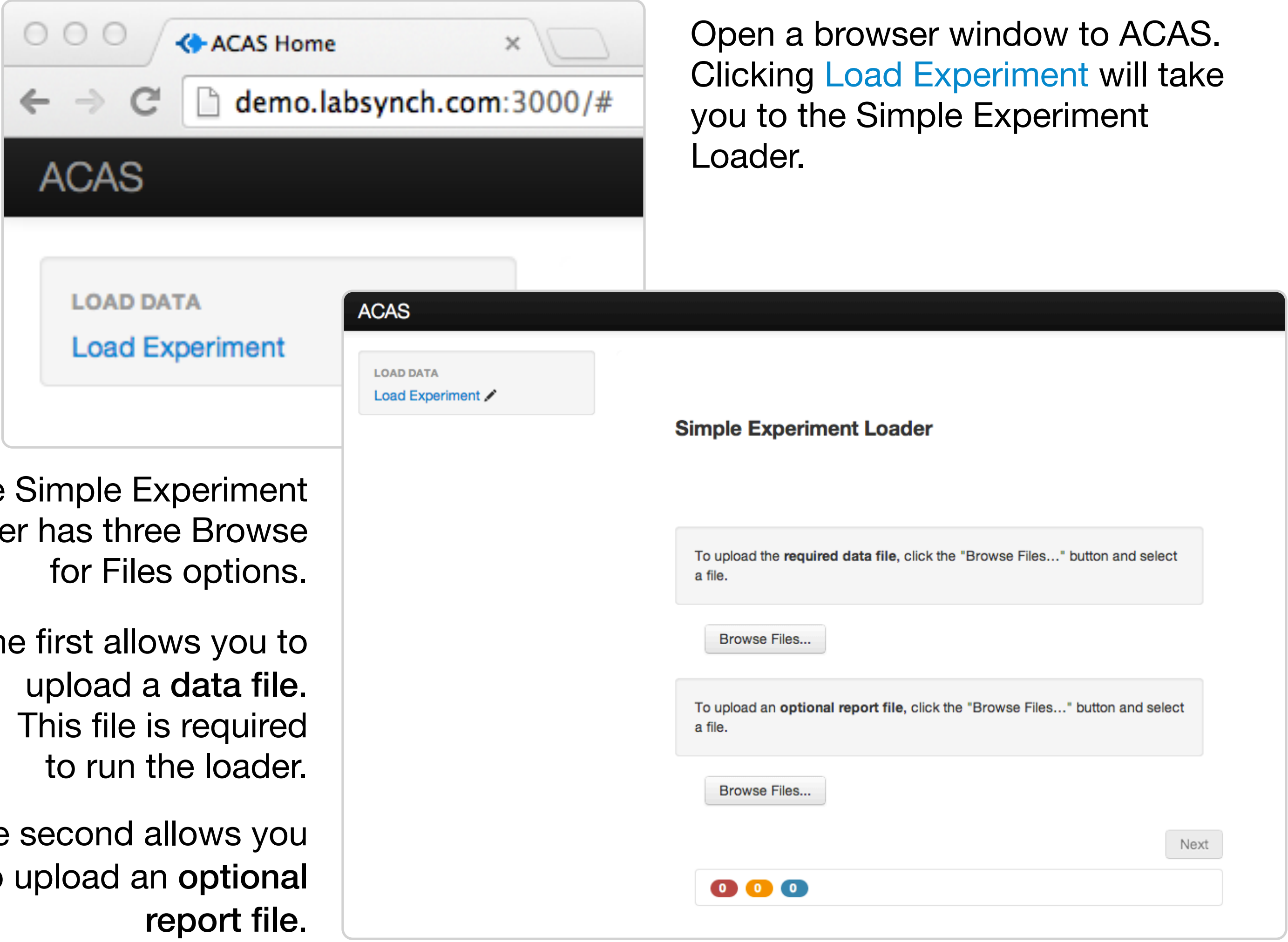
ACAS Tutorial

Simple Experiment Loader

Contents:

- Overall Workflow
- Loading a Generic Data File
- Loading a Concentration Data File
- Adding a Report File
- Adding Images
- Validation Errors
- Editing a Protocol
- Adding Files to Protocols

JOHN McNEIL
& Company, Inc.



To upload the **required data file**, click the "Browse Files..." button and select a file.

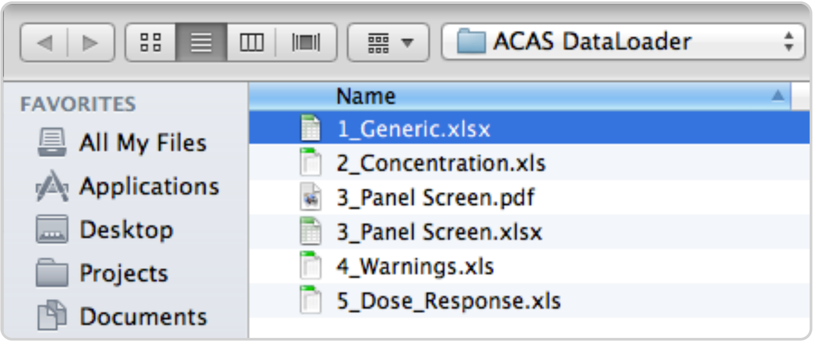
To upload an **optional report file**, click the "Browse Files..." button and select a file.

Open a browser window to ACAS. Clicking Load Experiment will take you to the Simple Experiment Loader.

The Simple Experiment Loader has three Browse for Files options.

The first allows you to upload a **data file.** This file is required to run the loader.

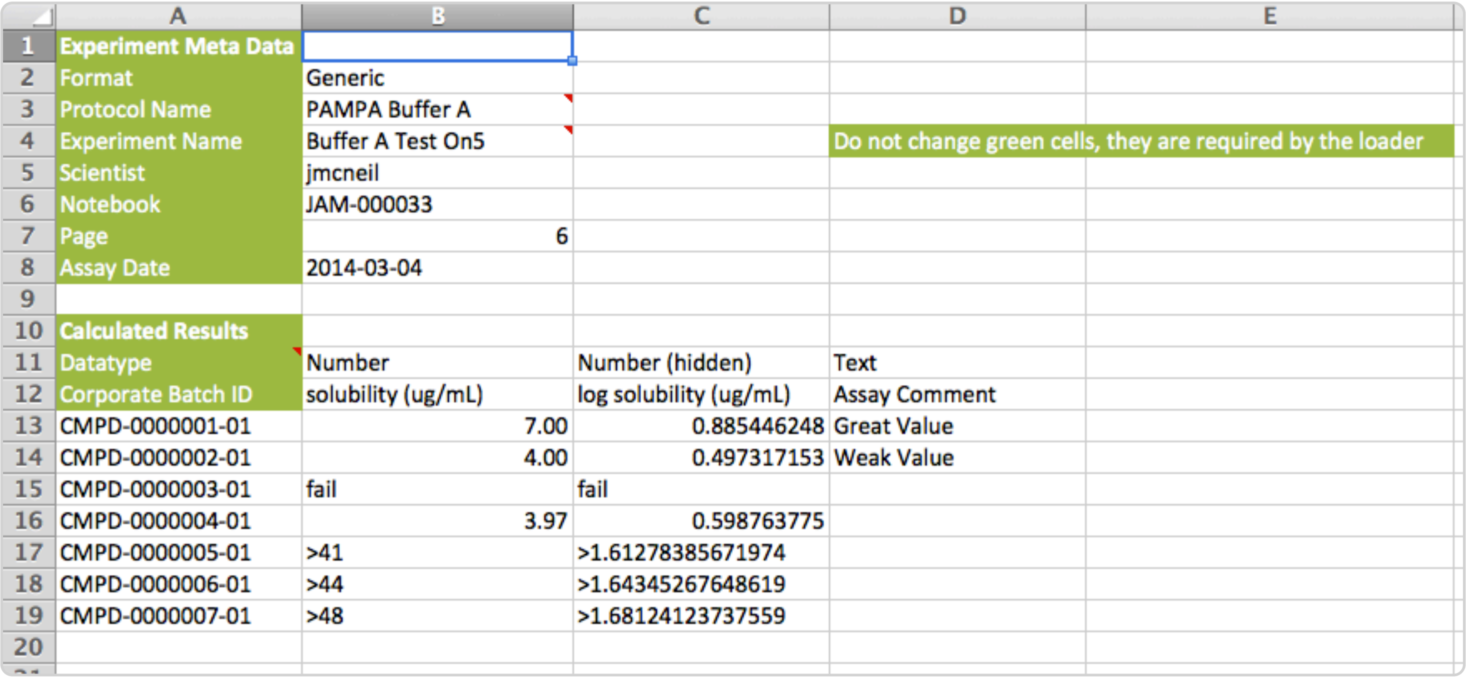
The second allows you to upload an **optional report file.**



Click Browse Files… and select the data file you would like to upload.

The data file browser accepts these file types: .xls, .xlsx, and .csv.

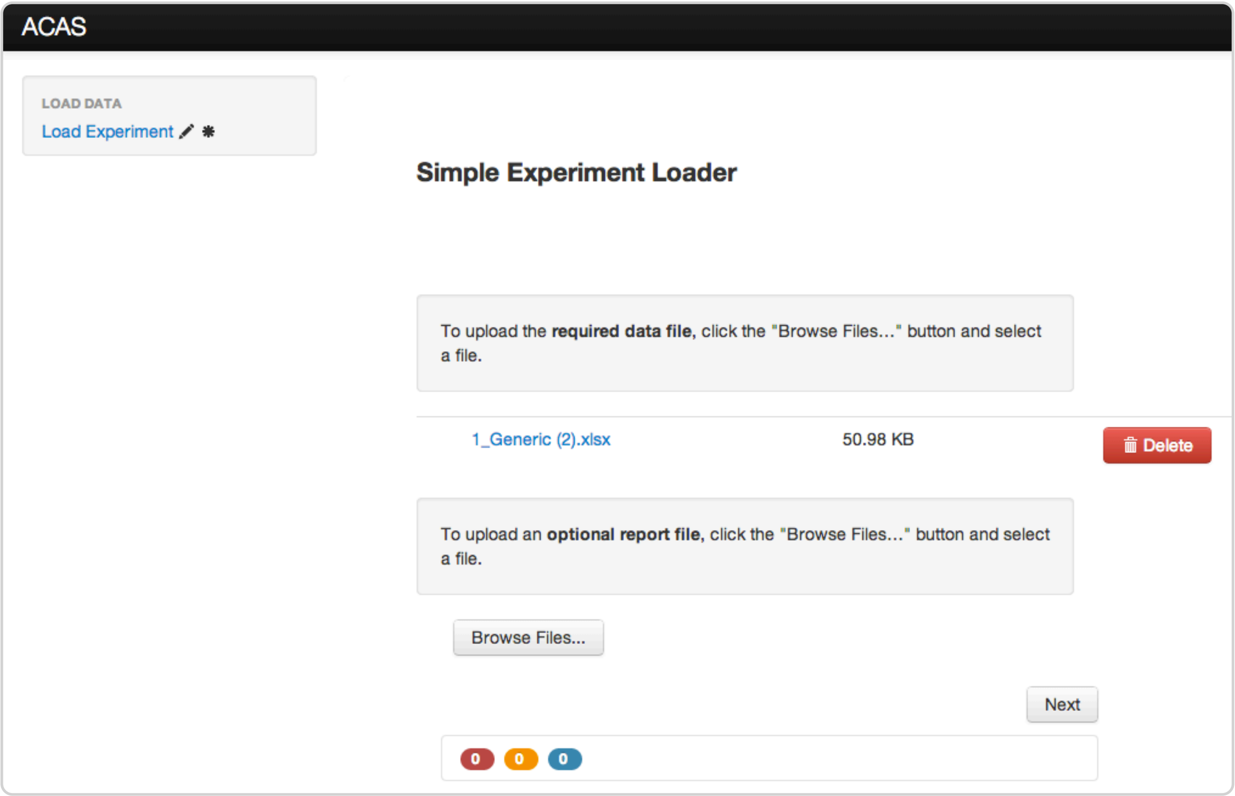
The report file browser accepts almost all file types except .exe.



	A	B	C	D	E
1	Experiment Meta Data				
2	Format	Generic			
3	Protocol Name	PAMPA Buffer A			
4	Experiment Name	Buffer A Test On5		Do not change green cells, they are required by the loader	
5	Scientist	jmcneil			
6	Notebook	JAM-000033			
7	Page	6			
8	Assay Date	2014-03-04			
9					
10	Calculated Results				
11	Datatype	Number	Number (hidden)	Text	
12	Corporate Batch ID	solubility (ug/mL)	log solubility (ug/mL)	Assay Comment	
13	CMPD-0000001-01	7.00	0.885446248	Great Value	
14	CMPD-0000002-01	4.00	0.497317153	Weak Value	
15	CMPD-0000003-01	fail	fail		
16	CMPD-0000004-01	3.97	0.598763775		
17	CMPD-0000005-01	>41	>1.61278385671974		
18	CMPD-0000006-01	>44	>1.64345267648619		
19	CMPD-0000007-01	>48	>1.68124123737559		
20					

This is what a generic sample data file looks like (in this case: solubility). The green cells are required by the loader to analyze the data in the file. However, all other fields may be changed. Keep in mind: some fields have format requirements.

Select the data file. It will appear in the Simple Experiment Loader, with options. If there is no report file, click the Next button.

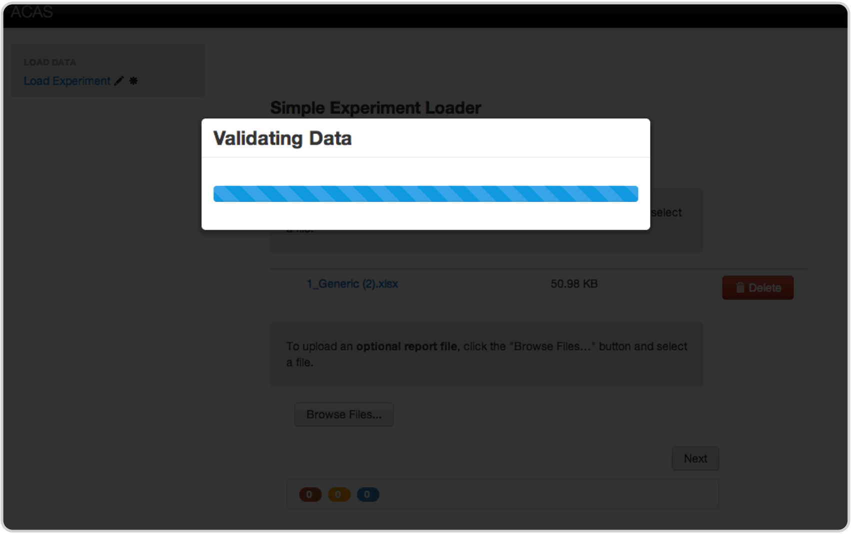


Simple Experiment Loader

To upload the **required data file**, click the "Browse Files..." button and select a file.

1_Generic (2).xlsx 50.98 KB

To upload an **optional report file**, click the "Browse Files..." button and select a file.



Simple Experiment Loader

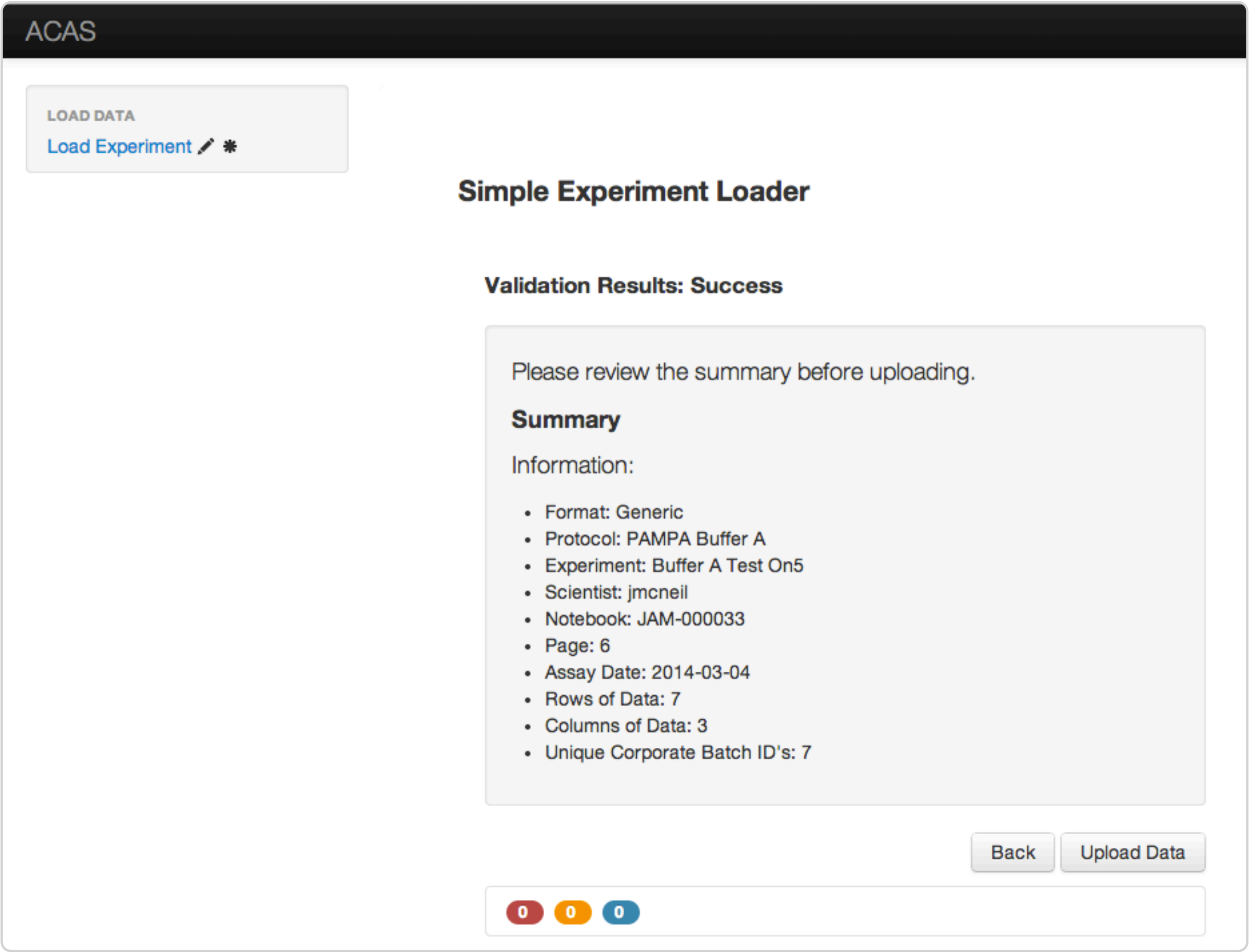
Validating Data

1_Generic (2).xlsx 50.98 KB

To upload an **optional report file**, click the "Browse Files..." button and select a file.

The file is then validated, and the results are displayed. Check the summary to make sure all the information is correct.

If correct, click the Upload Data button.



Simple Experiment Loader

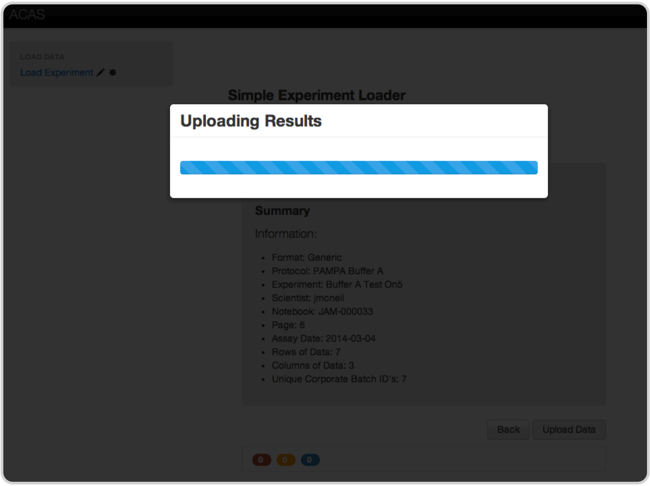
Validation Results: Success

Please review the summary before uploading.

Summary

Information:

- Format: Generic
- Protocol: PAMPA Buffer A
- Experiment: Buffer A Test On5
- Scientist: jmcneil
- Notebook: JAM-000033
- Page: 6
- Assay Date: 2014-03-04
- Rows of Data: 7
- Columns of Data: 3
- Unique Corporate Batch ID's: 7



Summary

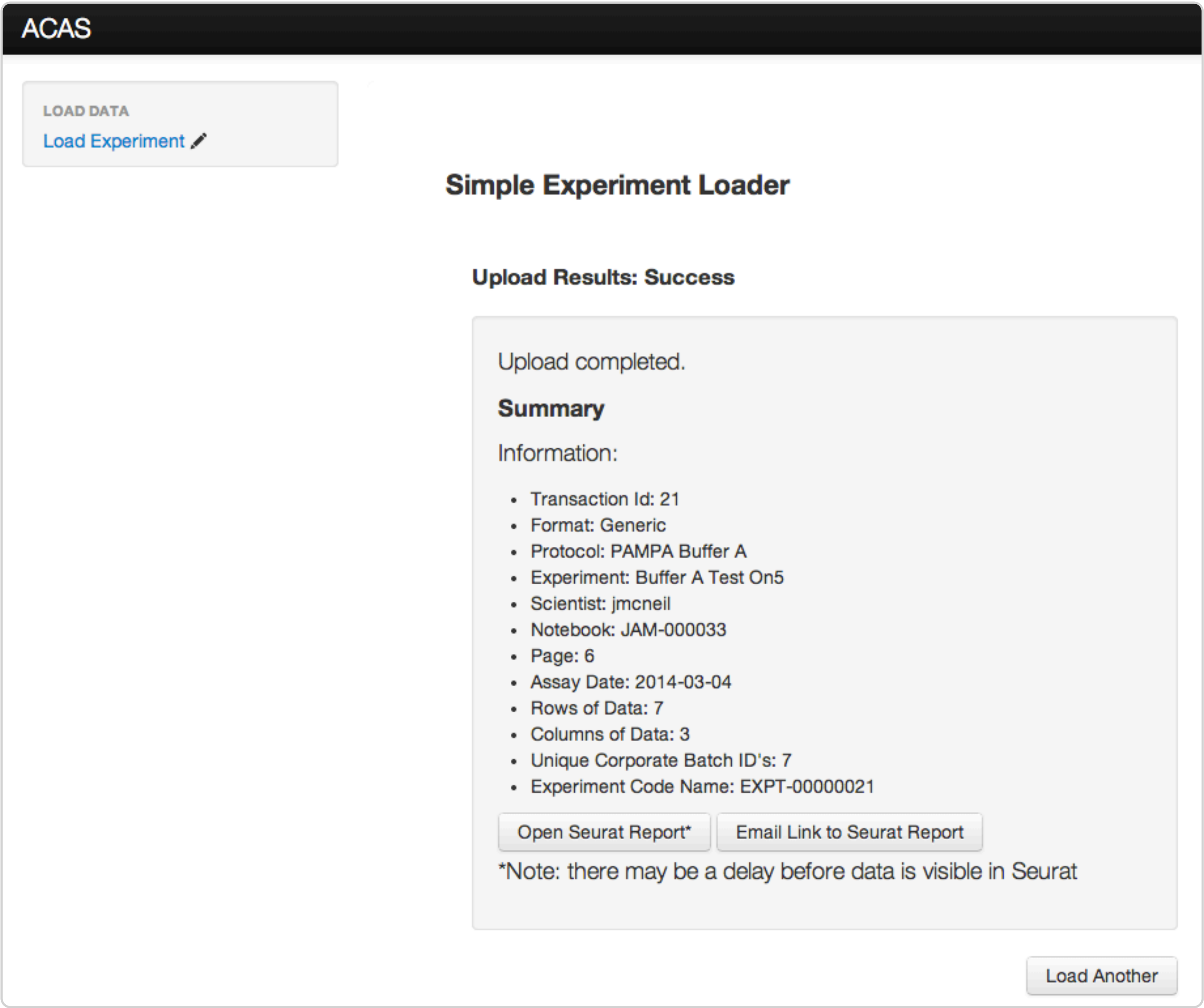
Information:

- Format: Generic
- Protocol: PAMPA Buffer A
- Experiment: Buffer A Test On5
- Scientist: jmcneil
- Notebook: JAM-000033
- Page: 6
- Assay Date: 2014-03-04
- Rows of Data: 7
- Columns of Data: 3
- Unique Corporate Batch ID's: 7

The results are uploaded, and a summary is displayed.

From there you can open the report in Seurat and email a link to the report. Clicking Open Seurat Report launches Seurat.

Alternatively, you can also load another experiment by clicking Load Another.



Simple Experiment Loader

Upload Results: Success

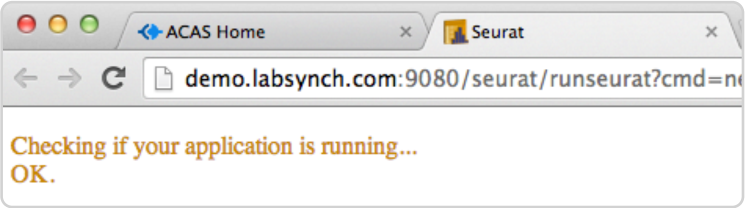
Upload completed.

Summary

Information:

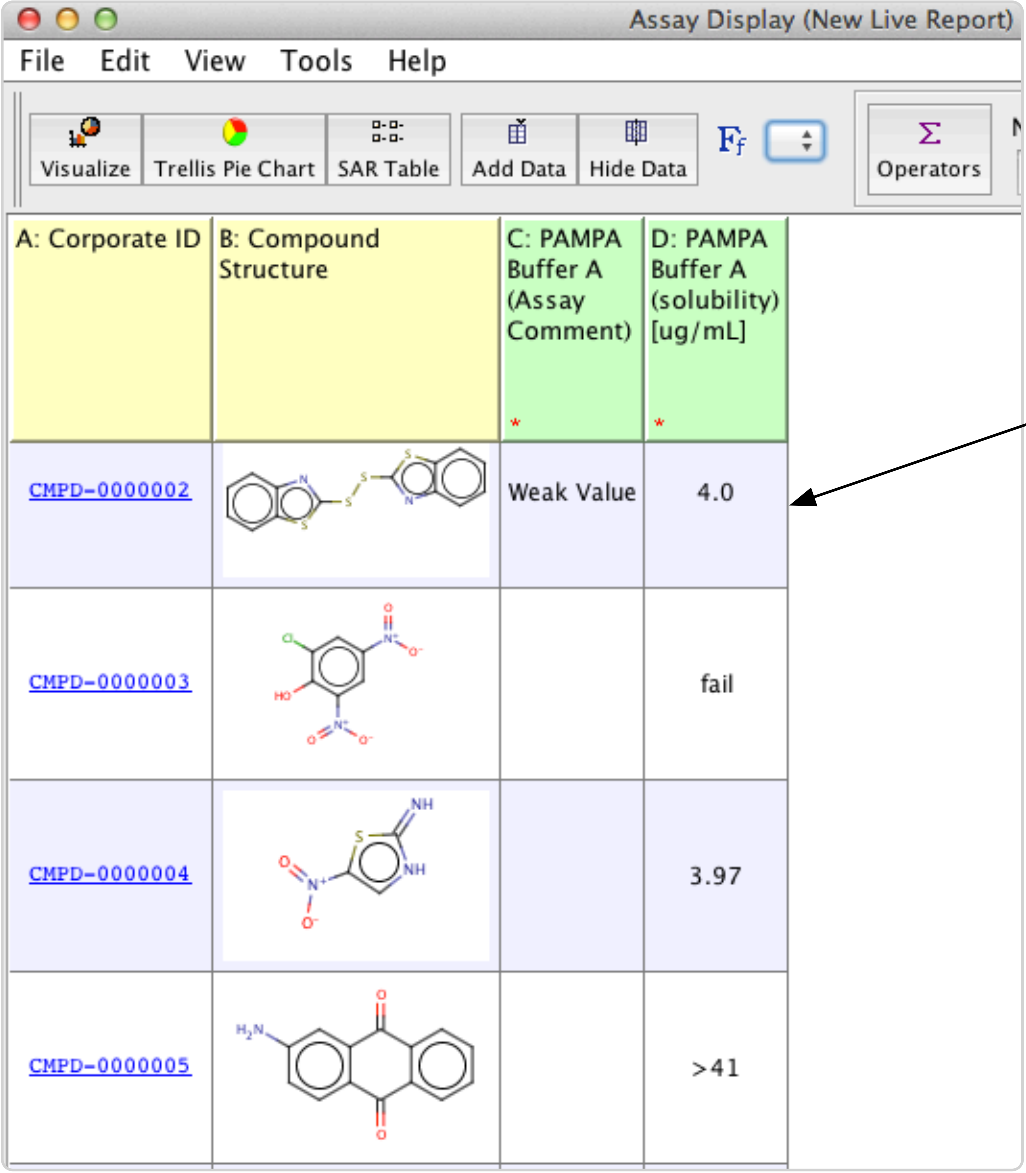
- Transaction Id: 21
- Format: Generic
- Protocol: PAMPA Buffer A
- Experiment: Buffer A Test On5
- Scientist: jmcneil
- Notebook: JAM-000033
- Page: 6
- Assay Date: 2014-03-04
- Rows of Data: 7
- Columns of Data: 3
- Unique Corporate Batch ID's: 7
- Experiment Code Name: EXPT-00000021

*Note: there may be a delay before data is visible in Seurat



Checking if your application is running...
OK.

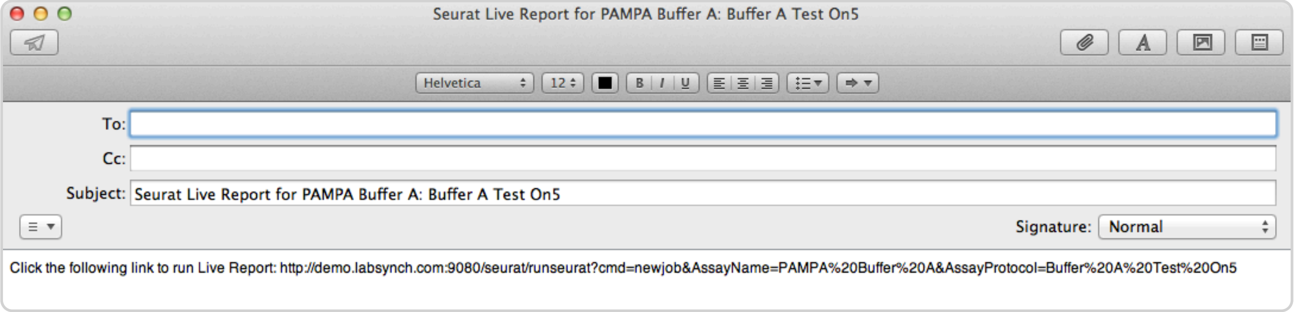
Seurat launches...



A: Corporate ID	B: Compound Structure	C: PAMPA Buffer A (Assay Comment) *	D: PAMPA Buffer A (solubility) [ug/mL] *
CMPD-0000002		Weak Value	4.0
CMPD-0000003			fail
CMPD-0000004			3.97
CMPD-0000005			>41

Data loaded.

This is the format for emailing a Seurat report.



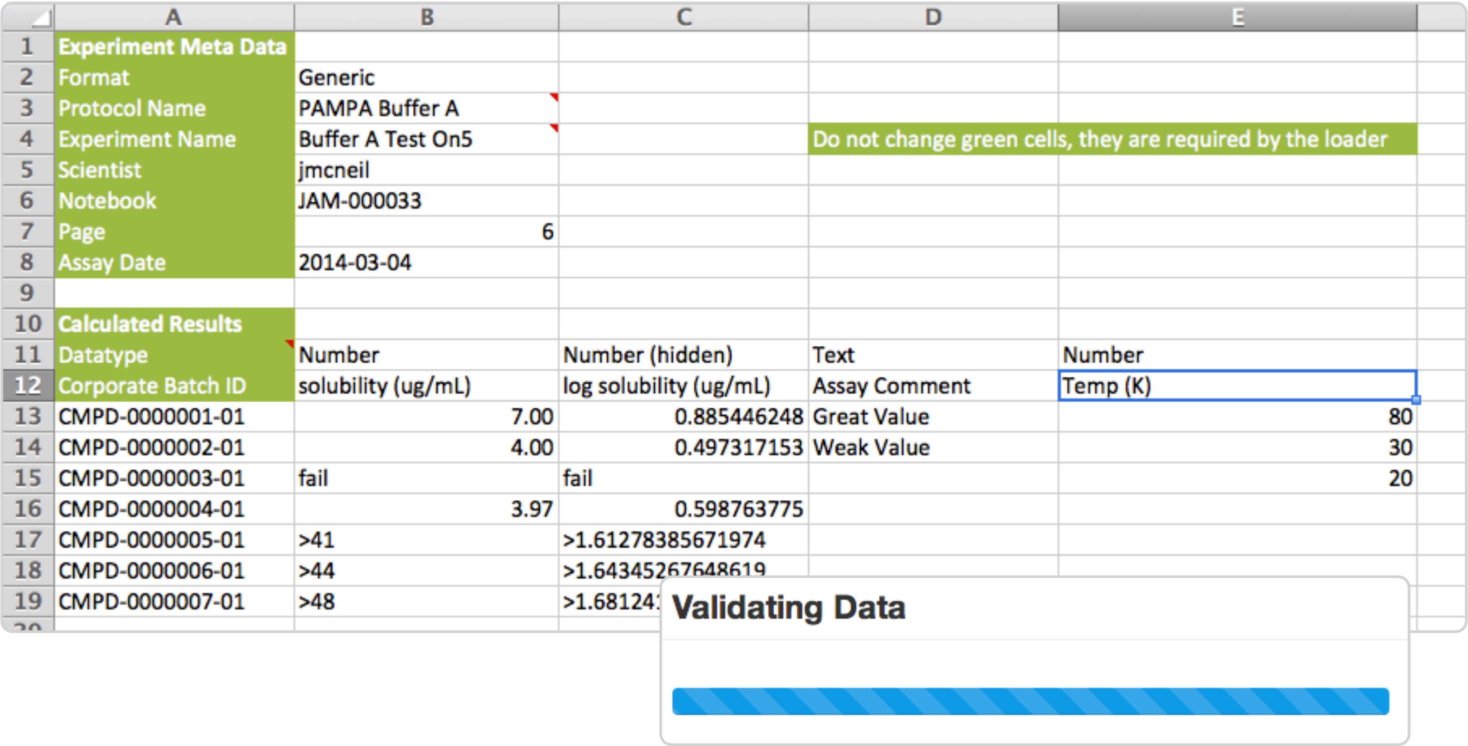
To:

Cc:

Subject: Seurat Live Report for PAMPA Buffer A: Buffer A Test On5

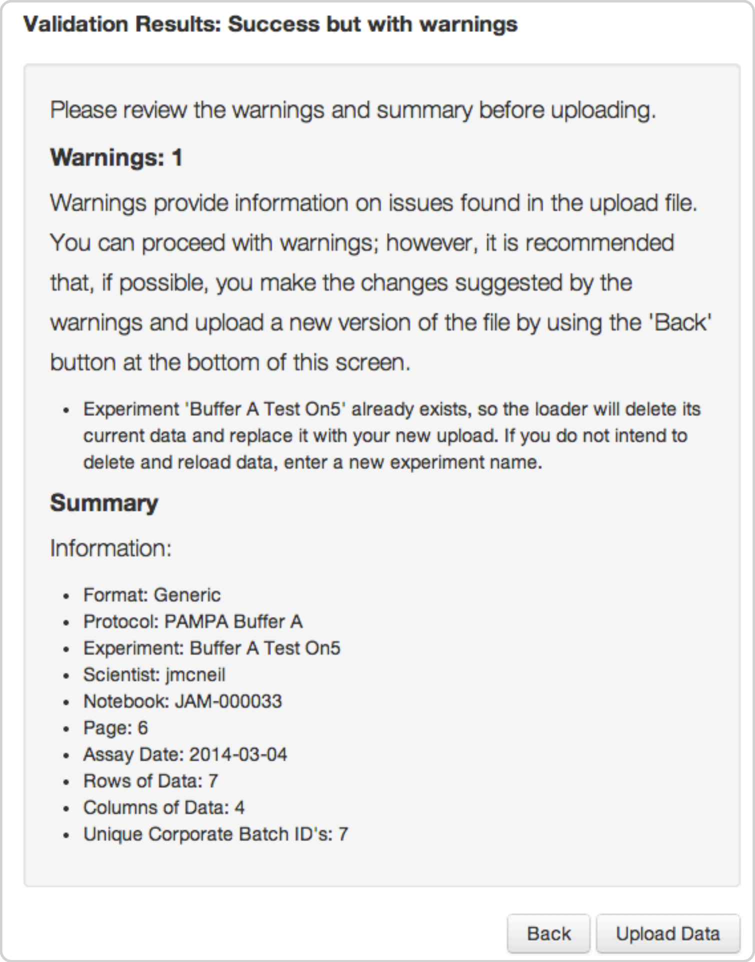
Signature: Normal

Click the following link to run Live Report: http://demo.labsynch.com:9080/seurat/runseurat?cmd=newjob&AssayName=PAMPA%20Buffer%20A&AssayProtocol=Buffer%20A%20Test%20On5



	A	B	C	D	E
1	Experiment Meta Data				
2	Format	Generic			
3	Protocol Name	PAMPA Buffer A			
4	Experiment Name	Buffer A Test On5		Do not change green cells, they are required by the loader	
5	Scientist	jmcneil			
6	Notebook	JAM-000033			
7	Page	6			
8	Assay Date	2014-03-04			
9					
10	Calculated Results				
11	Datatype	Number	Number (hidden)	Text	Number
12	Corporate Batch ID	solubility (ug/mL)	log solubility (ug/mL)	Assay Comment	Temp (K)
13	CMPD-0000001-01	7.00	0.885446248	Great Value	80
14	CMPD-0000002-01	4.00	0.497317153	Weak Value	30
15	CMPD-0000003-01	fail	fail		20
16	CMPD-0000004-01	3.97	0.598763775		
17	CMPD-0000005-01	>41	>1.61278385671974		
18	CMPD-0000006-01	>44	>1.64345267648619		
19	CMPD-0000007-01	>48	>1.68124		

Validating Data



Validation Results: Success but with warnings

Please review the warnings and summary before uploading.

Warnings: 1

Warnings provide information on issues found in the upload file. You can proceed with warnings; however, it is recommended that, if possible, you make the changes suggested by the warnings and upload a new version of the file by using the 'Back' button at the bottom of this screen.

- Experiment 'Buffer A Test On5' already exists, so the loader will delete its current data and replace it with your new upload. If you do not intend to delete and reload data, enter a new experiment name.

Summary

Information:

- Format: Generic
- Protocol: PAMPA Buffer A
- Experiment: Buffer A Test On5
- Scientist: jmcneil
- Notebook: JAM-000033
- Page: 6
- Assay Date: 2014-03-04
- Rows of Data: 7
- Columns of Data: 4
- Unique Corporate Batch ID's: 7

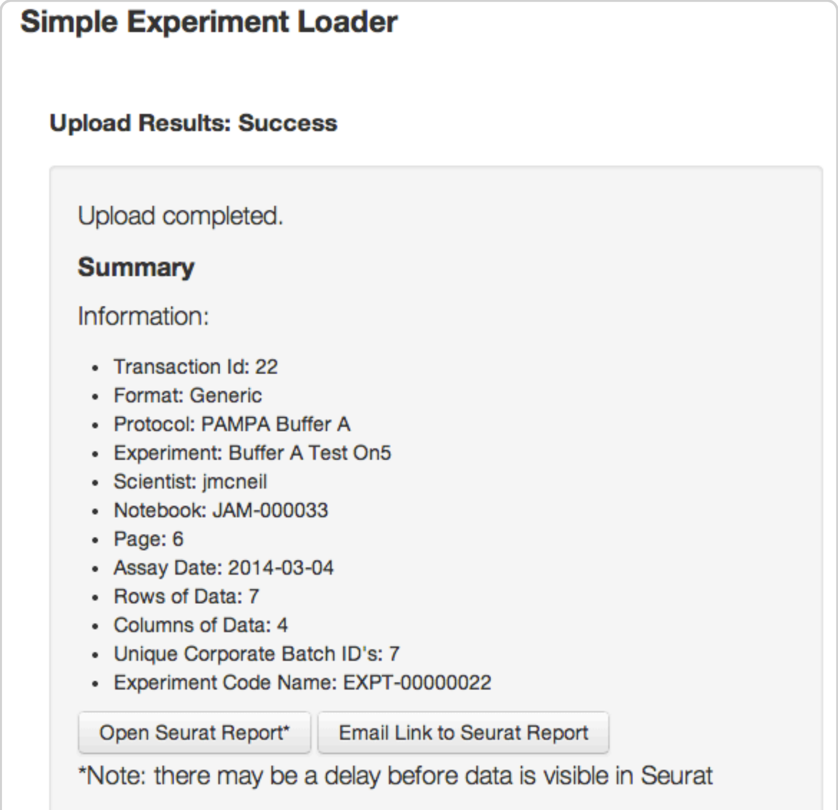
It is possible to upload a different data set for the same experiment. Just alter the file and reupload.

The loader will give you a warning stating that the experiment already exists. It will replace the existing data with the new data.

In this example, the user added an additional data column (temperature) to the file. This will be displayed when the user opens the Seurat report.

Uploading Results

Once uploaded, the results summary is shown, and again there are options to view the report in Seurat or email a link to the report.



Simple Experiment Loader

Upload Results: Success

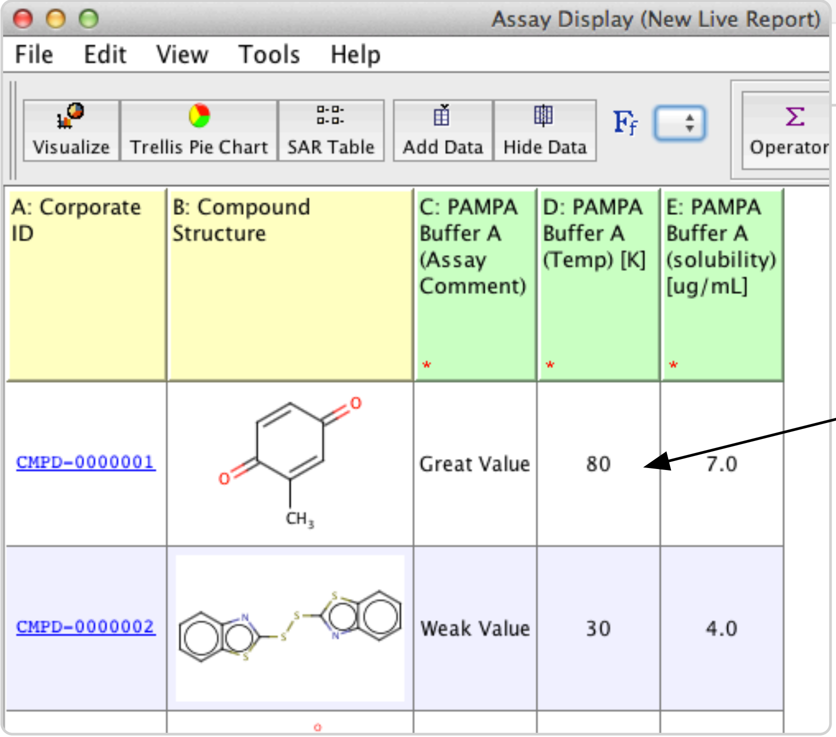
Upload completed.

Summary

Information:

- Transaction Id: 22
- Format: Generic
- Protocol: PAMPA Buffer A
- Experiment: Buffer A Test On5
- Scientist: jmcneil
- Notebook: JAM-000033
- Page: 6
- Assay Date: 2014-03-04
- Rows of Data: 7
- Columns of Data: 4
- Unique Corporate Batch ID's: 7
- Experiment Code Name: EXPT-00000022

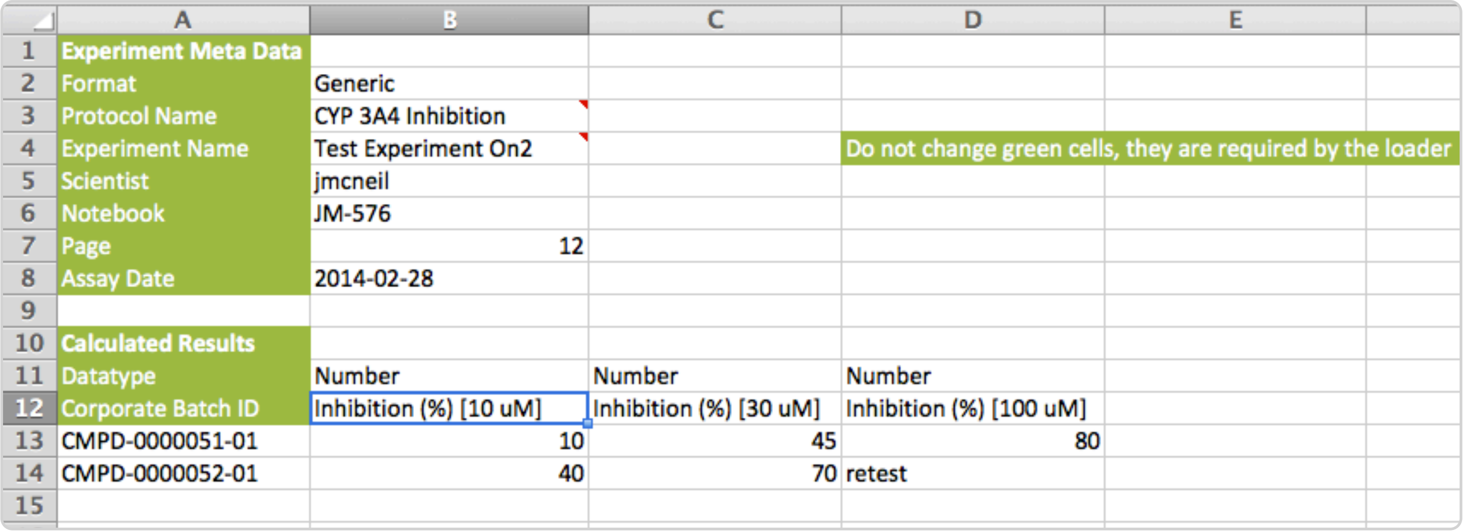
*Note: there may be a delay before data is visible in Seurat



Assay Display (New Live Report)

A: Corporate ID	B: Compound Structure	C: PAMPA Buffer A (Assay Comment) *	D: PAMPA Buffer A (Temp) [K] *	E: PAMPA Buffer A (solubility) [ug/mL] *
CMPD-0000001		Great Value	80	7.0
CMPD-0000002		Weak Value	30	4.0

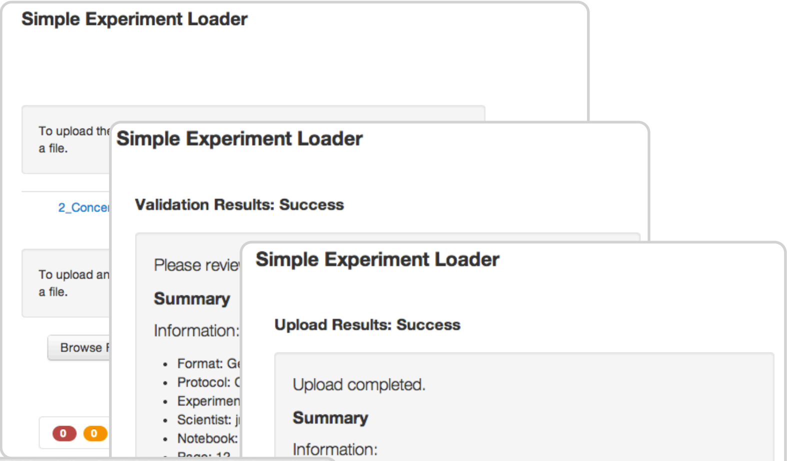
New temperature data.



	A	B	C	D	E
1	Experiment Meta Data				
2	Format	Generic			
3	Protocol Name	CYP 3A4 Inhibition			
4	Experiment Name	Test Experiment On2		Do not change green cells, they are required by the loader	
5	Scientist	jmcneil			
6	Notebook	JM-576			
7	Page	12			
8	Assay Date	2014-02-28			
9					
10	Calculated Results				
11	Datatype	Number	Number	Number	
12	Corporate Batch ID	Inhibition (%) [10 uM]	Inhibition (%) [30 uM]	Inhibition (%) [100 uM]	
13	CMPD-0000051-01	10	45	80	
14	CMPD-0000052-01	40	70	retest	
15					

In the first example, a solubility data file was used. Other data types may also be uploaded, like inhibition at different concentrations.

The steps to upload are the same.



Simple Experiment Loader

To upload the
a file.

2_Conce

To upload an
a file.

Browse F

0 0

Simple Experiment Loader

Validation Results: Success

Please revie

Summary

Information:

- Format: Ge
- Protocol: C
- Experimen
- Scientist: j
- Notebook:
- Page: 12

Simple Experiment Loader

Upload Results: Success

Upload completed.

Summary

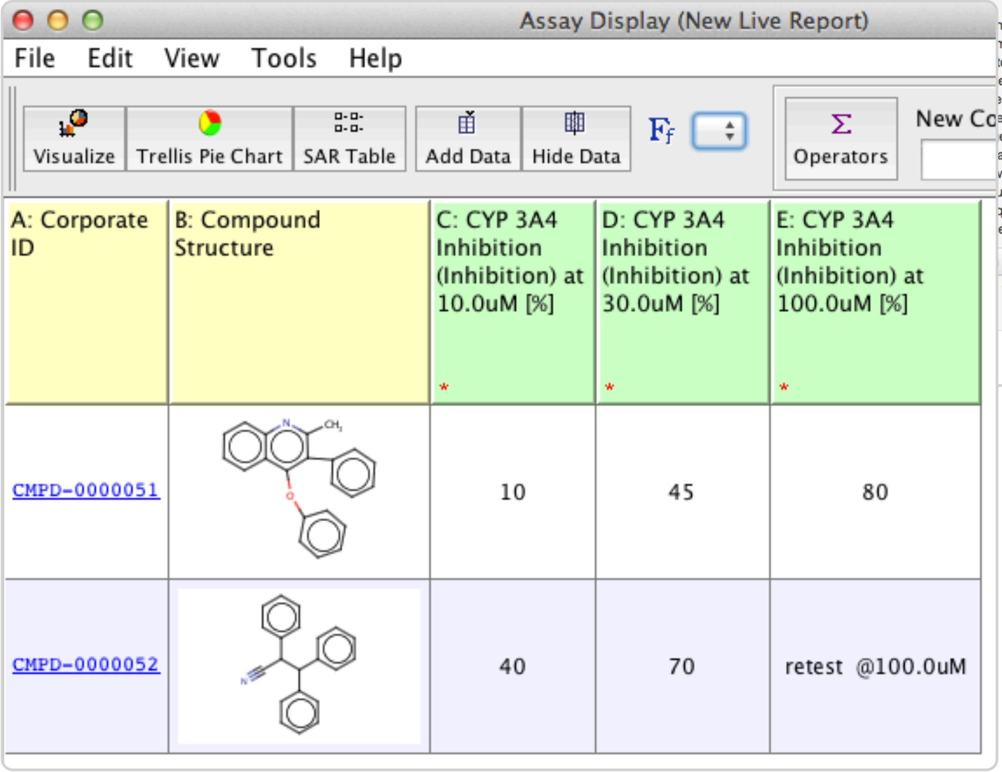
Information:

nsaction Id: 23
mat: Generic
tocol: CYP 3A4 Inhibition
eriment: Test Experiment On3
entist: jmcneil
ebook: JM-576
e: 12
ay Date: 2014-02-28
vs of Data: 2
umns of Data: 3
que Corporate Batch ID's: 2
eriment Code Name: EXPT-00000023

Seurat Report* | Email Link to Seurat Report

there may be a delay before data is visible in Seurat

Load Another

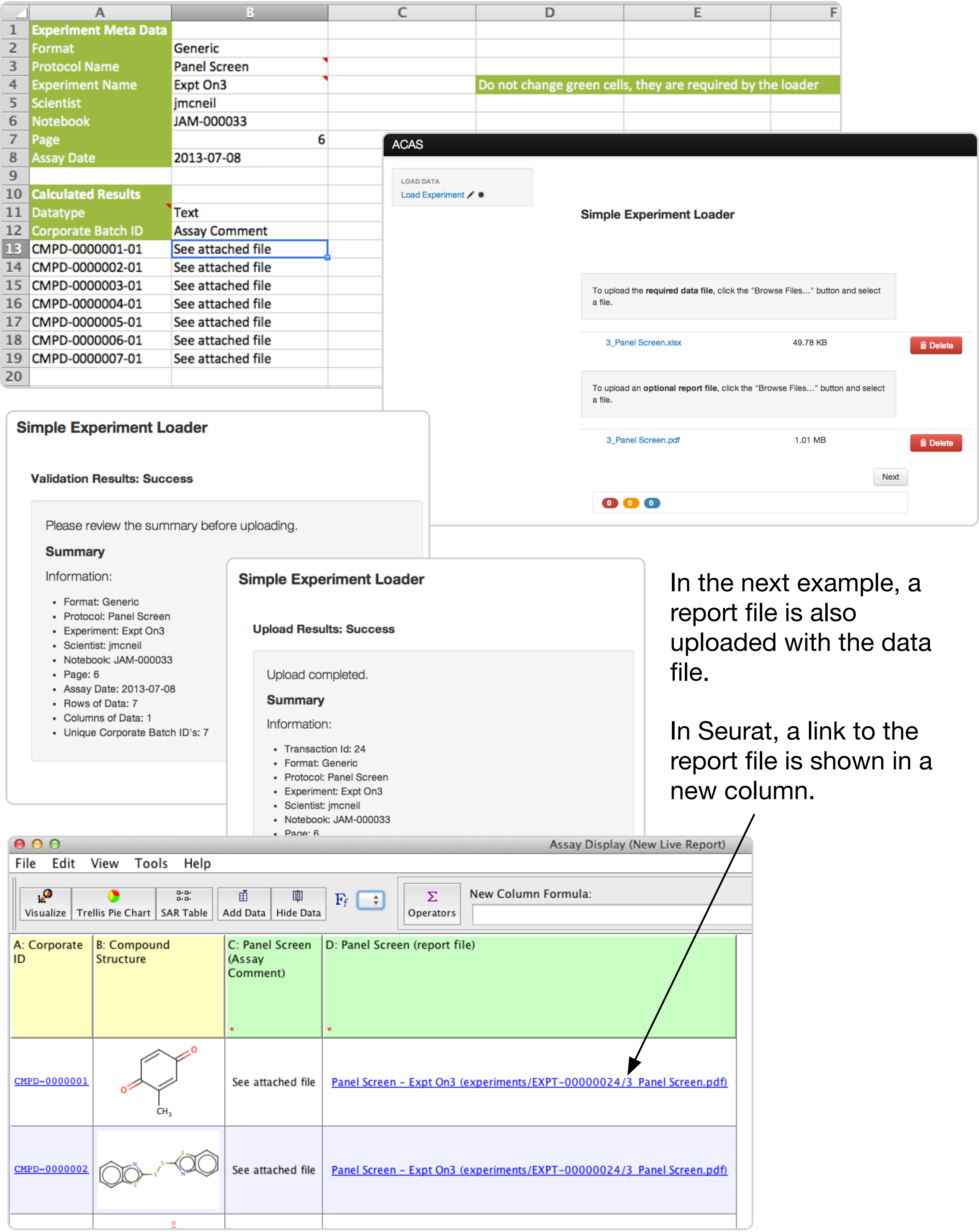


A: Corporate ID	B: Compound Structure	C: CYP 3A4 Inhibition (Inhibition) at 10.0uM [%]	D: CYP 3A4 Inhibition (Inhibition) at 30.0uM [%]	E: CYP 3A4 Inhibition (Inhibition) at 100.0uM [%]
CMPD-0000051		10	45	80
CMPD-0000052		40	70	retest @100.0uM

The concentration data is shown, in this case, in multiple columns.

ACAS Tutorial

Adding a Report File



	A	B	C	D	E	F
1	Experiment Meta Data					
2	Format	Generic				
3	Protocol Name	Panel Screen				
4	Experiment Name	Expt On3		Do not change green cells, they are required by the loader		
5	Scientist	jmcneil				
6	Notebook	JAM-000033				
7	Page	6				
8	Assay Date	2013-07-08				
9						
10	Calculated Results					
11	Datatype	Text				
12	Corporate Batch ID	Assay Comment				
13	CMPD-0000001-01	See attached file				
14	CMPD-0000002-01	See attached file				
15	CMPD-0000003-01	See attached file				
16	CMPD-0000004-01	See attached file				
17	CMPD-0000005-01	See attached file				
18	CMPD-0000006-01	See attached file				
19	CMPD-0000007-01	See attached file				
20						

ACAS

LOAD DATA
Load Experiment

Simple Experiment Loader

To upload the **required data file**, click the "Browse Files..." button and select a file.

3_Panel Screen.xlsx 49.78 KB Delete

To upload an **optional report file**, click the "Browse Files..." button and select a file.

3_Panel Screen.pdf 1.01 MB Delete

Next

0 0 0

Simple Experiment Loader

Validation Results: Success

Please review the summary before uploading.

Summary

Information:

- Format: Generic
- Protocol: Panel Screen
- Experiment: Expt On3
- Scientist: jmcneil
- Notebook: JAM-000033
- Page: 6
- Assay Date: 2013-07-08
- Rows of Data: 7
- Columns of Data: 1
- Unique Corporate Batch ID's: 7

Simple Experiment Loader

Upload Results: Success

Upload completed.

Summary

Information:

- Transaction Id: 24
- Format: Generic
- Protocol: Panel Screen
- Experiment: Expt On3
- Scientist: jmcneil
- Notebook: JAM-000033
- Page: 6

Assay Display (New Live Report)

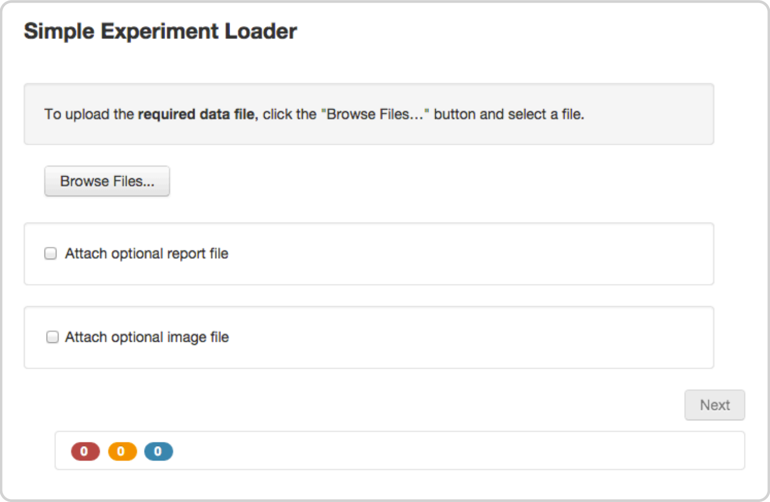
A: Corporate ID	B: Compound Structure	C: Panel Screen (Assay Comment)	D: Panel Screen (report file)
CMPD-0000001		See attached file	Panel Screen - Expt On3 (experiments/EXPT-00000024/3_Panel Screen.pdf)
CMPD-0000002		See attached file	Panel Screen - Expt On3 (experiments/EXPT-00000024/3_Panel Screen.pdf)

In the next example, a report file is also uploaded with the data file.

In Seurat, a link to the report file is shown in a new column.

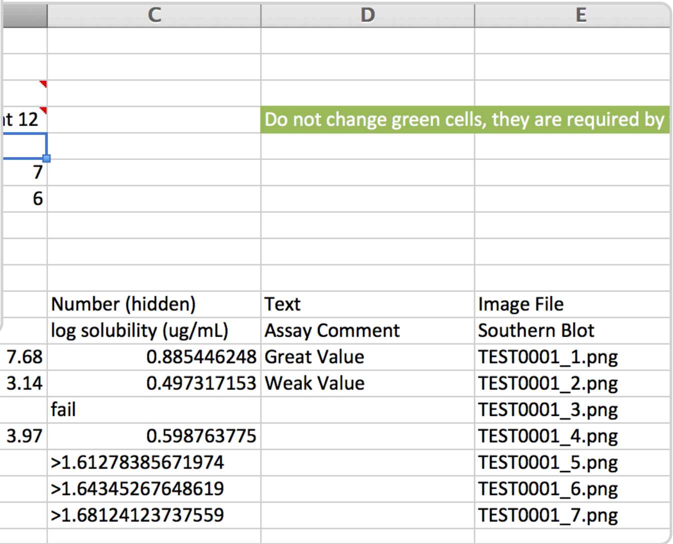
ACAS Tutorial

Adding Images

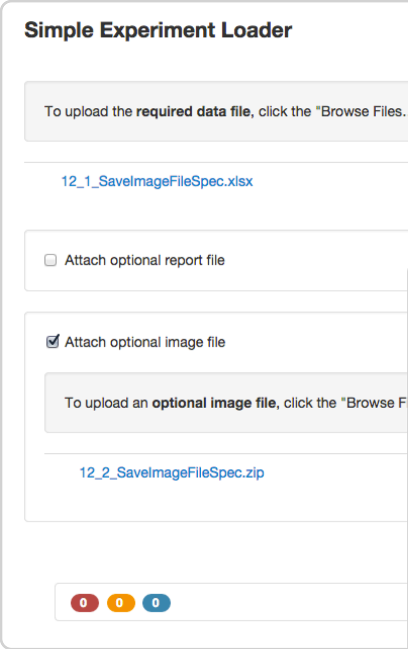


Simple Experiment Loader

To upload the **required data file,** click the "Browse Files..." button and select a file.



	C	D	E
t 12		Do not change green cells, they are required by	
7			
6			
	Number (hidden)	Text	Image File
	log solubility (ug/mL)	Assay Comment	Southern Blot
7.68	0.885446248	Great Value	TEST0001_1.png
3.14	0.497317153	Weak Value	TEST0001_2.png
	fail		TEST0001_3.png
3.97	0.598763775		TEST0001_4.png
	>1.61278385671974		TEST0001_5.png
	>1.64345267648619		TEST0001_6.png
	>1.68124123737559		TEST0001_7.png



Simple Experiment Loader

To upload the **required data file,** click the "Browse Files..." button and select a file.

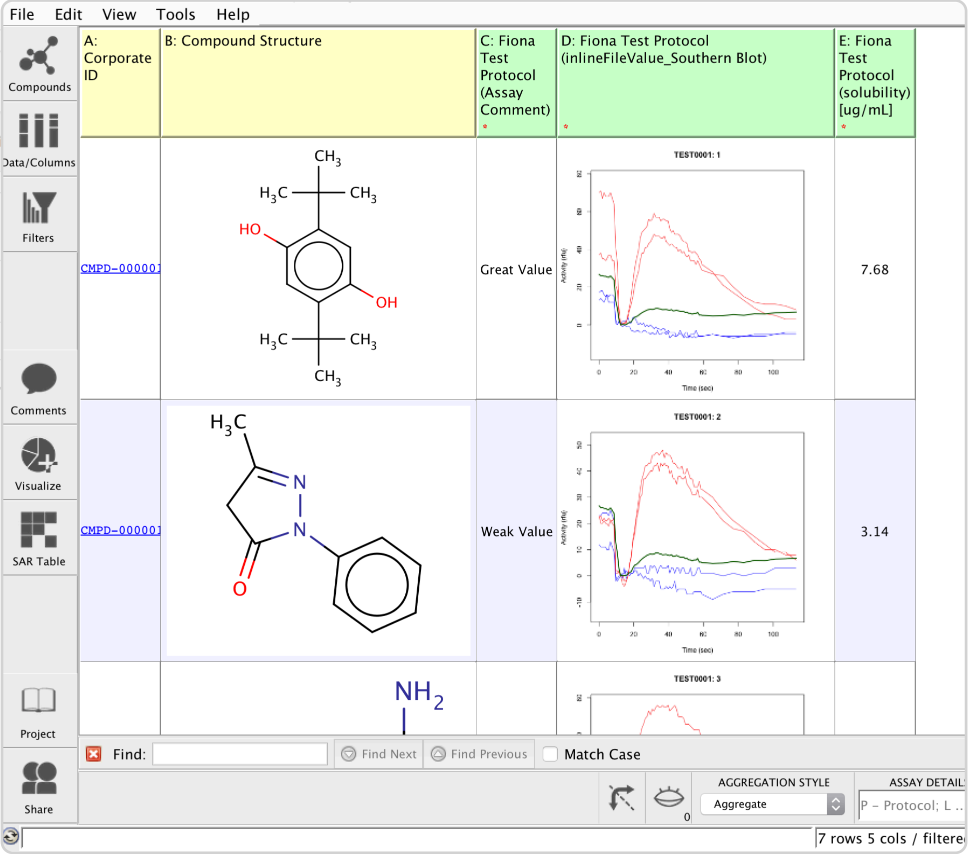
12_1_SaveImageFileSpec.xlsx 50.90 KB

☐ Attach optional report file

☑ Attach optional image file

To upload an **optional image file,** click the "Browse F

12_2_SaveImageFileSpec.zip



A: Corporate ID	B: Compound Structure	C: Fiona Test Protocol (Assay Comment) *	D: Fiona Test Protocol (inlineFileValue_Southern Blot) *	E: Fiona Test Protocol (solubility) [ug/mL] *
CMPD-000001		Great Value		7.68
CMPD-000001		Weak Value		3.14

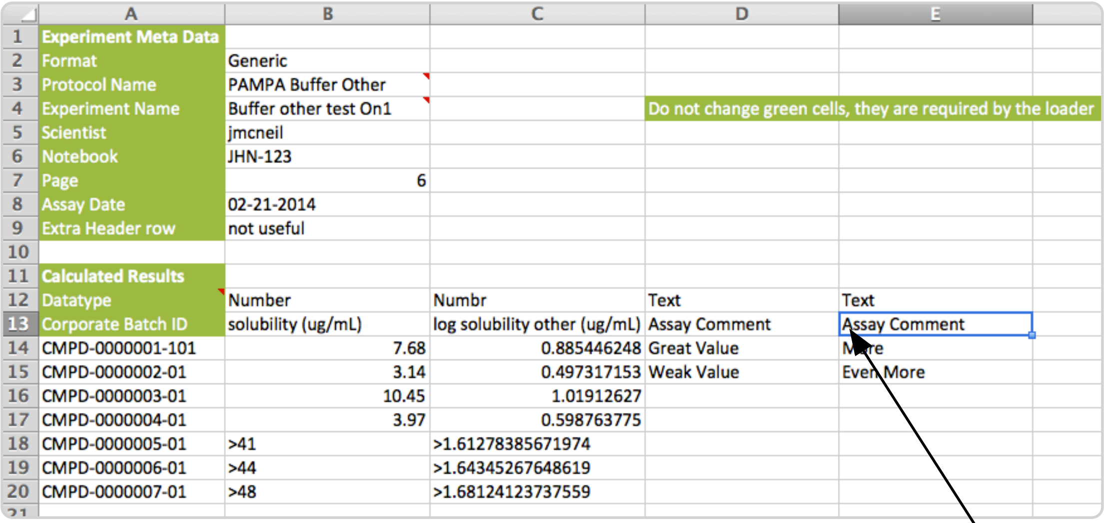
7 rows 5 cols / filtere

The next SEL file option is to upload an optional image file.

Adding inline images to Seurat is similar to adding a report file. Upload a data file, and then attach a zipped folder of images in the "Attach optional image file" browser.

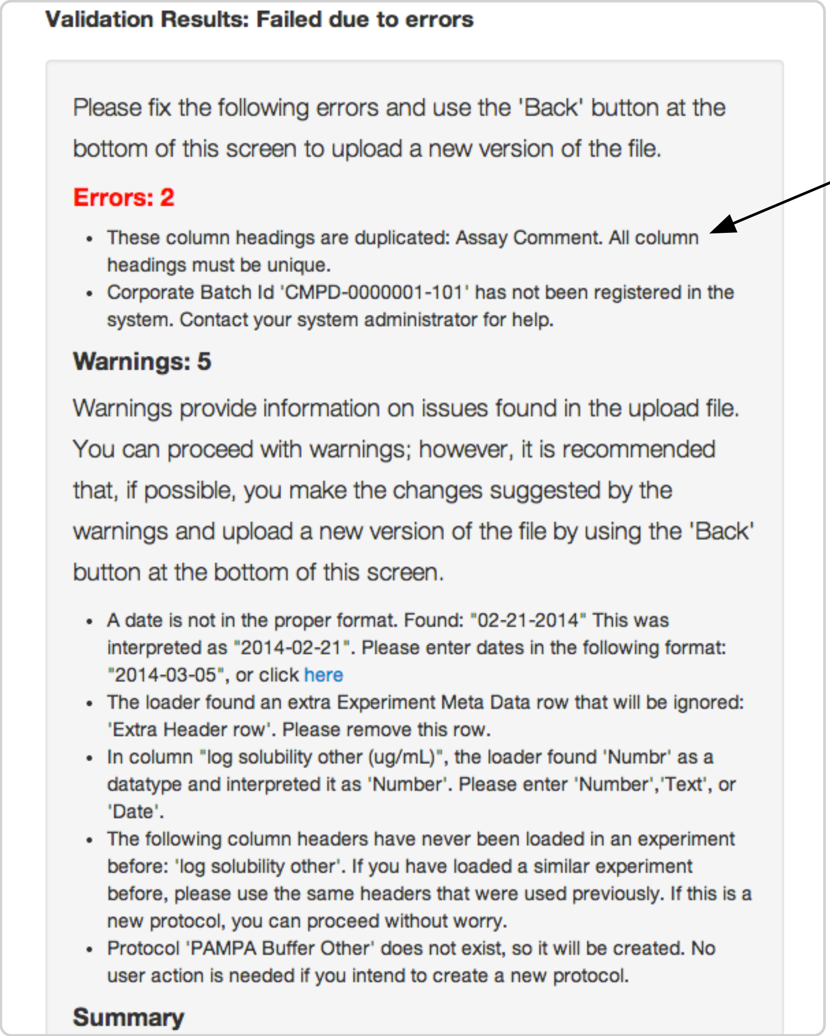
The image file names must be listed in the data file, and must also match what is in the compressed folder.

ACAS Tutorial



	A	B	C	D	E
1	Experiment Meta Data				
2	Format	Generic			
3	Protocol Name	PAMPA Buffer Other			
4	Experiment Name	Buffer other test On1		Do not change green cells, they are required by the loader	
5	Scientist	jmcneil			
6	Notebook	JHN-123			
7	Page	6			
8	Assay Date	02-21-2014			
9	Extra Header row	not useful			
10					
11	Calculated Results				
12	Datatype	Number	Numbr	Text	Text
13	Corporate Batch ID	solubility (ug/mL)	log solubility other (ug/mL)	Assay Comment	Assay Comment
14	CMPD-0000001-101	7.68	0.885446248	Great Value	More
15	CMPD-0000002-01	3.14	0.497317153	Weak Value	Even More
16	CMPD-0000003-01	10.45	1.01912627		
17	CMPD-0000004-01	3.97	0.598763775		
18	CMPD-0000005-01	>41	>1.61278385671974		
19	CMPD-0000006-01	>44	>1.64345267648619		
20	CMPD-0000007-01	>48	>1.68124123737559		

If there is an error in the data file, the loader will fail to validate the file and report the errors. The errors can then be fixed and the file re-uploaded.



Validation Results: Failed due to errors

Please fix the following errors and use the 'Back' button at the bottom of this screen to upload a new version of the file.

Errors: 2

- These column headings are duplicated: Assay Comment. All column headings must be unique.
- Corporate Batch Id 'CMPD-0000001-101' has not been registered in the system. Contact your system administrator for help.

Warnings: 5

Warnings provide information on issues found in the upload file. You can proceed with warnings; however, it is recommended that, if possible, you make the changes suggested by the warnings and upload a new version of the file by using the 'Back' button at the bottom of this screen.

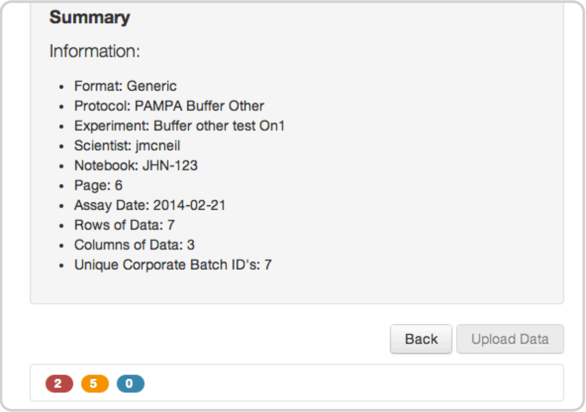
- A date is not in the proper format. Found: "02-21-2014" This was interpreted as "2014-02-21". Please enter dates in the following format: "2014-03-05", or click here
- The loader found an extra Experiment Meta Data row that will be ignored: 'Extra Header row'. Please remove this row.
- In column "log solubility other (ug/mL)", the loader found 'Numbr' as a datatype and interpreted it as 'Number'. Please enter 'Number','Text', or 'Date'.
- The following column headers have never been loaded in an experiment before: 'log solubility other'. If you have loaded a similar experiment before, please use the same headers that were used previously. If this is a new protocol, you can proceed without worry.
- Protocol 'PAMPA Buffer Other' does not exist, so it will be created. No user action is needed if you intend to create a new protocol.

Summary

In this example, the Assay Comment headers are duplicated. This is one of the errors listed.

The date format is also incorrect, the loader has detected and ignored an extra header row, etc. If it can, the loader will correct these issues.

The loader will try to allow you to continue uploading if there are only warnings, but true errors will cause a failure.



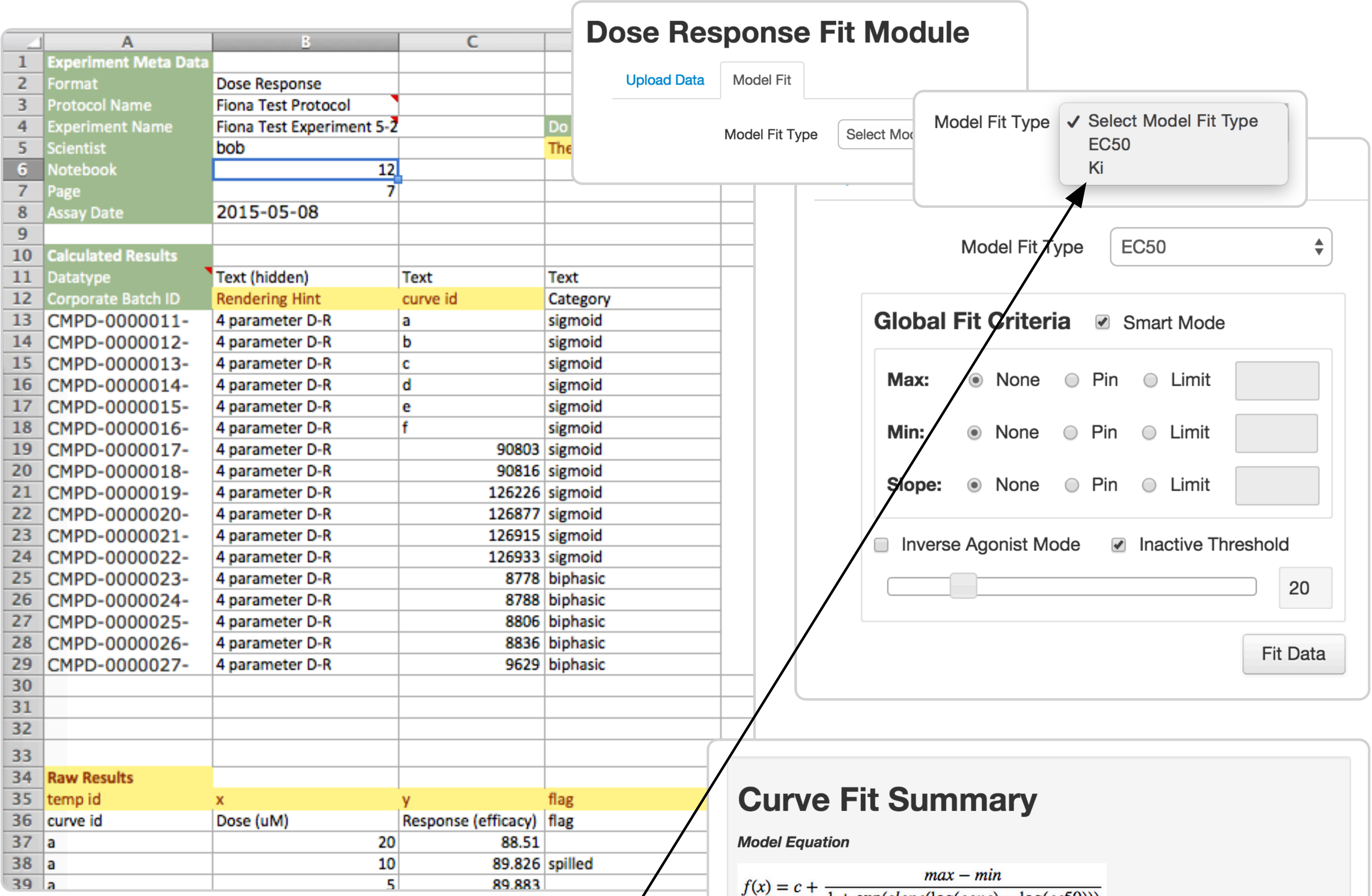
Summary

Information:

- Format: Generic
- Protocol: PAMPA Buffer Other
- Experiment: Buffer other test On1
- Scientist: jmcneil
- Notebook: JHN-123
- Page: 6
- Assay Date: 2014-02-21
- Rows of Data: 7
- Columns of Data: 3
- Unique Corporate Batch ID's: 7

ACAS Tutorial

Loading a Dose Response Data File



	A	B	C	D
1	Experiment Meta Data			
2	Format	Dose Response		
3	Protocol Name	Fiona Test Protocol		
4	Experiment Name	Fiona Test Experiment 5-2		Do
5	Scientist	bob		The
6	Notebook	12		
7	Page	7		
8	Assay Date	2015-05-08		
9				
10	Calculated Results			
11	Datatype	Text (hidden)	Text	Text
12	Corporate Batch ID	Rendering Hint	curve id	Category
13	CMPD-0000011-	4 parameter D-R	a	sigmoid
14	CMPD-0000012-	4 parameter D-R	b	sigmoid
15	CMPD-0000013-	4 parameter D-R	c	sigmoid
16	CMPD-0000014-	4 parameter D-R	d	sigmoid
17	CMPD-0000015-	4 parameter D-R	e	sigmoid
18	CMPD-0000016-	4 parameter D-R	f	sigmoid
19	CMPD-0000017-	4 parameter D-R	90803	sigmoid
20	CMPD-0000018-	4 parameter D-R	90816	sigmoid
21	CMPD-0000019-	4 parameter D-R	126226	sigmoid
22	CMPD-0000020-	4 parameter D-R	126877	sigmoid
23	CMPD-0000021-	4 parameter D-R	126915	sigmoid
24	CMPD-0000022-	4 parameter D-R	126933	sigmoid
25	CMPD-0000023-	4 parameter D-R	8778	biphasic
26	CMPD-0000024-	4 parameter D-R	8788	biphasic
27	CMPD-0000025-	4 parameter D-R	8806	biphasic
28	CMPD-0000026-	4 parameter D-R	8836	biphasic
29	CMPD-0000027-	4 parameter D-R	9629	biphasic
30				
31				
32				
33				
34	Raw Results			
35	temp id	x	y	flag
36	curve id	Dose (uM)	Response (efficacy)	flag
37	a	20	88.51	
38	a	10	89.826	spilled
39	a	5	89.883	

Dose Response Fit Module

Model Fit Type: Select Mod

Model Fit Type: ✓ Select Model Fit Type

Model Fit Type: EC50

Global Fit Criteria ☑ Smart Mode

Max: ● None ○ Pin ○ Limit

Min: ● None ○ Pin ○ Limit

Slope: ● None ○ Pin ○ Limit

☐ Inverse Agonist Mode ☑ Inactive Threshold

20

Curve Fit Summary

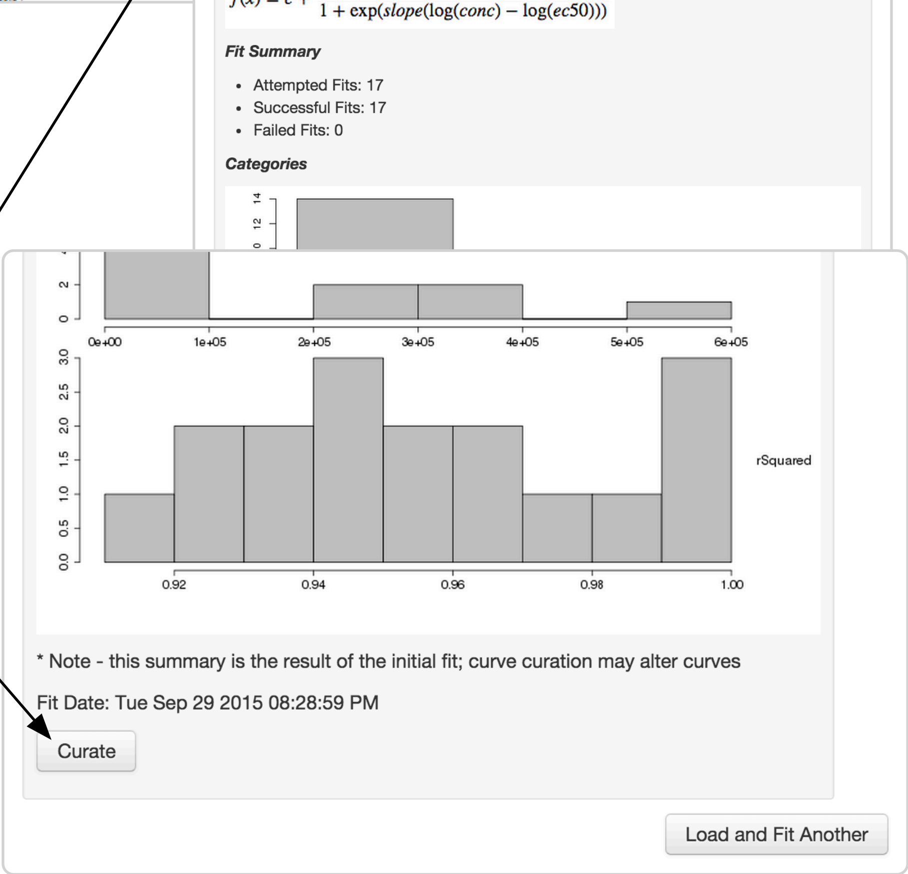
Model Equation

$$f(x) = c + \frac{max - min}{1 + \exp(slope(\log(conc) - \log(ec50)))}$$

Fit Summary

- Attempted Fits: 17
- Successful Fits: 17
- Failed Fits: 0

Categories

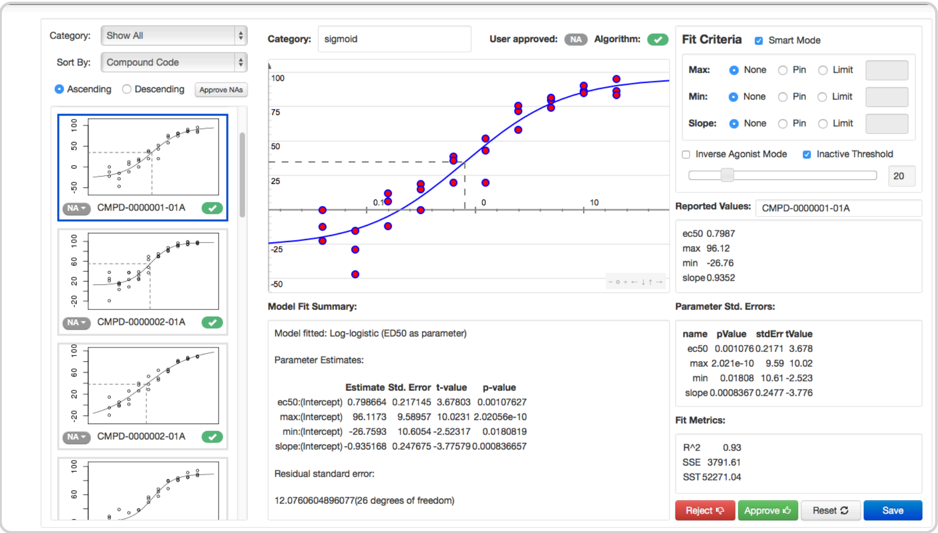


* Note - this summary is the result of the initial fit; curve curation may alter curves

Fit Date: Tue Sep 29 2015 08:28:59 PM

Load dose response data by going to the Dose Response module. Loading a file here is exactly like loading a file in SEL. Once the file has been uploaded successfully, it will ask you to choose between EC50 and KD. It will then show you a curve fit summary. From there, click the Curate button to open the curve curator.

In curve curator, you can reject and approve curves, knock out points, and change fit criteria. There is also a link to open the curves in Seurat.



Category: Show All

Sort By: Compound Code

● Ascending ○ Descending

Category: sigmoid

User approved: NA Algorithm: ✓

Fit Criteria ☑ Smart Mode

Max: ● None ○ Pin ○ Limit

Min: ● None ○ Pin ○ Limit

Slope: ● None ○ Pin ○ Limit

☐ Inverse Agonist Mode ☑ Inactive Threshold 20

Reported Values: CMPD-0000001-01A

```
ec50 0.7987
max  96.12
min  -26.76
slope0.9352
```

Model Fit Summary:

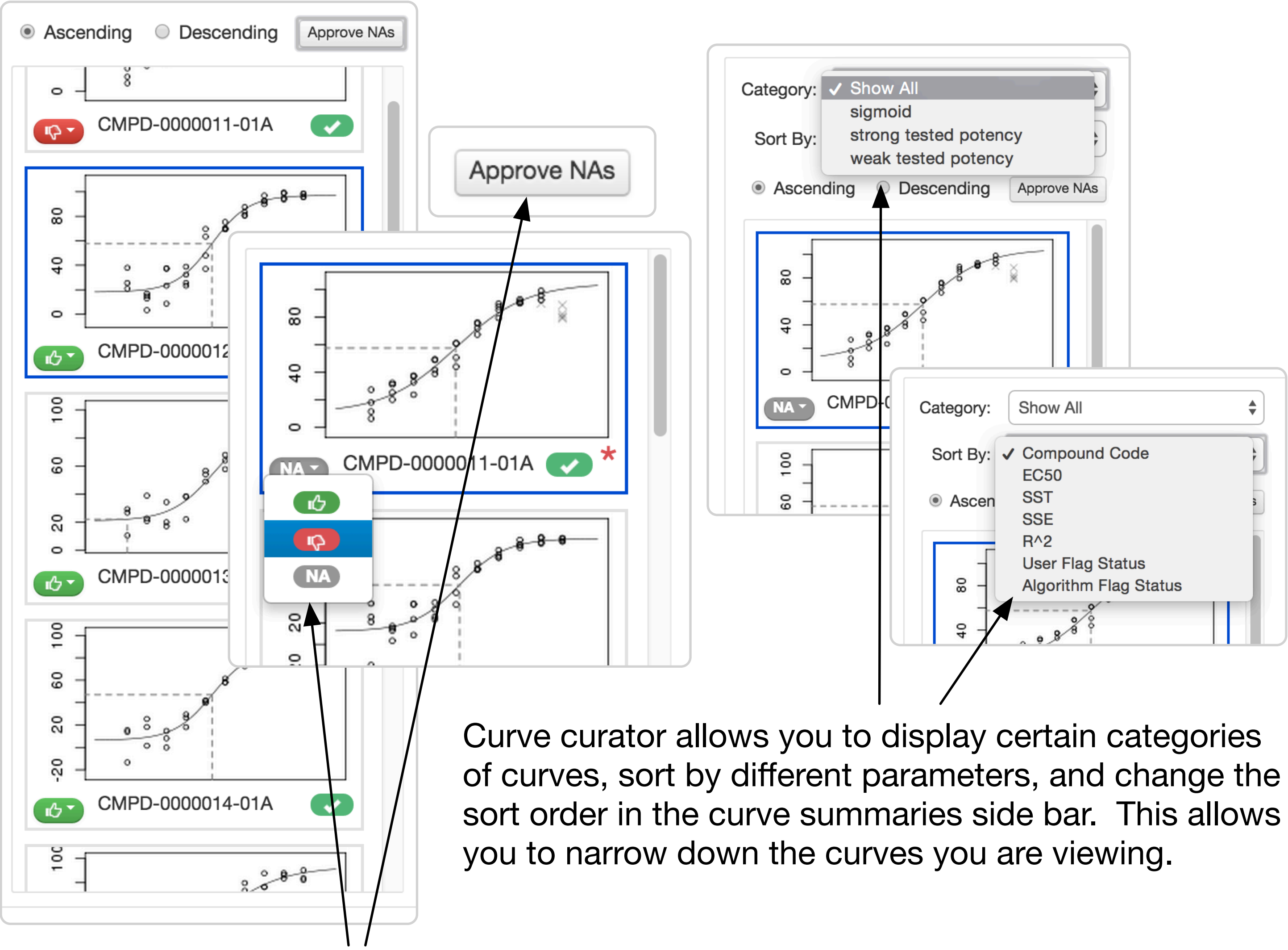
```
Model fitted: Log-logistic (ED50 as parameter)

Parameter Estimates:

                  Estimate Std. Error  t-value     p-value
 ec50:(Intercept)  0.798664  0.217145  3.67803  0.00107627
  max:(Intercept)   96.1173   9.58957  10.0231 2.02056e-10
  min:(Intercept)  -26.7593   10.6054 -2.52317   0.0180819
slope:(Intercept) -0.935168  0.247675 -3.77579 0.000836657

Residual standard error:

12.0760604896077(26 degrees of freedom)
```

Parameter Std. Errors:

```
name   pValue   stdErr tValue
 ec50  0.001076 0.2171  3.678
  max 2.021e-10   9.59  10.02
  min   0.01808  10.61 -2.523
slope 0.0008367 0.2477 -3.776
```

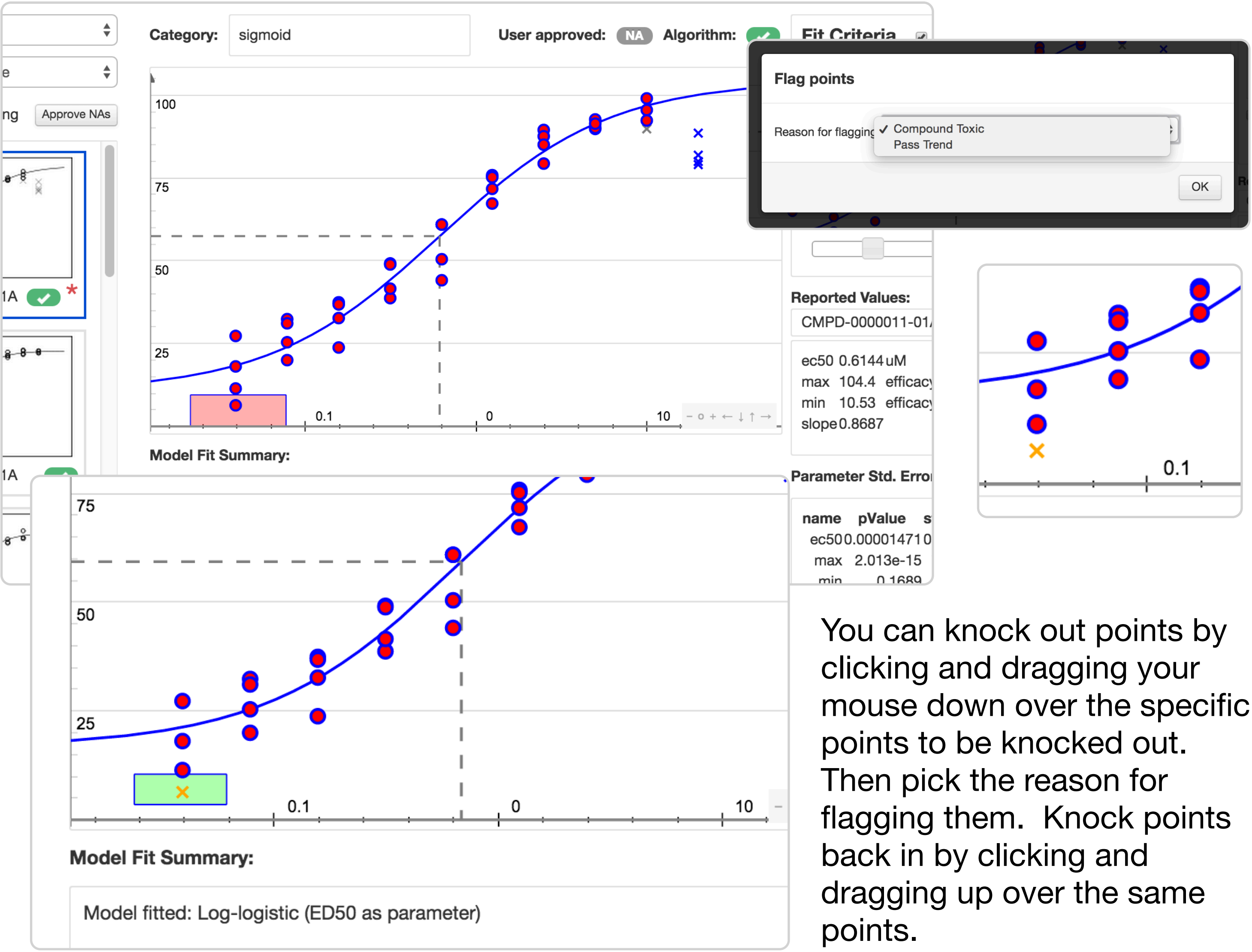
Fit Metrics:

```
R^2     0.93
SSE  3791.61
SST 52271.04
```



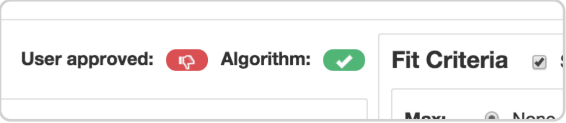
Curve curator allows you to display certain categories of curves, sort by different parameters, and change the sort order in the curve summaries side bar. This allows you to narrow down the curves you are viewing.

From here you can also quick approve and reject curves, and approve all NA curves.

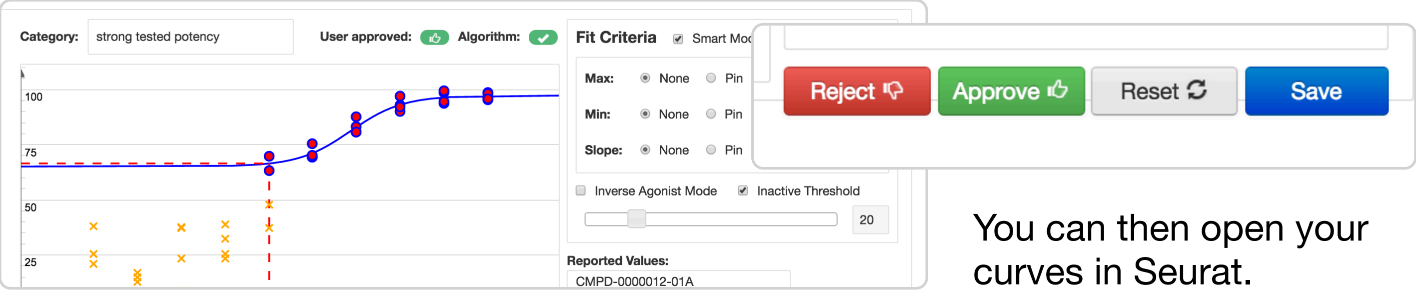


You can knock out points by clicking and dragging your mouse down over the specific points to be knocked out. Then pick the reason for flagging them. Knock points back in by clicking and dragging up over the same points.

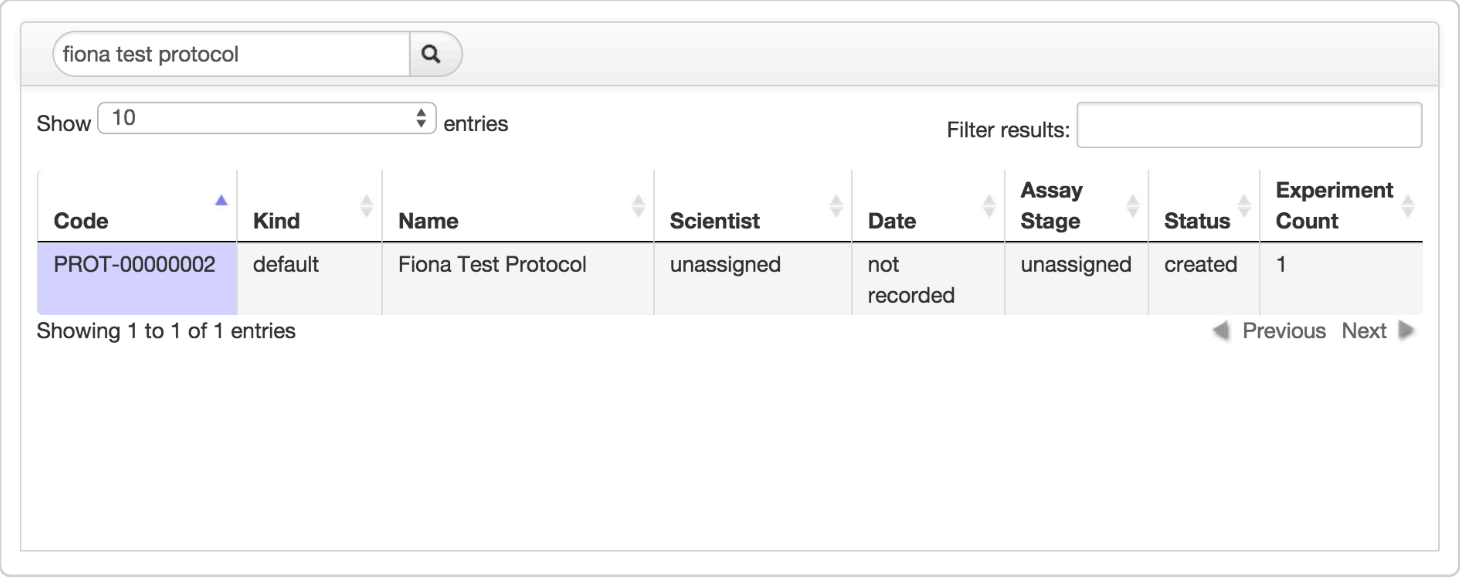
You can reset a curve to it's last save point by clicking the reset button. This will get rid of any changes made since the curve was first loaded or saved last.



You can also reject or approve a curve from the detailed view. Click Save once you are satisfied with your changes.



You can then open your curves in Seurat.



fiona test protocol

Show 10 entries

Filter results:

Code	Kind	Name	Scientist	Date	Assay Stage	Status	Experiment Count
PROT-00000002	default	Fiona Test Protocol	unassigned	not recorded	unassigned	created	1

Showing 1 to 1 of 1 entries

To edit a protocol, go to Protocol Browser and use the search bar to find the protocol. You can search using a number of criteria, like protocol name and protocol code. You can also search for something in the description or details of a protocol.

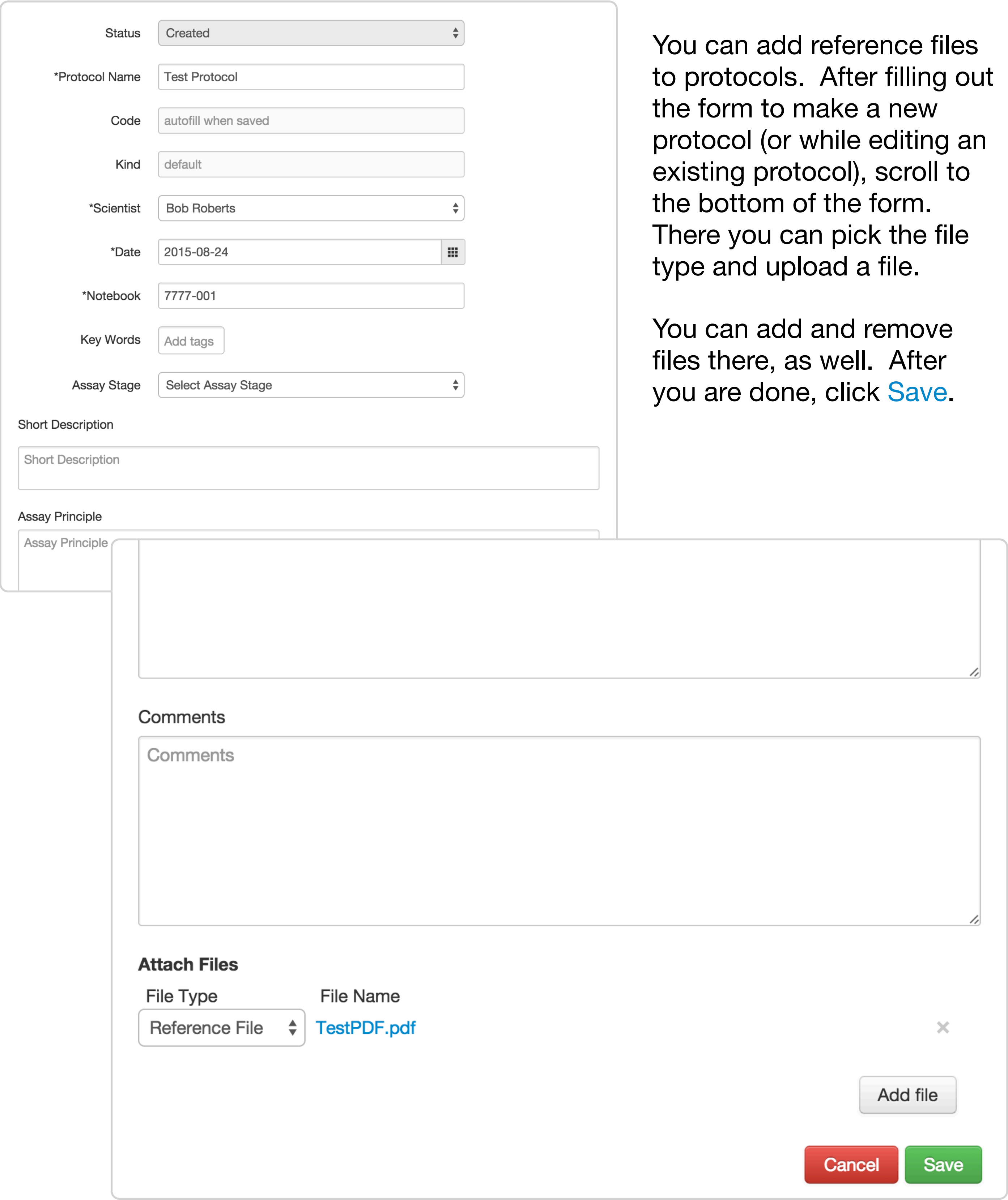
Once you have found your protocol, click on it. It will open a preview below the search results. From there you can delete it, edit it, duplicate it, or create an experiment from it. Clicking Edit will open the edit view of the protocol in a new tab.

Status: Created

*Protocol Name: Fiona Test Protocol

Code: PROT-00000002

Kind: default



Status: Created

*Protocol Name: Test Protocol

Code: autofill when saved

Kind: default

*Scientist: Bob Roberts

*Date: 2015-08-24

*Notebook: 7777-001

Key Words: Add tags

Assay Stage: Select Assay Stage

Short Description: Short Description

Assay Principle: Assay Principle

Comments: Comments

Attach Files

File Type	File Name
Reference File	TestPDF.pdf

You can add reference files to protocols. After filling out the form to make a new protocol (or while editing an existing protocol), scroll to the bottom of the form. There you can pick the file type and upload a file.

You can add and remove files there, as well. After you are done, click Save.