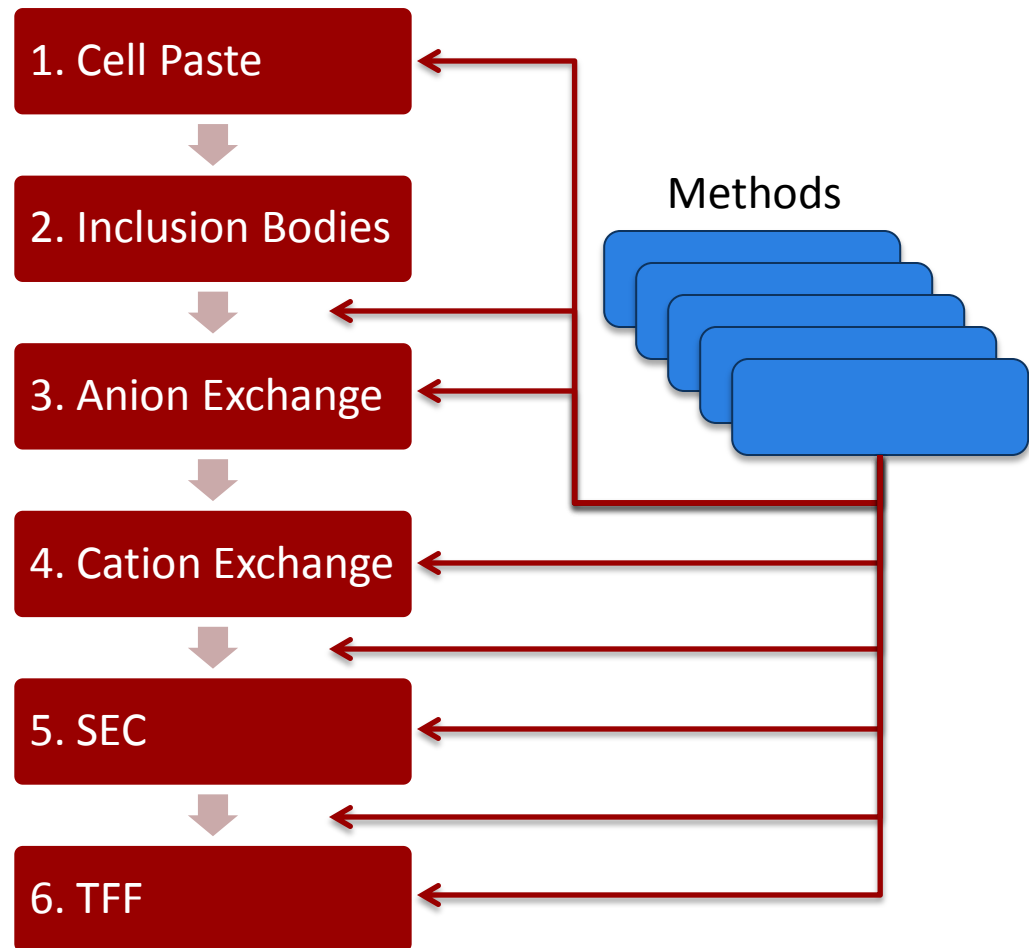
- *Understand processes*
 - Steps
 - Variability
 - Data collected, observations made
- *Understand data*
 - Meaning of data
 - Relationship between data and steps/objects

Broad Overview of Steps



Detailed Understanding of Processes

This scheme is applied to each antigen lot.



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

| User | Task |
|------------------------|-------------------------------|
| Produced by | Enter data |
| Purified by | Enter data |
| Checked by | Review and enter data |
| Analytics performed by | Enter data |
| Internal Collaborators | View reports, request samples |
| External Collaborators | View reports, request samples |

Simplifying Schema

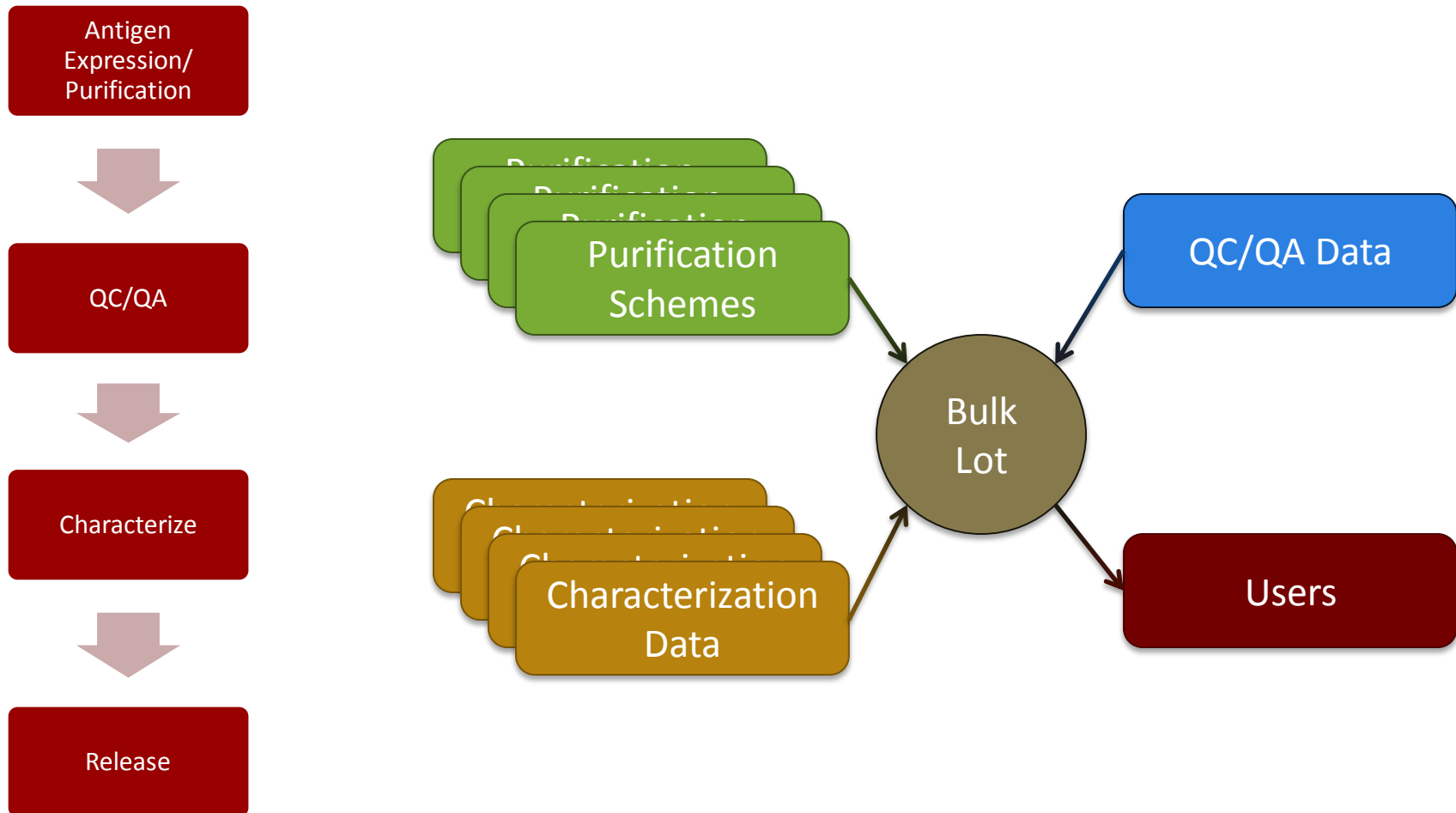
Define the basic object(s)

- *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



User Groups and Needs

Data Entry Group

- Produced by
- Purified by
- Analytics performed by

Data Viewer Group

- Internal Collaborators
- External Collaborators
- Checked by

Needs

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

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

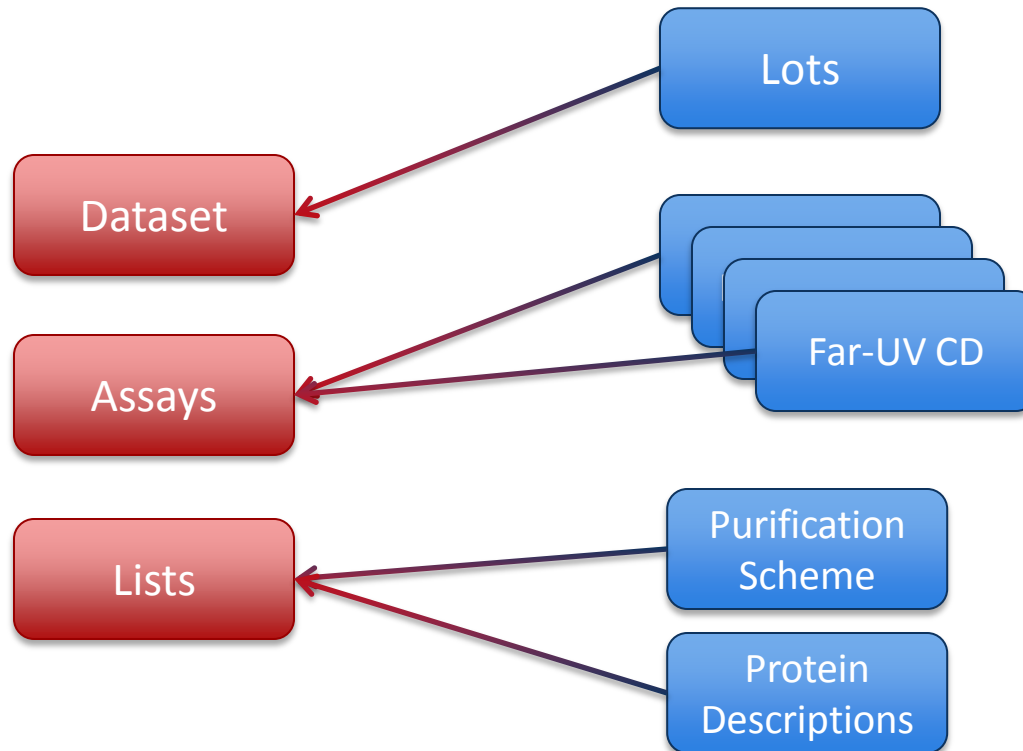
Mapping to LabKey

- *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

Process Development



To Study or Not to Study

Select which modules to use by identifying analogous structure:

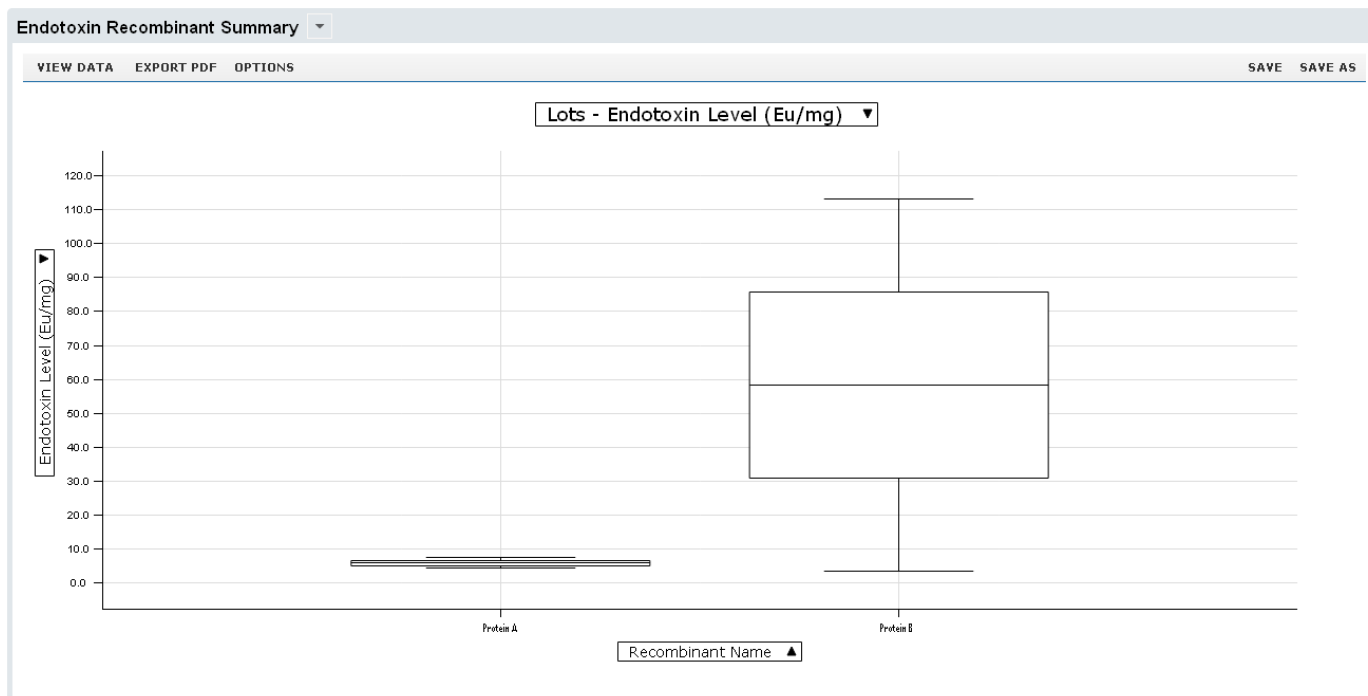
- Basic “unit” of module
- Relationships between data types/tables in module
- Tools available
- Customizability of Module

The Study Module is well developed

Advantages of using Study Module

Groups!

- Study module understands grouping relationships
- Easy development of views/analysis



Custom Development

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

Formulations

| | | | |
|---------------------------------------|---------------------------------------|----------------------|---|
| Lot Number* | <input type="text" value="QF290"/> | Date of Manufacture* | <input type="text" value="07/22/2010"/> |
| Formulation Type* | <input type="text" value="Liposome"/> | Batch Size* | <input type="text" value="100"/> |
| Comments | <input type="text"/> | Notebook Page* | <input type="text" value="355-133"/> |
| | | Stability Watch | <input type="checkbox"/> |
| <input type="text" value="IRM-0259"/> | <input type="text" value="7.2"/> | %w/vol | Remove |
| <input type="text" value="IRM-0258"/> | <input type="text" value="0.8"/> | %w/vol | Remove |
| <input type="text" value="IRM-0058"/> | <input type="text" value="2"/> | %w/vol | Remove |

Custom Development

Data Views

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

Formulation QF384

HOME PAGE | EDIT QF384 | BROWSE FORMULATIONS | SAMPLE VIEW

Information

Date of Manufacture: Thu Jan 06 00:00:00 PST 2011
 Type: Emulsion
 Lot Size: 500
 Notebook Page: 408-161
 Comments:
 Raw Materials: IRM-0279, IRM-0270, IRM-0255, IRM-0235, IRM-0234, IRM-0108, IRM-0249

Particle Size Stability

REFRESH

| | DM | 1 wk | 2 wk | 1 mo | 3 mo | 6 mo | 12 mo | Me... |
|------|-------|-------|-------|-------|-------|--------|-------|-------|
| Mean | 80.69 | 77.72 | 77.57 | 75.7 | 77.22 | 75.26 | 75.78 | 78 |
| Mean | 77.16 | 78.28 | 75.9 | 79.08 | 90.44 | | | 78 |
| Mean | 78.11 | 79.92 | 76.95 | 78.59 | 75.45 | 186.69 | | 78 |
| Mean | 78.96 | 87.81 | 197.6 | | | | | 78 |

Displaying 1 - 4 of 4

Concentrations

| Name | Name | Concentration Unit | Name |
|------|----------|--------------------|-----------------------|
| EDIT | IRM-0279 | QF384 | 1.9 %w/vol IRM-0279 |
| EDIT | IRM-0270 | QF384 | 10.0 %w/vol IRM-0270 |
| EDIT | IRM-0255 | QF384 | 1.8 %w/vol IRM-0255 |
| EDIT | IRM-0235 | QF384 | 25.0 mM IRM-0235 |
| EDIT | IRM-0234 | QF384 | 25.0 mM IRM-0234 |
| EDIT | IRM-0108 | QF384 | 0.9 %w/vol IRM-0108 |
| EDIT | IRM-0249 | QF384 | 0.025 %w/vol IRM-0249 |
| EDIT | | QF384 | 0.025 %w/vol IRM-0249 |
| EDIT | | QF384 | 25.0 mM IRM-0235 |
| EDIT | | QF384 | 25.0 mM IRM-0234 |
| EDIT | | QF384 | 1.8 %w/vol IRM-0255 |
| EDIT | | QF384 | 10.0 %w/vol IRM-0270 |
| EDIT | | QF384 | 0.9 %w/vol IRM-0108 |
| EDIT | | QF384 | 1.9 %w/vol IRM-0279 |

Stability Charts

PS QF384 aps

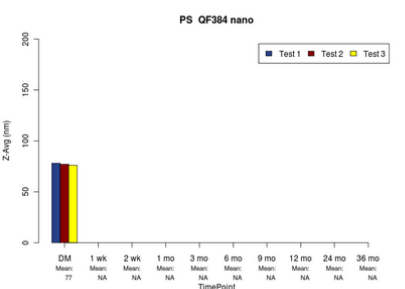


Z-Avg (nm)

TimePoint

2012-01-06 09:22

PS QF384 nano



Z-Avg (nm)

TimePoint

2012-01-06 09:22

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