

Adjuvant Formulations: Applied LabKey Server in Process Development

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Formulations Department

IDRI Background

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



IDRI Background

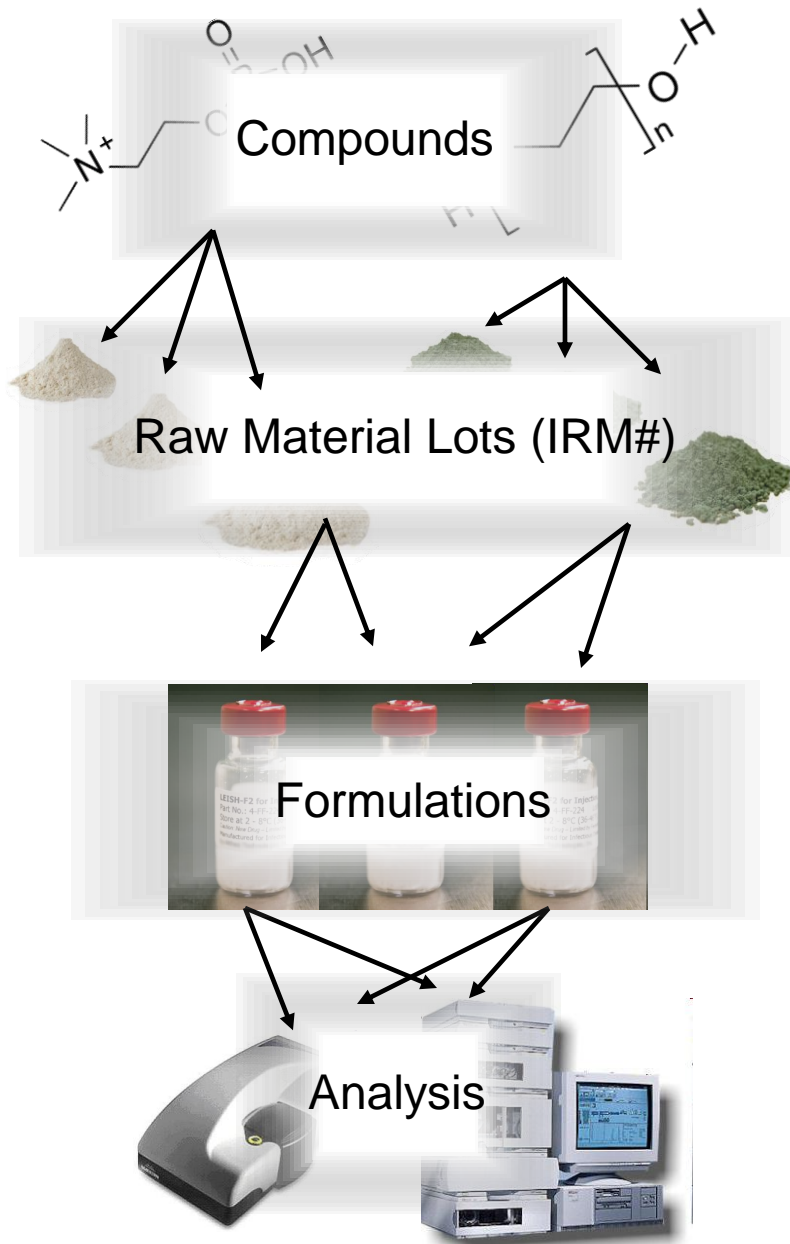
- Seattle-based not-for-profit
- R+D of products to prevent, detect and treat infectious diseases of poverty.
- IDRI integrates capabilities to bring scientific innovation from the lab to the people who need it most.

IDRI Research Programs

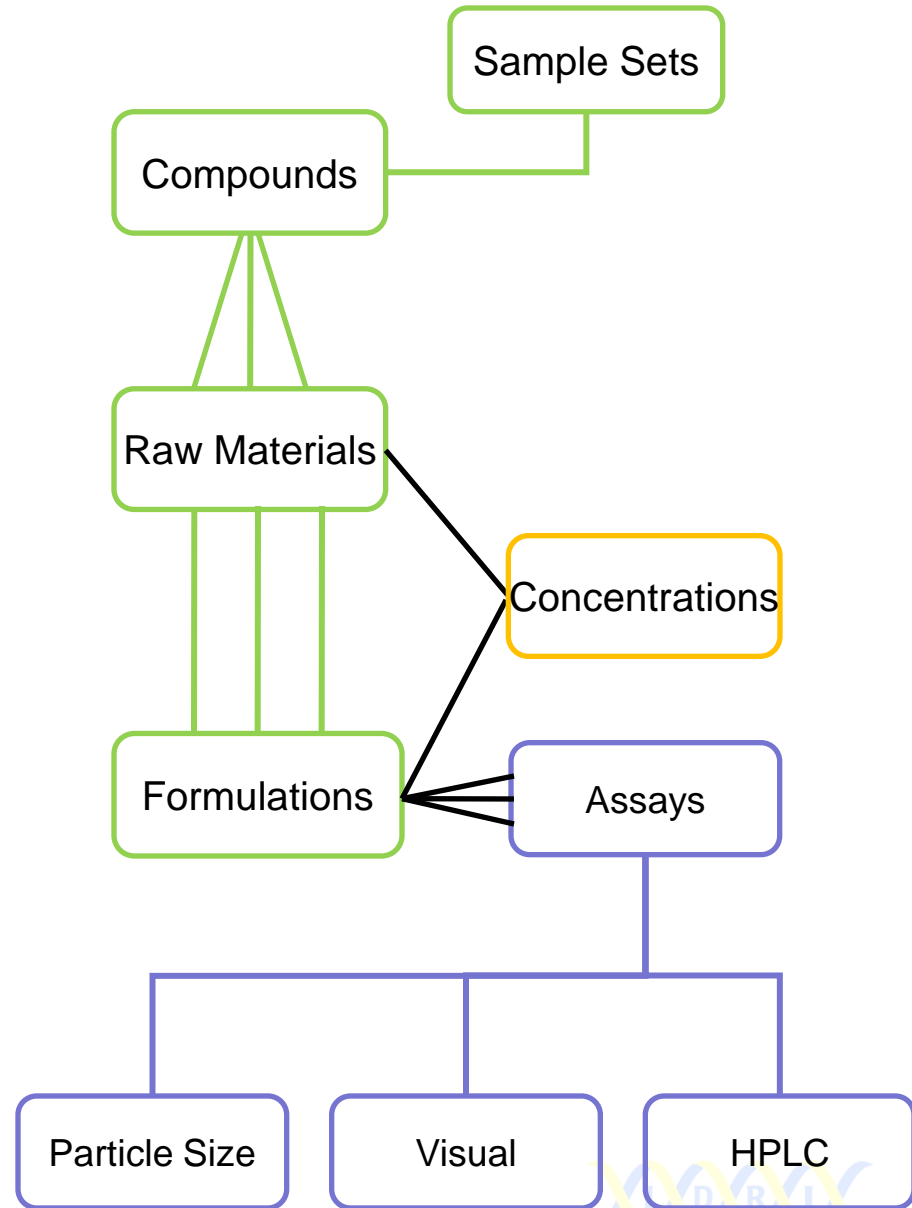
- Antigen/Drug Discovery
- Preclinical Biology
- Clinical Development
- Process Development
- **Adjuvant and Delivery Systems**



Physical Reality

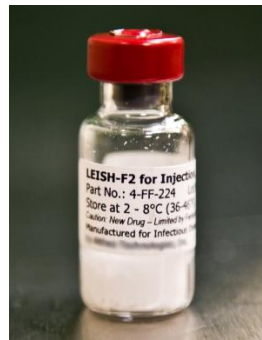


IDRI LabKey



LabKey: Tracking/Analysis

- Individual Tracking and Analysis



- Population Tracking and Analysis



What's the Goal?

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



Questions About Individuals

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



Individual Lot Tracking/Analysis

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Search IDRI LabKey Server

XXXXXX
Infectious Disease Research Institute
The Research Institute for

IDRI LabKey Server

Formulation QF055

FORMULATIONS HOME PAGE > EDIT QF055 > FORMULATIONS SAMPLE SET > OLD SAMPLE VIEW >

Information

Date of Manufacture: Mon Nov 30 00:00:00 PST 2009
 Type: Emulsion
 Lot Size: 100
 Notebook Page: 7961
 Comments: Terminated: Visual fail @ 25C (9 mo); Visual & PS fail @ 37C (3 mo), 60C (1 mo)
 Raw Materials: IRM-0027, IRM-0097, IRM-0107, IRM-0110, IRM-0109, IRM-0108

Particle Size Stability

REFRESH

...	DM	1 wk	2 wk	1 mo	3 mo	6 mo	12 mo	Me...
...		94.98	95.16	96.64	94.34	94.88	95.59	92
...		94.49	96.68	95.52	94.51	146.24		92
...		96.55	105.24	103	270.09			92
...		289.97	361.7	449.79				92

Page 1 of 1 | Displaying 1 - 4 of 4

Concentrations

Compound Name	Lot Name	Concentration	Unit	Material Name
	QF055	25.0	mM	IRM-0109
	QF055	25.0	mM	IRM-0110
IRM-0027	QF055	1.8	%w/vol	IRM-0107
IRM-0097	QF055	1.9	%w/vol	IRM-0027
IRM-0107	QF055	10.0	%w/vol	IRM-0097
IRM-0108	QF055	1.8	%w/vol	IRM-0107
IRM-0109	QF055	0.09	%w/vol	IRM-0108
IRM-0110	QF055	25.0	mM	IRM-0109
	QF055	25.0	mM	IRM-0110
	QF055	1.9	%w/vol	IRM-0027
	QF055	0.09	%w/vol	IRM-0108
	QF055	10.0	%w/vol	IRM-0097

Stability Charts

PS QF055 aps

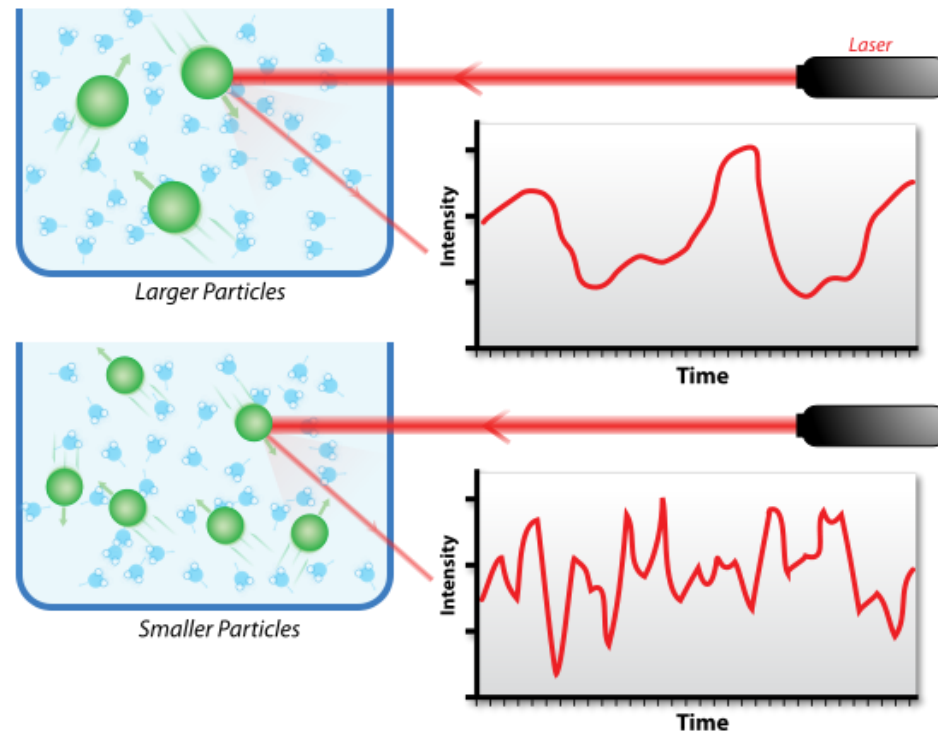
TimePoint	Test 1 Mean	Test 2 Mean	Test 3 Mean
DM	NA	NA	NA
1 wk	95	95	95
2 wk	95	95	95
1 mo	96.67	96.67	96.67
3 mo	94.33	94.33	94.33
6 mo	94.67	94.67	94.67
9 mo	90.67	90.67	90.67
12 mo	95.33	95.33	95.33
24 mo	NA	NA	NA
36 mo	NA	NA	NA

PS QF055 nano

TimePoint	Test 1 Mean	Test 2 Mean	Test 3 Mean
DM	92.33	92.33	92.33
1 wk	NA	NA	NA
2 wk	NA	NA	NA
1 mo	NA	NA	NA
3 mo	NA	NA	NA
6 mo	NA	NA	NA
9 mo	NA	NA	NA
12 mo	NA	NA	NA
24 mo	NA	NA	NA
36 mo	NA	NA	NA

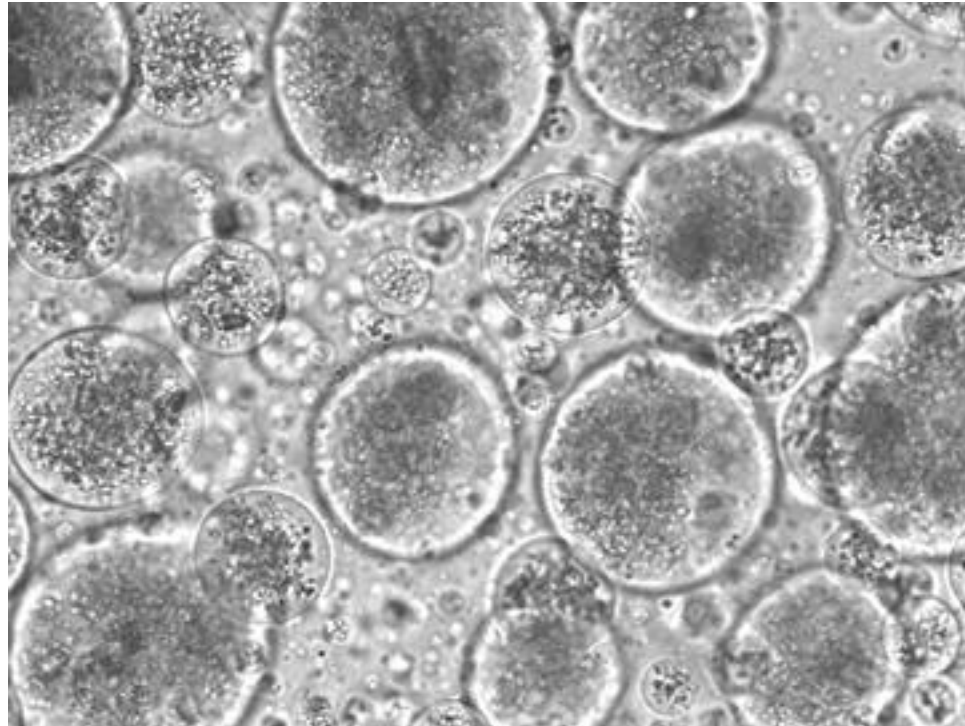
Particle Size Data

- Dynamic light scattering

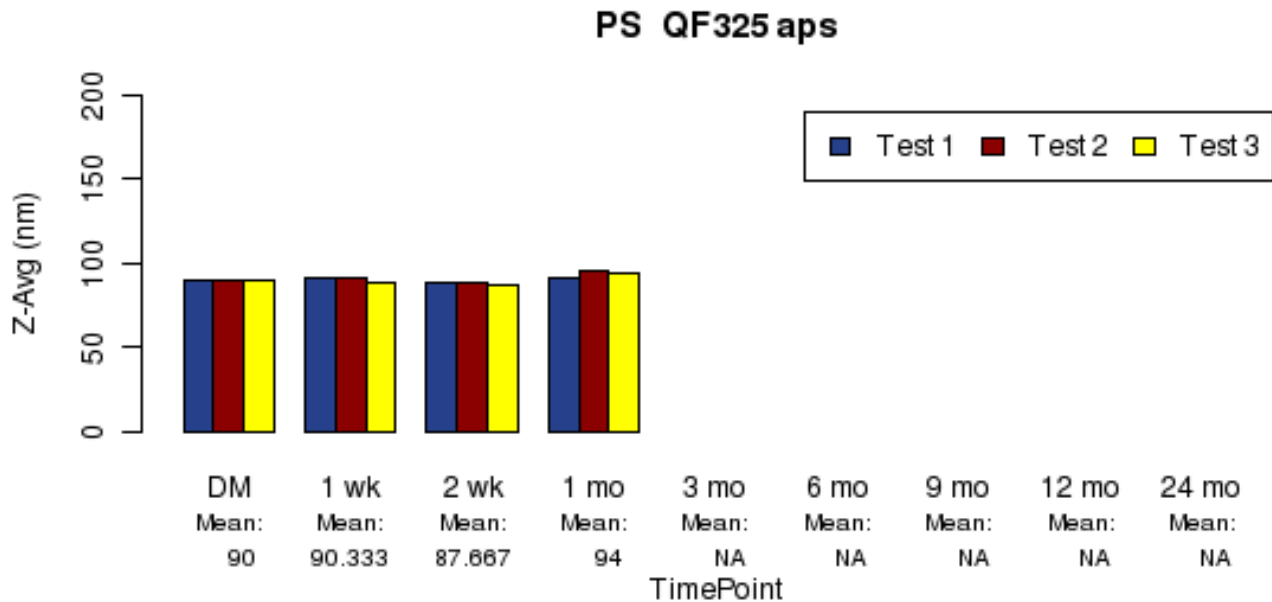


Particle Size Data

- Larger particles tend to aggregate



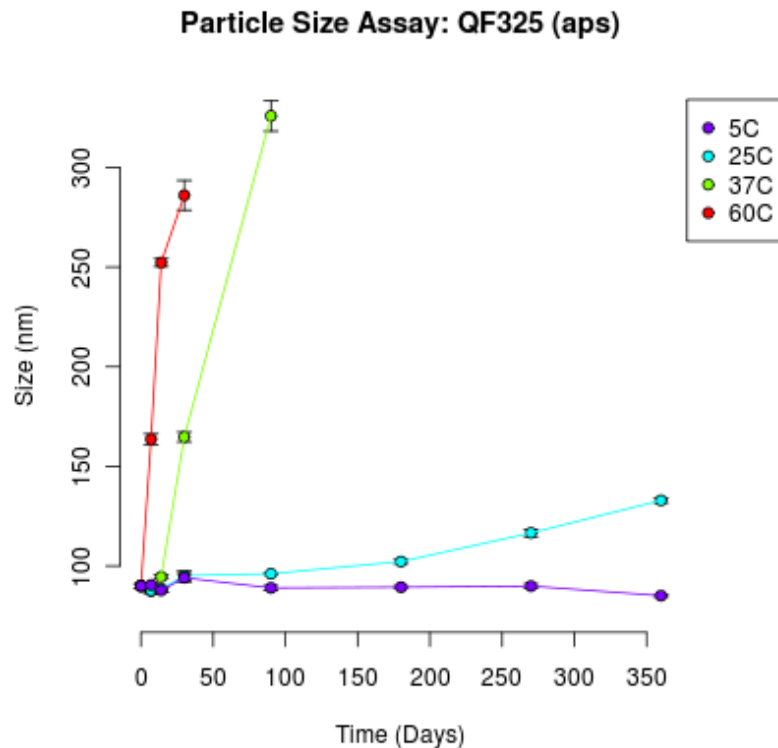
View Development



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

View Development

- Multiple temps
- Quantitative error
- Infinitely scalable



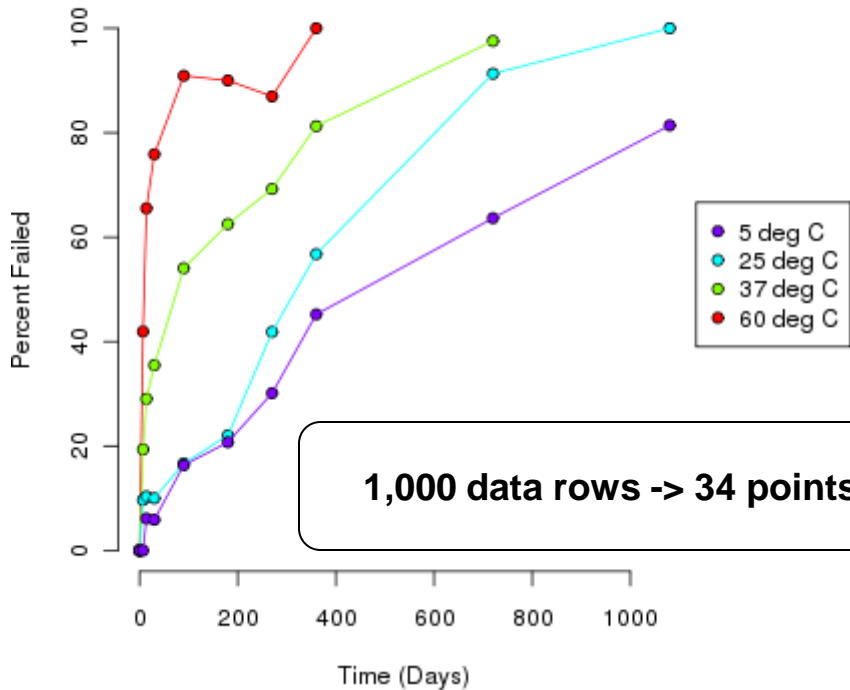
The True Power of LabKey

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

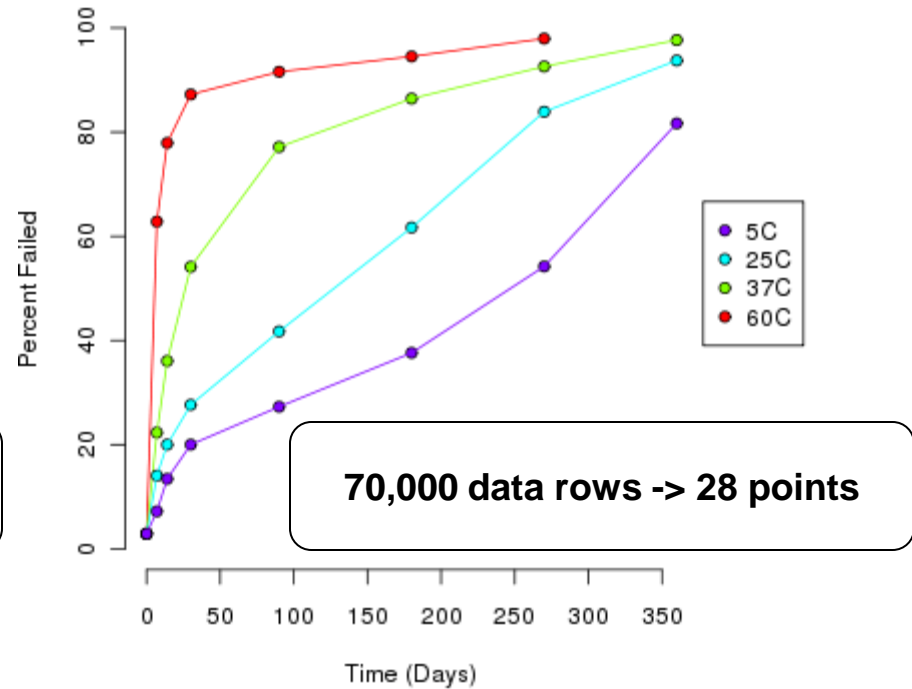


Views

**Visual Assay:
Percent Failure by Storage Time and Temperature**



**Particle Size Assay:
Percent Failure of Emulsion formulations (aps)**



White-boarding

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

- Now start writing code.



Method: SQL

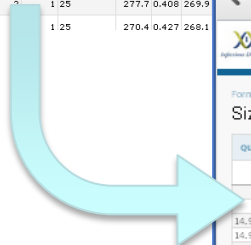
Assay

Particle Size Results

MANAGE ASSAY DESIGN VIEW BATCHES VIEW RUNS VIEW RESULTS VIEW COPY-TO-STUDY HISTORY

Time Label	Extraction Number	Test Number	Measuring Temperature	Z-Ave	PdI	Mean Count Rate (cps)	Cumulant	Measurement Date and Time	Storage Temperature	Record Name	Sample Name	Analysis Tool	Run IDRI Batch Number	Run Ave	Run Z-Error
T=0	1	1	1.25	1467.0	0.958	94.0	0.0080	Tue, Oct 13, 2009 at 09:59:34 AM	5C	1 DM 1	nano	1003	1146		
T=0	2	1	2.25	966.6	0.908	85.3	0.00856	Tue, Oct 13, 2009 at 10:02:42 AM	5C	2 DM 2	nano	1003	1146		
T=0	3	1	2.25	1361.0	1.0	84.2	0.0104	Tue, Oct 13, 2009 at 10:05:50 AM	5C	3 DM 3	nano	1003	1146		
T=0	1	2	2.25	893.2	0.757	360.4	0.00719	Tue, Oct 13, 2009 at 10:09:24 AM	5C	4 DM 1	nano	1003	1146		
T=0	2	2	2.25	2299.0	1.0	377.0	0.00864	Tue, Oct 13, 2009 at 10:11:30 AM	5C	5 DM 2	nano	1003	1146		
T=0	3	2	2.25	2771.0	1.0	381.9	0.0126	Tue, Oct 13, 2009 at 10:13:36 AM	5C	6 DM 3	nano	1003	1146		
T=0	1	3	2.25	875.2	0.798	255.9	0.0128	Tue, Oct 13, 2009 at 10:16:05 AM	5C	7 DM 1	nano	1003	1146		
T=0	2	3	2.25	873.4	0.729	277.1	0.012	Tue, Oct 13, 2009 at 10:15:32 AM	5C	8 DM 2	nano	1003	1146		
T=0	3	3	2.25	1464.0	0.978	288.4	0.0171	Tue, Oct 13, 2009 at 10:52:58 AM	5C	9 DM 3	nano	1003	1146		
1 dy	1	1	1.25	286.1	0.415	269.6									
1 dy	2	1	1.25	277.7	0.408	269.9									
1 dy	3	1	1.25	270.4	0.427	268.1									

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



idri.labkey.com/query/Formulations/executeQuery.view?schemaName=assay&query.queryName=SizeFail

Formulations > Query Schema Browser > assay Schema > SizeFail

QUERY	VIEW	EXPORT	PRINT	PAGE SIZE	Mean Z-Ave	Mean PdI	Std Dev PdI	Mean Cumulants	Std Dev Cumulants	Mean Mean Count	Std Dev Mean Count	Name	Analysis Tool	Storage Temperature	Sort Order	Type	Index Name	Failed		
					0.0	0.0	0.0	0.0	0.0	279.83333333333333	11.787422675603805	QF065	aps	5C		0	Aqueous	QF065.0.5C	TRUE	
					0.0	0.0	0.0	0.10414573122952919	0.0027366666666666666	308.8	1.8999999999999999	QF065	aps	5C		7	Aqueous	QF065.7.5C	TRUE	
14.917833333333334					126.18888888888889	6.68214869688786	0.32644444444444444	0.0361182471581578	0.0013899999999999999	5.0829814085829675	308.77777777777777	6.360380841148881	QF187	aps	5C		7	Aqueous	QF187.7.5C	TRUE
14.917833333333334					136.87777777777778	9.509702647529663	0.31255555555555556	0.040660518660953625	0.0013877777777777778	1.8410443899909795	314.61111111111111	7.474698061535357	QF187	aps	5C		14	Aqueous	QF187.14.5C	TRUE
14.917833333333334					195.47777777777778	11.364137007478775	0.375	0.015297058540778948	0.0013633333333333334	2.17715410570773375	305.02222222222222	10.791521878051425	QF187	aps	5C		90	Aqueous	QF187.90.5C	TRUE
14.917833333333334					14.917833333333334	12.971348198369103	0.7996666666666666	0.17689073840462463	0.0050	0.0012501199999999999	312.56666666666666	9.151138362704714	QF187	aps	5C		0	Aqueous	QF187.0.5C	FALSE
36.291111111111114					42.056666666666666	0.7362234715387851	0.23333333333333335	0.010499999999999999	6.246666666666666	1.42841367213820575	277.96666666666667	9.78199877325603	QF096	nano	30C		7	Liposome	QF096.7.30C	FALSE
36.291111111111114					117.323232323232327	3.60276705928677	0.44966666666666666	0.02154059522953848	0.0029866666666666667	3.9496835162628365	192.57777777777778	5.620671172840896	QF096	nano	60C		7	Liposome	QF096.7.60C	TRUE
36.291111111111114					36.291111111111114	0.6190202832793713	0.15788888888888888	0.008313309275560208	3.6955555555555556	5.2948390094951385	388.87777777777778	64.84479118976694	QF096	nano	5C		0	Liposome	QF096.0.5C	FALSE
36.291111111111114					42.088888888888889	1.2472213560997802	0.26433333333333333	0.026272609310838995	7.238888888888889	3.312895048471666	277.63333333333334	121.88545852561732	QF096	nano	90C		90	Liposome	QF096.90.5C	FALSE
36.291111111111114					48.608888888888889	1.98246339464611	0.393	0.024494897427830432	0.0015955555555555559	0.001211705149969742	342.38888888888889	47.5088266527449	QF096	nano	5C		0	Liposome	QF096.0.5C	FALSE
36.291111111111114					43.471111111111112	2.361934823637314	0.275	0.029870554062487724	0.0026902222222222222	0.004345864061892002	271.78888888888889	114.50377116545997	QF096	nano	5C		0	Liposome	QF096.0.5C	FALSE
36.291111111111114					39.484444444444445	0.6517497815709747	0.19011111111111112	0.007888375063114099	5.108888888888889	8.67603660153135	231.36666666666667	11.211601134538824	QF096	nano	5C		0	Liposome	QF096.0.5C	FALSE
36.291111111111114					37.705555555555556	0.4312803934539643	0.17177777777777778	0.009121099861674875	4.453333333333334	1.398811999994513	279.76666666666667	78.75212695540324	QF096	nano	5C		0	Liposome	QF096.0.5C	FALSE

SQL View

Method: R

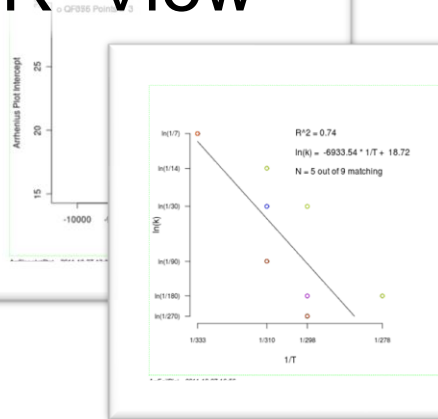
Grouping
Metadata

Individual Metadata

Use R to find individuals in group

Group
Result

R View

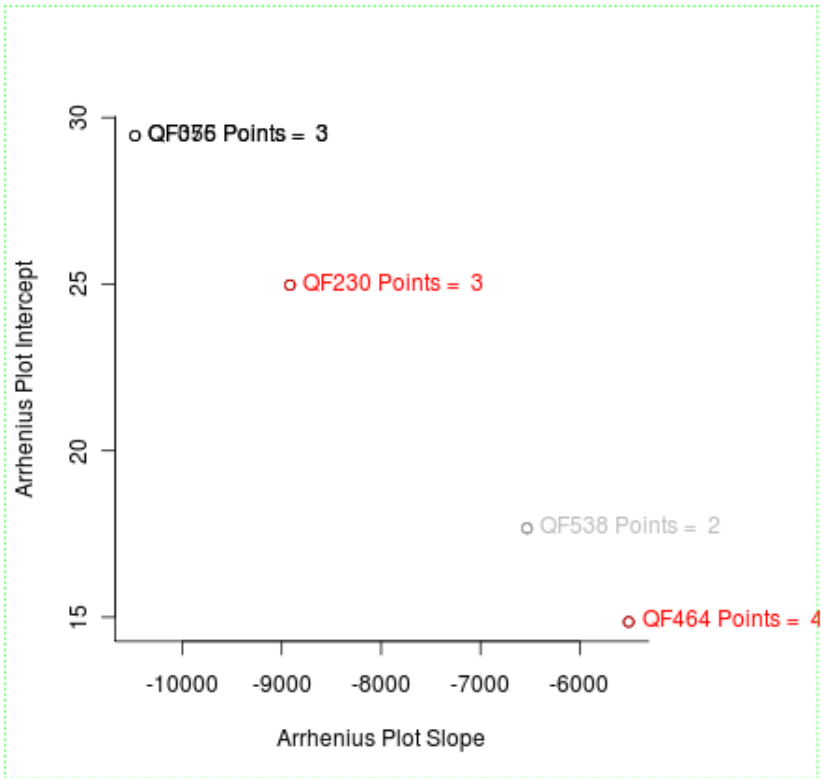


SQL View

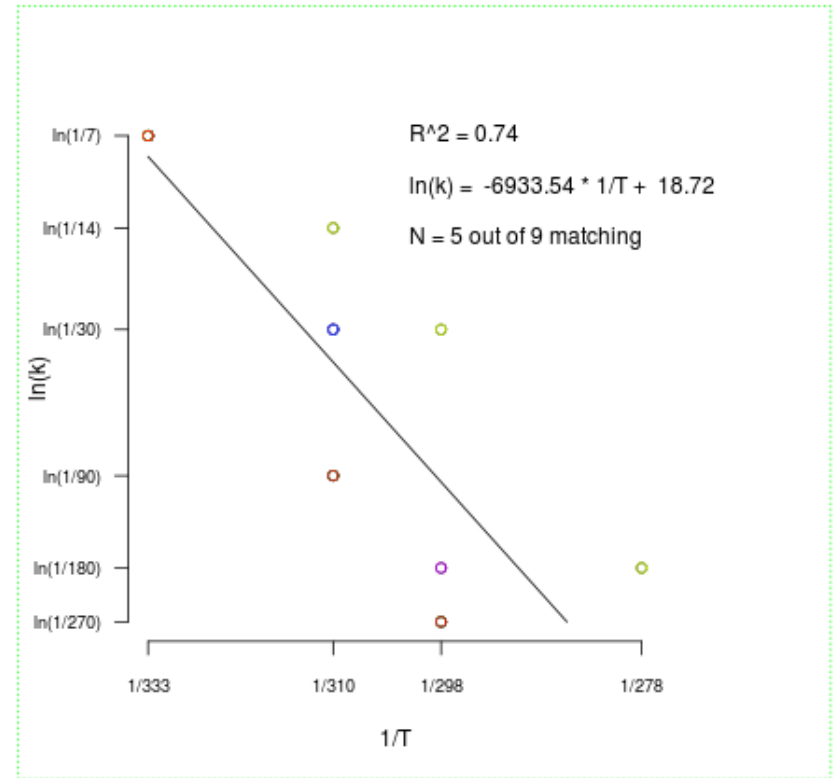
Filter View, pass group data
to R for processing/display

```
34,91763333333333 1.8647777777777778 0.5400000000000000 0.2300000000000000 0.0000000000000000 1.8647777777777778 1.8647777777777778 394.45  
34,91763333333333 2.8647777777777778 1.1400000000000000 0.4700000000000000 0.0000000000000000 2.8647777777777778 2.8647777777777778 395.45  
34,91763333333333 4.8647777777777778 2.3400000000000000 0.9400000000000000 0.0000000000000000 4.8647777777777778 4.8647777777777778 396.45  
36,29133333333333 42.80000000000000 0.7900000000000000 0.2800000000000000 0.0000000000000000 42.80000000000000 42.80000000000000 271.88  
36,29133333333333 137.20000000000000 0.4000000000000000 0.1400000000000000 0.0000000000000000 137.20000000000000 137.20000000000000 292.57  
36,29133333333333 36,29133333333333 0.4000000000000000 0.1400000000000000 0.0000000000000000 36,29133333333333 36,29133333333333 288.57  
36,29133333333333 42.80000000000000 0.7900000000000000 0.2800000000000000 0.0000000000000000 42.80000000000000 42.80000000000000 271.88
```

Group Analysis



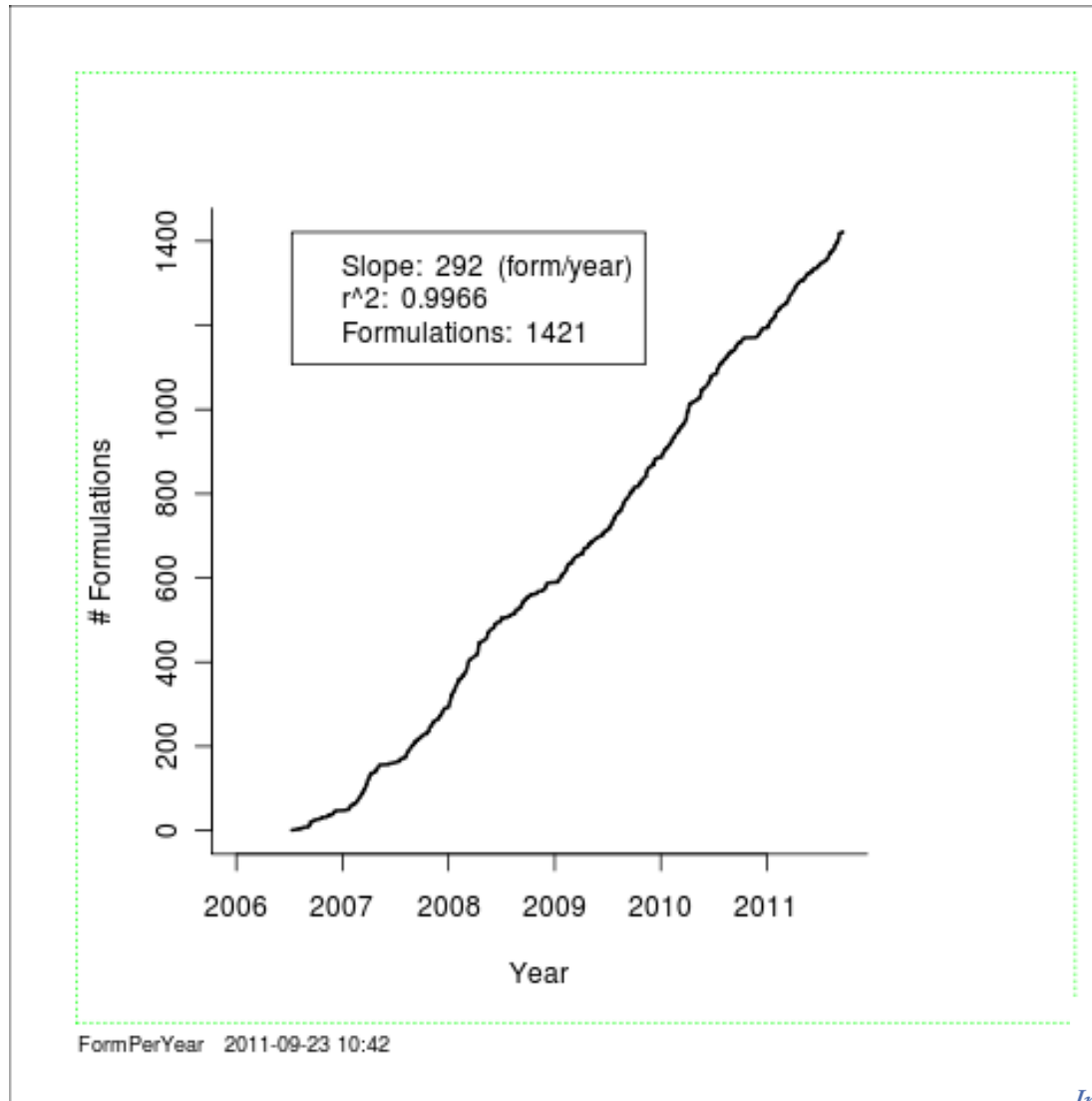
ArrSlopeIntPlot 2011-10-27 13:06



ArrFailPlot 2011-10-27 16:56



LabKey: Database Statistics



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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