Adjuvant Formulations: Applied LabKey Server in Process Development

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IDRI Background

- Outline:
  - IDRI, LabKey and IDRI LabKey
    - Why a LIMS?
  - The power of relational databases
  - Custom views in R and SQL

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IDRI Background

- Seattle-based not-for-profit
- R+D of products to prevent, detect and treat infectious diseases of poverty.
- IDRI integrates capabilities to bring scientific innovation from the lab to the people who need it most.

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IDRI Research Programs

- Antigen/Drug Discovery
- Preclinical Biology
- Clinical Development
- Process Development
- **Adjuvant and Delivery Systems**

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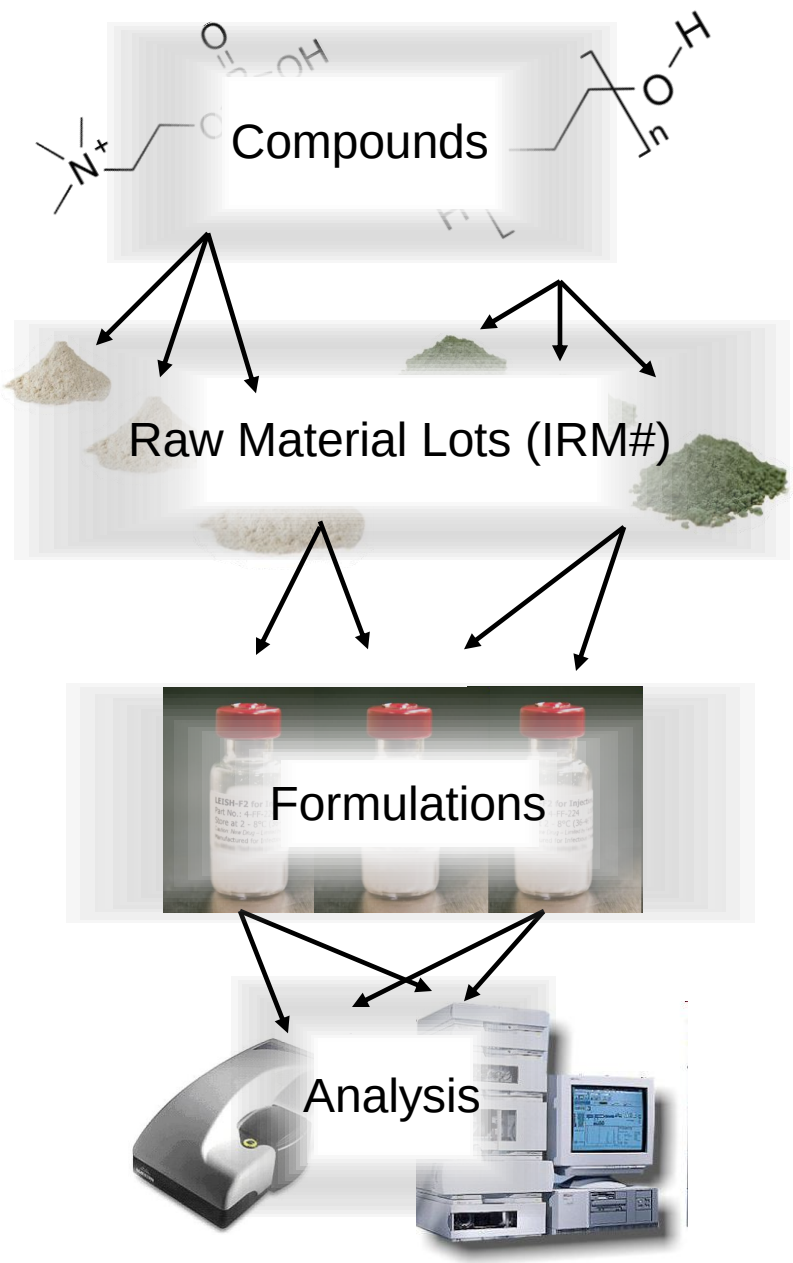
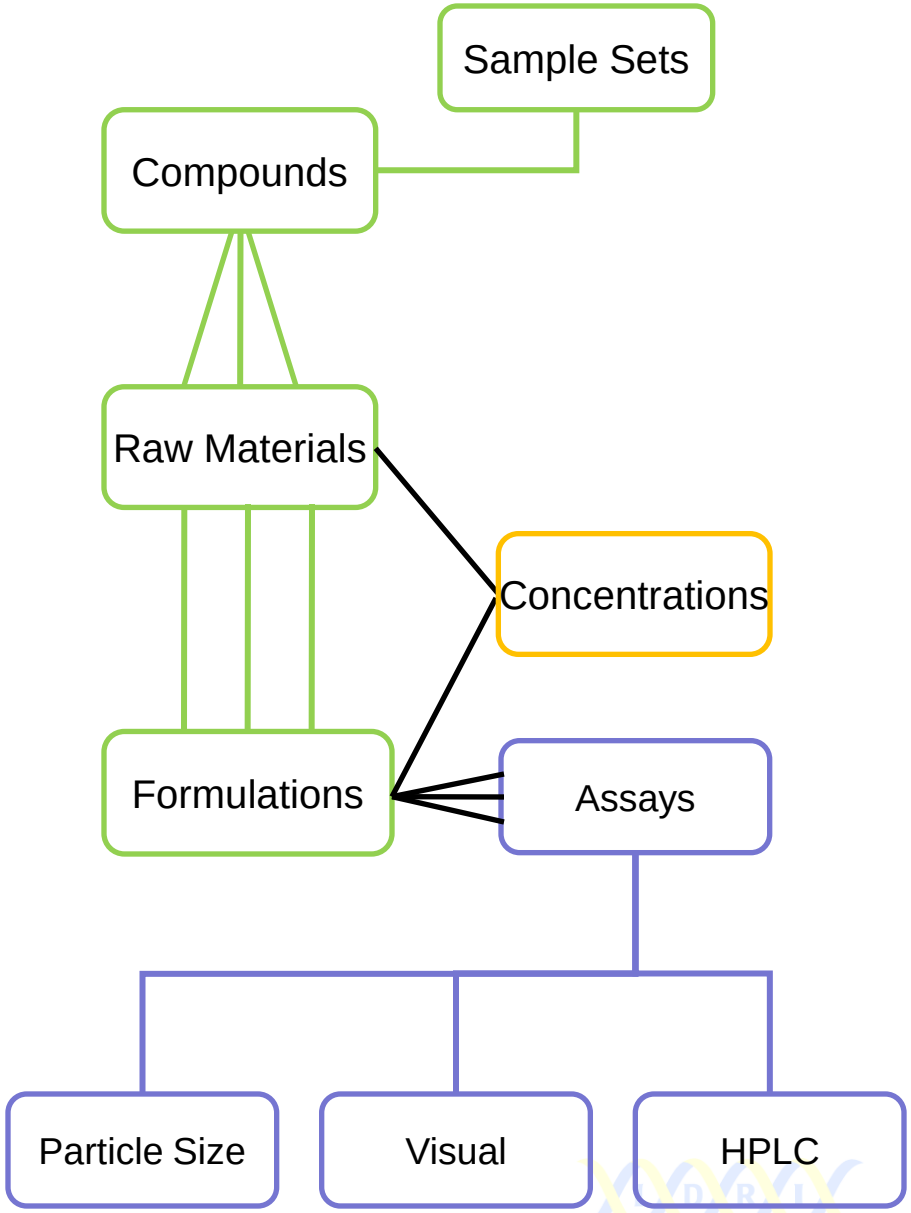
Physical Reality



IDRI LabKey



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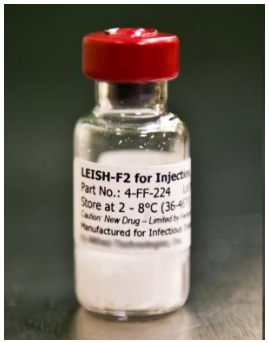
LabKey: Tracking/Analysis

- Individual Tracking and Analysis



- Population Tracking and Analysis

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What's the Goal?

- Ask and Answer questions about…
  - An individual.
  - A class or group of individuals.
  - The database.

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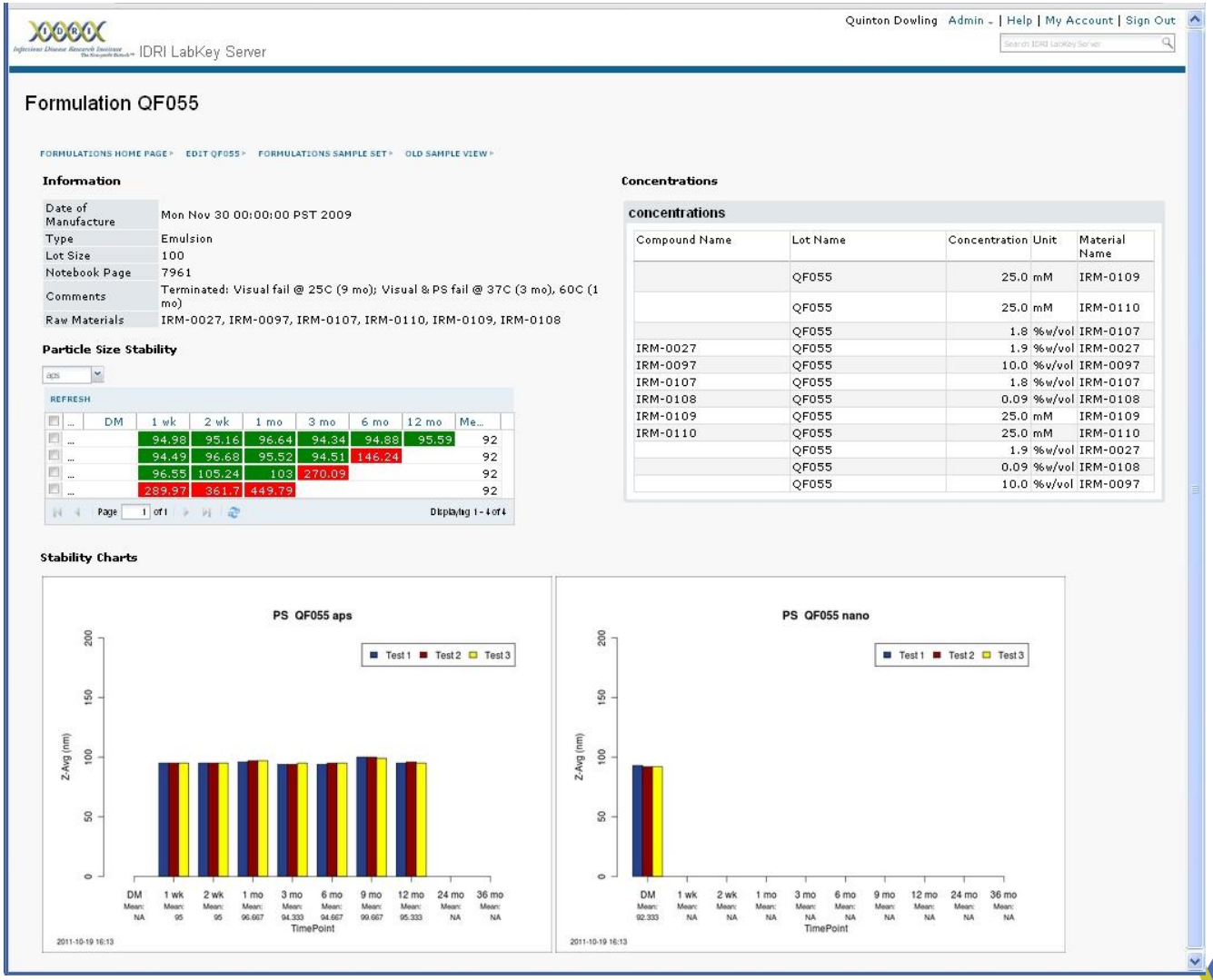
Questions About Individuals

- What properties does an individual have?
- Individual behavior over time?
- Individual history?

Individual Lot Tracking/Analysis



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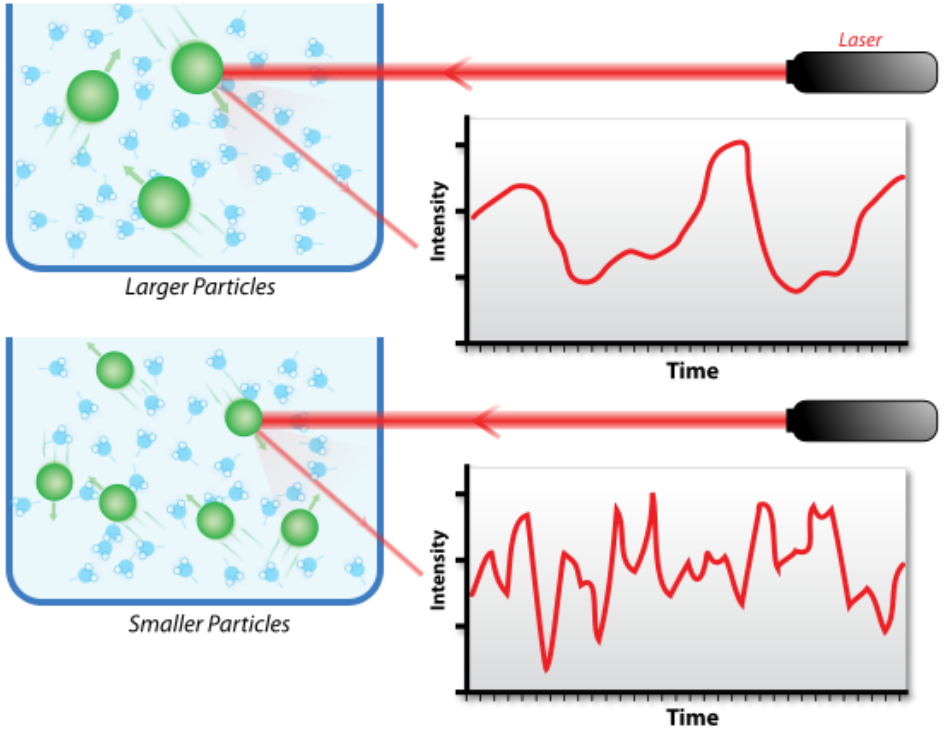
Particle Size Data

- Dynamic light scattering



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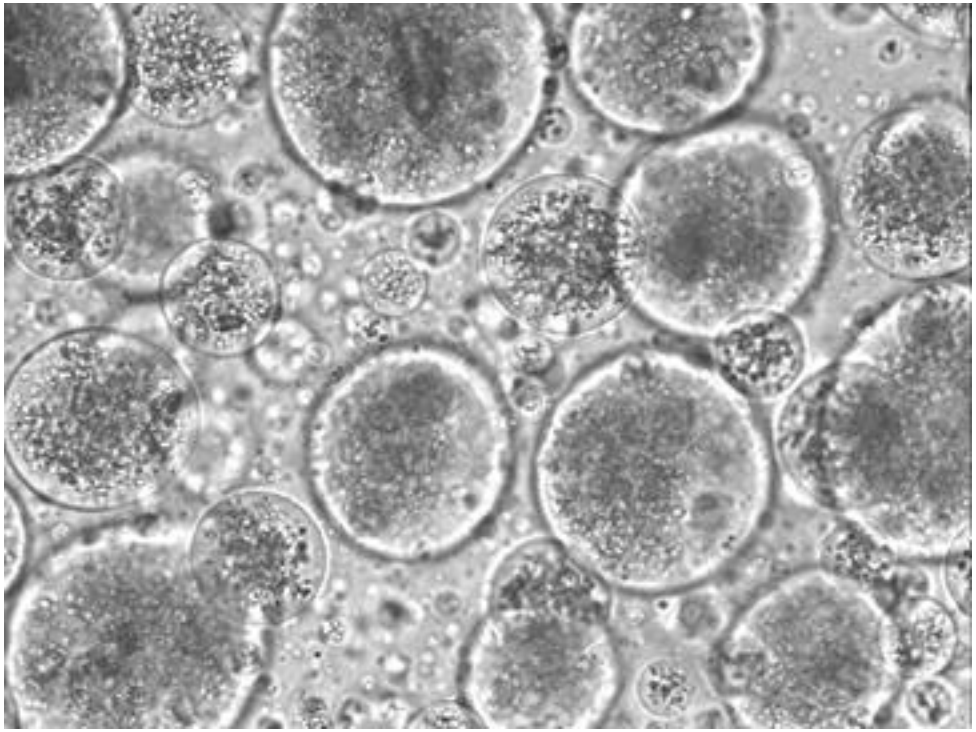
Particle Size Data

- Larger particles tend to aggregate



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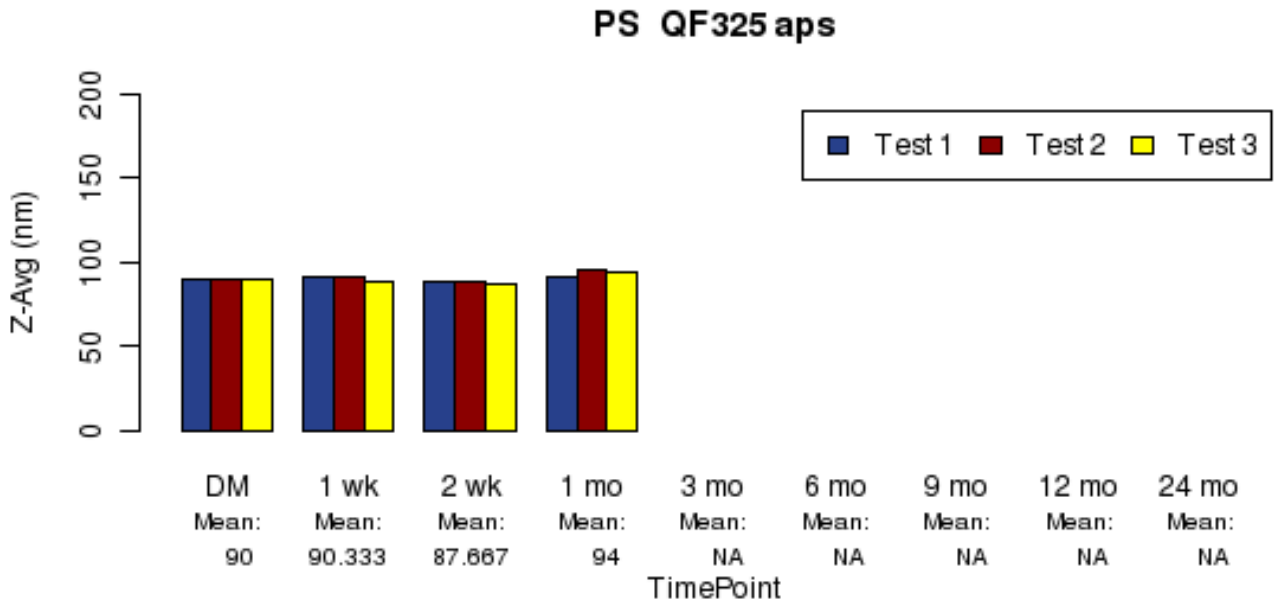
View Development



- **One temperature**
- **Qualitative error**
- **Finitely scalable (view gets cluttered over time)**

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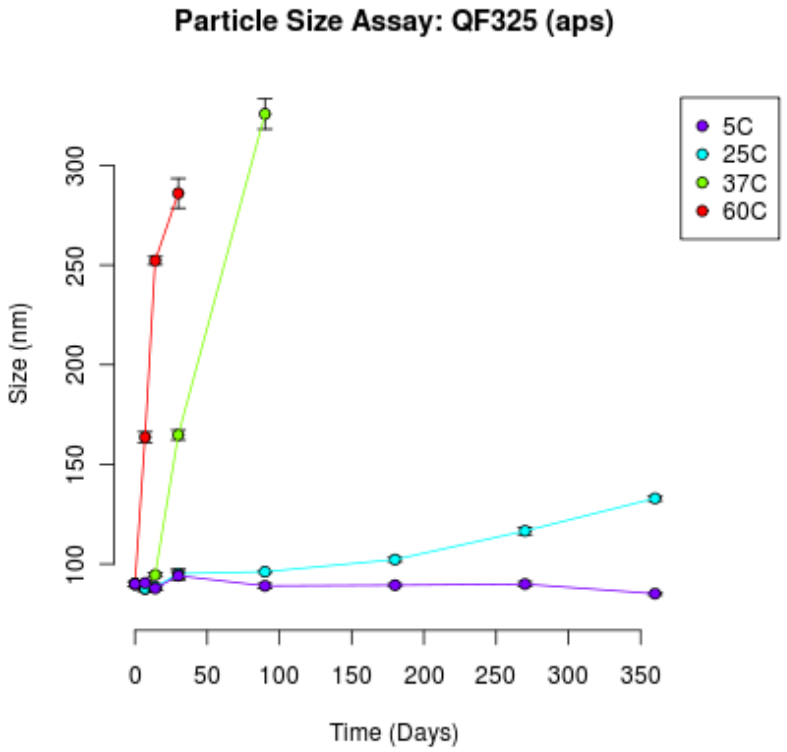
View Development



- **Multiple temps**
- **Quantitative error**
- **Infinitely scalable**

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The True Power of LabKey

- Population Level Analysis
  - Relational Structure facilitates analysis of large datasets.
  - Data mining for generating and testing predictive models.

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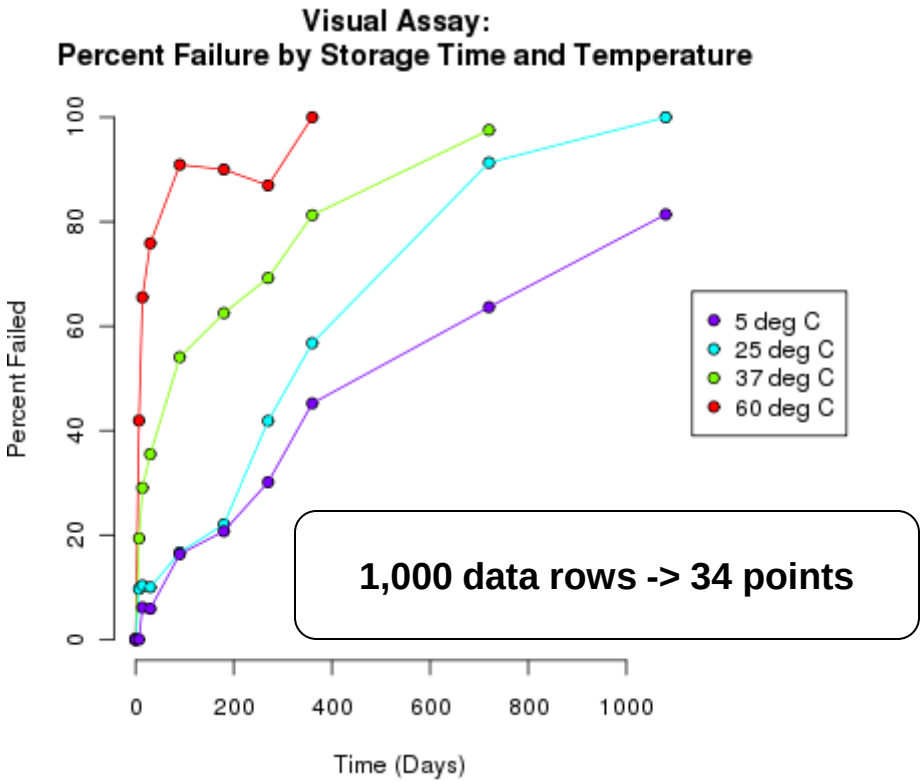
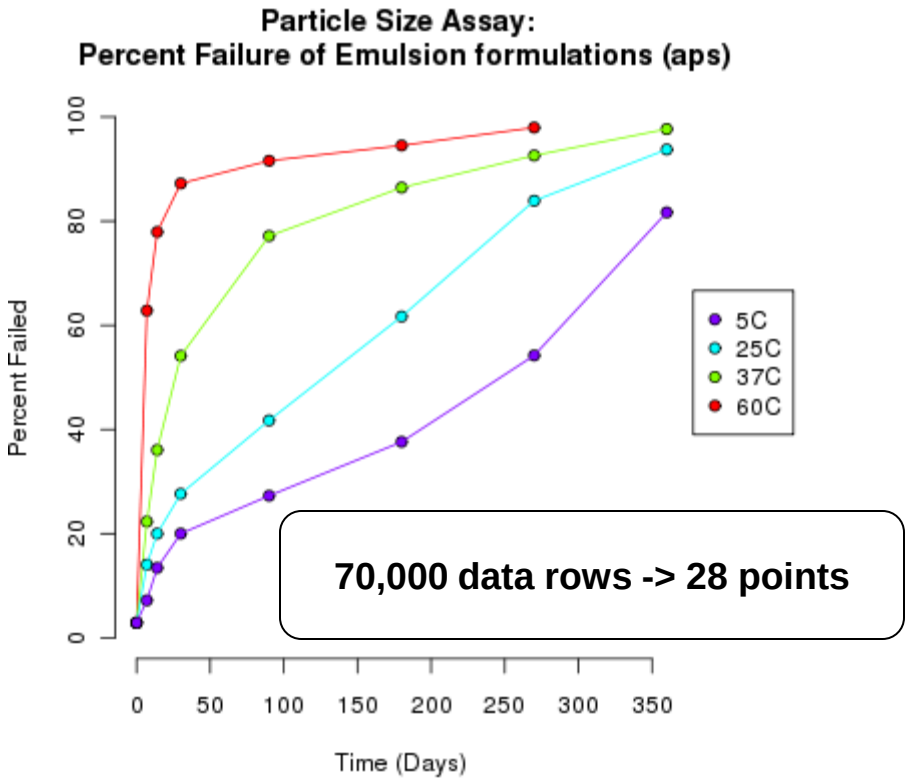
Views





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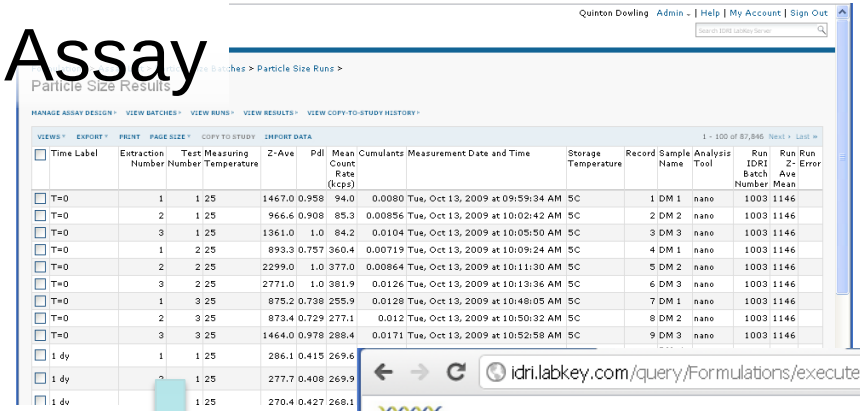
White-boarding

- Identify goal
- Locate needed starting data
- Map out transformations
  - SQL vs. R, or both?
- Consider UX

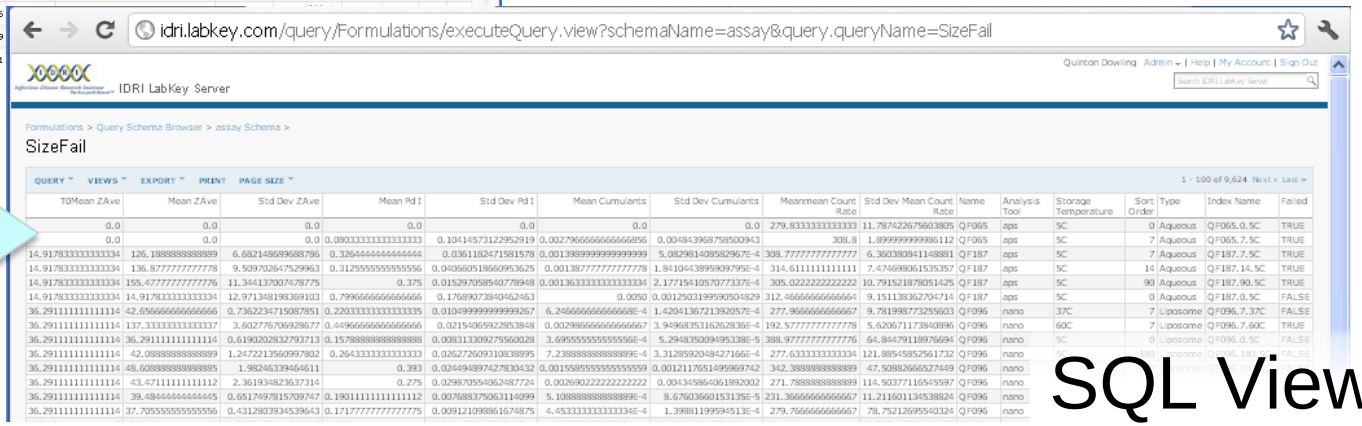
- Now start writing code.

Method: SQL

Assay



Use SQL to generate a view that contains data needed to reach goal (in this case a graphic)



SQL View

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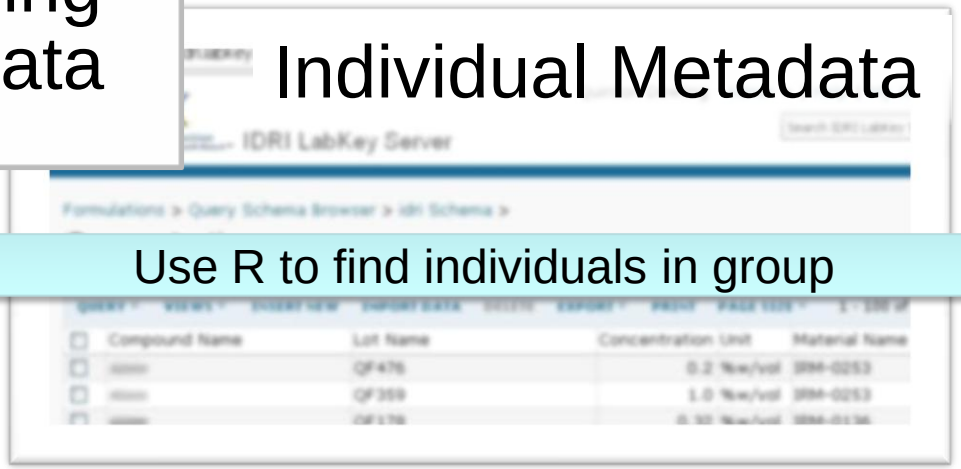
Method: R

Grouping Metadata

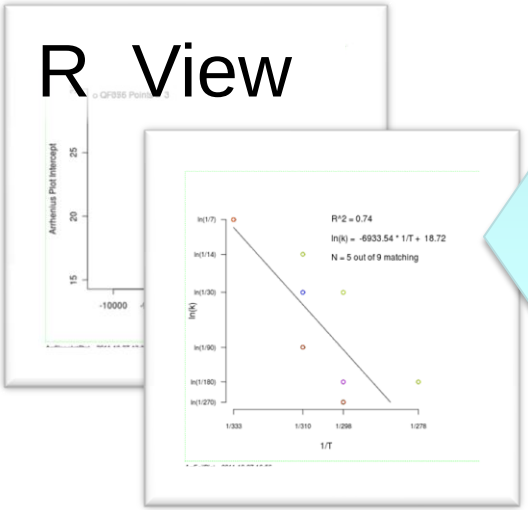
Individual Metadata



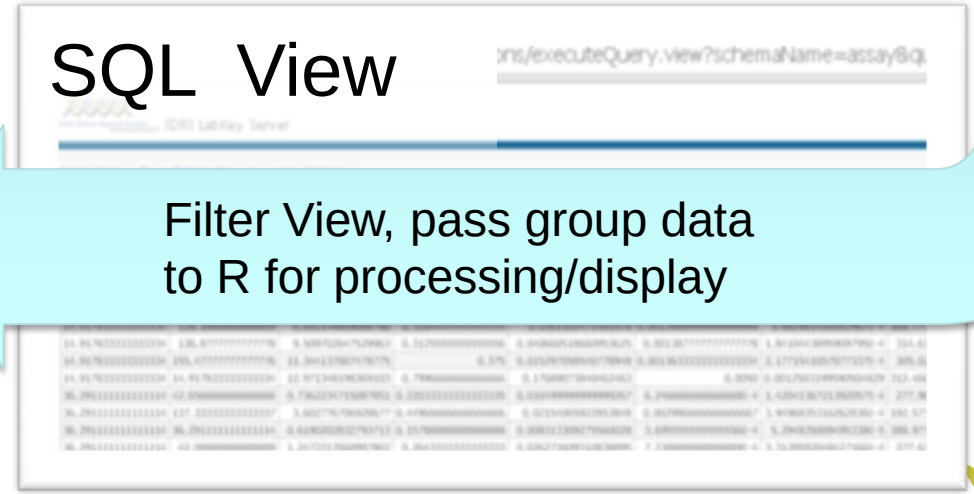
Use R to find individuals in group

Group Result

R View



SQL View



Filter View, pass group data to R for processing/display

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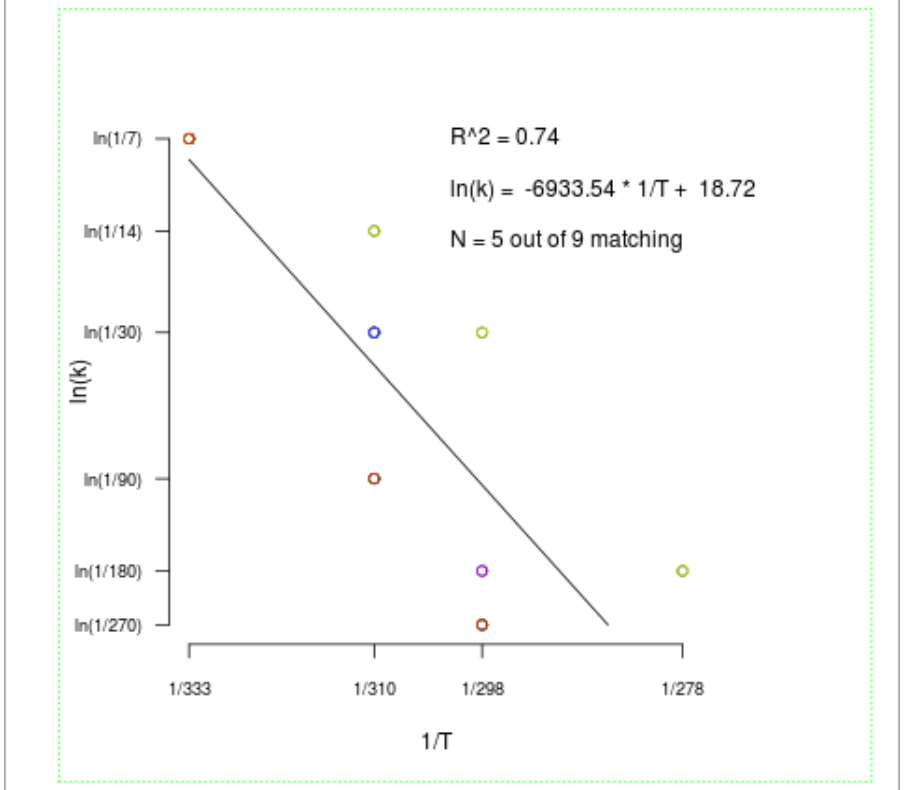
Group Analysis



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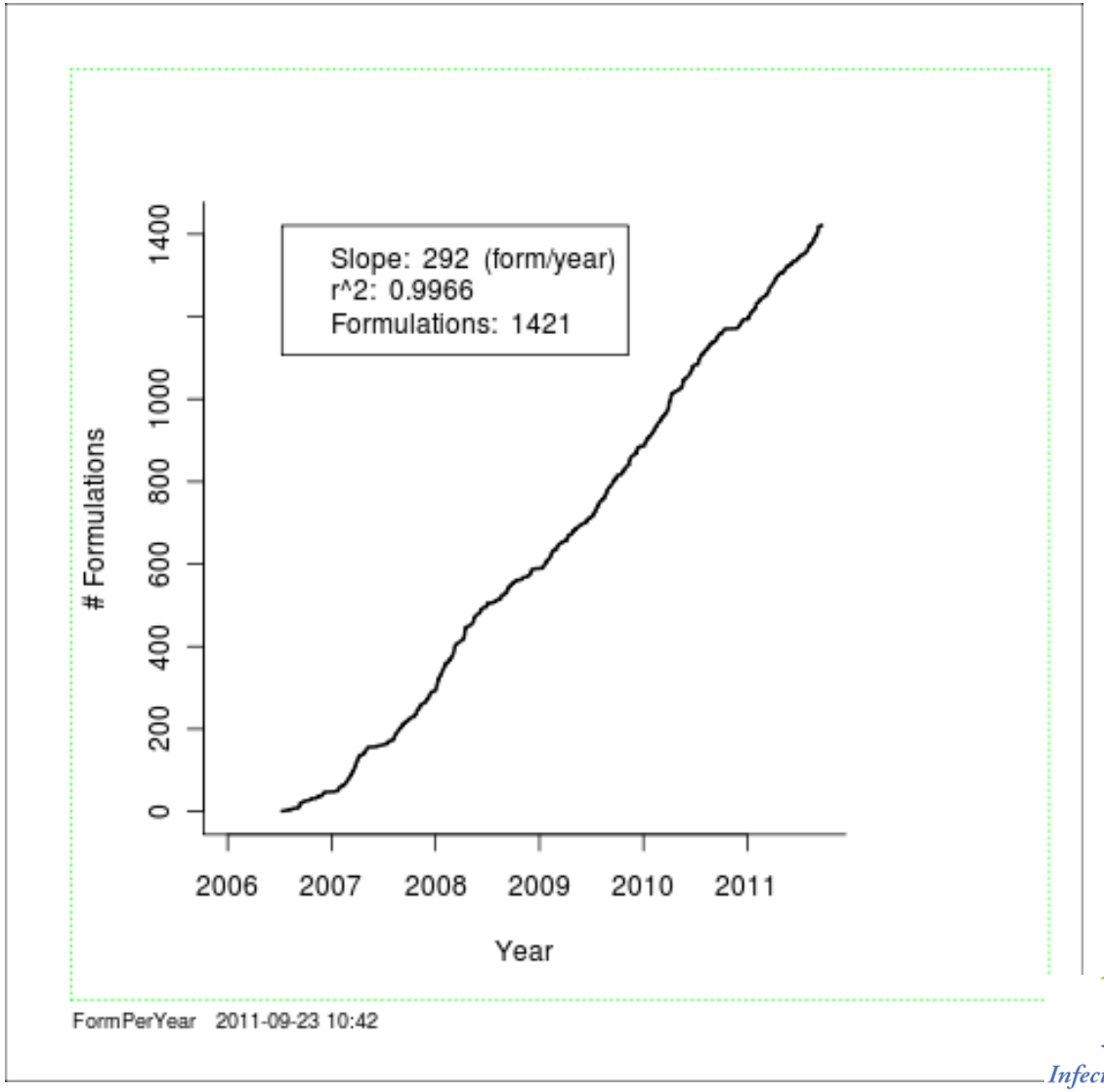
LabKey: Database Statistics



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Challenges

- Well defined relationships
  - A good model is priceless
- Know your data; be creative!
  - Carefully framed questions reveal powerful insight into your data

Conclusions

- LabKey at IDRI allows easy tracking of 14,000 “Samples.”

- Also allows data mining to answer relevant questions about sample population behavior

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Acknowledgements

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