ScienceCloud Project Data
Biological Registration Guide

Summary: This guide provides instructions for using ScienceCloud Project Data and Project Documents to perform biological registration tasks.

Covered Topics

Getting Started with Biological Registration

Introduction

Biological Registration can be completed both in Project Data via New Biological Data as well as Project Documents via batch registration.

ScienceCloud supports registration for the following kinds of biological data:

- Single Biological, ADME or PK result (online via Project Data)

- Multiple biological, ADME or PK results (from a file via Project Documents)

Biological Data Template Registration

The following information explains how to configure and register the Excel biological templates that are available for use within ScienceCloud during batch registration in Project Documents.

Getting Started with Biological Data Templates

The following Excel biological templates are available in ScienceCloud and can be found in the Details section of New Data Entry | Register Multiple Biological, ADME, or PK Results from a File.

- Generic
- In Vitro Generic
- MTS & in vitro Generic
- PK
- DMPK

These templates are equivalent—they all place data into ScienceCloud in the same way. They were designed to offer different data entry solutions based on the characteristics of the assay. Each template is described in more detail below.

Generic Template

The Generic template offers maximum flexibility, but might require some information to be entered more than once. It is possible to repeat the same batch number from one line to another.

Generic biological template (Generic.xlsm)

In Vitro Generic Template

The In Vitro Generic template selects all parameter information once in the top header, and then only fills up Batch Number values. It offers the entry of multiple assays at the same time. It is possible to repeat the same assay from one column to another.

	A	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z	AA	AB
					HAT in vitro			Chagas in vitro				Leish axenic in vitro				Leish macro in vitro				Malaria in vitro				Cytotoxicity			
			Screener	Rob Brown			Rob Brown																	Rob Brown			
			Organism	T.b. rhodesiense--STIB 900			T. cruzi--Tulahuen C4 (LacZ)																	MRC-5 cells--fibroblast			
			Date (dd-mmm-yyyy)	11-Dec-2013			11-Dec-2013																	11-Dec-2013			
			SOP	SCYIVTHAT			SCYVTCHA																	SCYVTCYT			
			Unit	ug/ml		ug/ml	ug/ml		ug/ml															ug/ml		ug/ml	
			Dose																								
			Time Point																								
	*Batch No.	Container ID	Well	EC50	EC90		EC50	EC90		EC50	IC50		EC50	EC90		EC50	EC90		EC50	EC90		EC50	EC50	
	DEACC1234				0.4																			35	
	DEACC1235			>	16																			16	
	DEACC1236						0.568	0.98																32	>	
	DEACC1237						10																	19	
	DEACC1238			>			32																		

In Vitro Generic template (In Vitro generic.xlsm)

MTS & in vitro Generic Template

The MTS & in vitro Generic template accepts data entry for multiple doses and types of assays (e.g., percent inhibition at multiple doses).

		Malaria MTS									Malaria in vitro		Malaria in vitro	
	Screener	Rob Brown									Rob Brown		Rob Brown	
	Organism	P. falciparum--K1									P. falciparum--K1		P. falciparum--NF54	
	Date (dd-mmm-yyyy)	11-Dec-2013									11-Dec-2013		11-Dec-2013	
	SOP													
	Test unit										uM		uM	
	Concentrations	100	50	25	12.5	6.25	3.12	2	1.5	1	1.56			
	Concentration Unit						uM							
	*Batch No.	External ID	% inhibition								IC50	IC90	IC50	IC90
	DEACC1234		100	95	91	90	80	70	50			12	5		
	DEACC1235			89	54	30	27	10	5					
	DEACC1236									100	98	98 <	0.5	31	1.4	3.2

MTS and Vitro Generic template (MTS & in vitro generic.xlsm)

PK Template

The PK template supports data entry for the PK assay. Select the number of data sets to enter, the relevant PK parameters, and then fill them out. You can also enter PK raw data (concentration vs. doses) that will be used to draw the PK curves.

Number of Set :	2			
Experiment Summary	**Set 1**		**Set 2**	
Compound ID				
Batch No / External Id	PCUTSMG-0001		PCUTSMG-0002	
Contain ID + Well				
Exp No	077-09		077-09	
Group	1		2	
Route	PO		PO	
Matrix	Plasma		Plasma	
Organism	Rat		Rat	
Tester Name	Rob Brown		Rob Brown	
Test Date	11-Dec-2013		11-Dec-2013	
Vehicle	20% EtOH 80% PEG400		20% EtOH 80% PEG400	
In Life Facility	Stillmeadow		Stillmeadow	
Comments				

pK Parameters	Paste pK value		Paste pK value	
Dose mg/kg	100		100	
tlast hr	6		6	
NCA AUC(0-last) hr*ug/mL	6.535		0.97	
NCA AUC(0-INF) hr*ug/mL	15.85			
Comp AUC(0-INF) hr*ug/mL				
% Extrapolation %	65.62%			
Cl L/kg/hr				
Cl/F L/kg/hr	6.32			
Vdss L/kg	NA			
t1/2 hr	4.91		Elimination phase not defined	
F % of IV				
Cmax ug/mL	1.95		033	
Tmax hr	1		6	

File				
Name				
Display Name				

Graph				

Raw Data	Timepoint	Obs Conc	Calc Conc	Timepoint	Obs Conc	Calc Conc
Units	hour	ug/mL		hour	ug/ml	

PK template (PK.xlsm)

DMPK Template

The DMPK template is a preconfigured template intended for all types of ADMET information. The assay name can be used to switch from one assay to another. It is always possible to use any other biological template to register ADMET data.

	A	B	E	F	G	H	I	J	K	L	M	N	O
			select assay:	Solubility									
	*Batch No.	External Id	Lipophilicity Metabolism Permeability PK pKa measurement protein binding Solubility Stability				Value Unit	Dose	Dose Unit	Time Point	Time Unit	*Test Date (dd-mmm-yyyy)	*Tester Name
	DEACC1234						/ml					11-Dec-2013	Rob Brown
	DEACC1235						/ml					11-Dec-2013	Rob Brown

DMPK template (DMPK.xlsm)

Define a Biological Data Model

ScienceCloud provides three hierarchal levels to describe and organize the biological values. These levels include:

- **Level 1** – Assay
- **Level 2** – Organism/Descriptor
- **Level 3** – Test Parameter

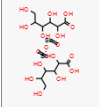To report a biological value, each level needs to be defined. Examples are provided in the table below.

Biological Values Examples

Level 1 (Assay)	Level 2 (Organism/Descriptor)	Level 3 (Test Parameter)
Malaria in vitro	P. Falciparum / K1 P. Falciparum / 3D7 P. Falciparum / NF54	EC50 % inhibition
Solubility	PBS - pH 7.4 /OD_RT PBS - pH 6.0 /LCMS_RT 0.01M HCl - pH 2 /NEPH_RT	Kinetic Thermodynamic
PK	Mouse / Plasma po Mouse / Plasma iv Rat / Blood iv	Cmax CL

Enter your data into these three levels in whatever way makes sense for organizing your information. It is not necessary to use all three levels. ScienceCloud will dynamically build the SAR table by creating a new column every time information changes at any level.

Level 2 is made out of two fields – organism name and descriptor, in case you want to describe one organism name and multiple variations (for example, multiple strains or multiple conditions). Any change in either of those two fields will create a new column in the SAR table.

If your biological value has more than three hierarchy levels, it will be necessary to combine extra levels to fit into the proposed levels. For example, in the table shown below, the route information is merged in Level 2 with species and matrix for PK. Regardless, the SAR table will be preserved, as the change of any of this information creates a separate column.

Display more values
Hide structures
Group by Compound
Template:
Open Save Delete Reset

	CYTOTOXICITY (i)		Chagas in Vitro (i)			Eff-SecA (i)	HAT in vitro (i)			Malaria in Vitro (i)	
Organism	MRC5hu (i)	IL929 (i)	T. cruzi Tulahuen LacZ, Clone C4 (i)			enzym1 (i)	T.b. rhodesiense STIB 900 (i)			P. falciparum K1 (i)	
Test Parameter	IC50	IC50	IC50	SI	Score	IC50	IC50	SI	Score	IC50	SI
Dose / Timepoint		72 hour									
	Value	Value	Value	Value	Value	Value	Value	Value	Value	Value	Value
Filters reset	Filter	Filter	Filter	Filter	Filter	Filter	Filter	Filter	Filter	Filter	Filter
	↑ OK ↓	↑ OK ↓	↑ OK ↓	↑ OK ↓	↑ OK ↓	↑ OK ↓	↑ OK ↓	↑ OK ↓	↑ OK ↓	↑ OK ↓	↑ OK ↓
SCYX0000902918 SURAMIN — Batch Tag: SP-002, Batch group Name: STANDARDS	54 ug/mL		11.85 ug/mL	4.6 none	1 none		.03 ug/mL	1.8E3 none	3 none	3.18 ug/mL	17 none
SCYX0000902928 IMMITICIDE, SP-0012 — Batch group Name: STANDARDS	4.12 ug/mL		10.17 ug/mL	.4 none	1 none		7.3 ug/mL	.6 none	1 none	8.39 ug/mL	.5 none
SCYX0000902932 SBV — Batch Tag: SP-0016, Batch group Name: STANDARDS	2.1 ug/mL		16.93 ug/mL	.1 none	1 none		11.33 ug/mL	.2 none	1 none	9.78 ug/mL	.2 none
SCYX0001734671 PCCR015-0113, SC... — Batch group Name: COMPOUNDS-P028-03		1.15 ug/mL				.04 ug/mL					

SAR table generated in Project Data

Configure the Biological Template Assay Header Sheet

To provide a convenient method for data entry, all biological templates are in Microsoft Excel .xlsm format. These templates can be populated with biological results and uploaded into Project Documents for registration.

Each template includes a first worksheet named "Assay Header" that configures the template for the assay. It describes the three hierarchy levels designed for your assay, as explained previously.

The following information is required when configuring the template.

Required Information for Biology Registration Templates

Field Name	Description	Example
Assay Name Assay Type	Name of Assay (500 characters max). Type of Assay (20 characters max).	Malaria In vitro
Organism Name and Organism Descriptor	Enter the authorized Organism Names (100 characters max) and Organism Descriptors (500 characters max). If Descriptor is left empty, "unknown" is used.	P. falciparum/K1 P.falciparum/NF54 P.falciparum/GHA P.falciparum/3D7
Test Parameter	Enter the authorized test parameters (100 characters max).	% inhibition IC50

An example of the Generic template is illustrated below.

Assay header for Generic template

The Assay Header sheet can be used to list the authorized values for the other key parameters. The table below provides details.

Authorized Values for Key Parameters

Field Name	Description	Example
Project ID	Project in ScienceCloud to check compound existence (Team ID can also be used)	P027; BIOVIA
Tester Information: First name, Last name, Username, Email	Authorized testers (must be valid ScienceCloud user accounts)	Bob Nare; BNARE; bnare@sciencecloud.com John Smith; JSMITH; jsmith@sciencecloud.com
Test Unit	Authorized value units	%, uM, nM, mg/kg
Test Operator	Authorized value operators	>, <, =, <=, >=
SOP/Trial ID	SOP or Trial IDs (or experiment #)	SOPMALVT1, SOPMALVT2
Time Point	Time point values	12, 24, 48, 72, 96
Time Unit	Authorized time point units	hour, minute, second

IMPORTANT! All entries on the Assay Header tab must already exist in the Team dictionary. If any values do not exist in the dictionary (for example, operator, organism, test parameter, units, assays), contact the Team Admin to get these entries added). Note that Time Point and SOP/Trial ID are not controlled by the Team dictionary.

Enter Result Values into the Assay Info Sheet

After the template is configured, use the Assay Info sheet to enter the biological values. When a list of authorized values is managed from the Assay Header sheet, a drop-down list of options is available.

*Batch No.	External Id	*Organism Name/Descriptor	*Test Parameter	*Operator	*Value	*Value Unit	Dose	Dose Unit	Time Point	Time Unit	*Test Date (dd-mmm-yyyy)	*Tester Name	Trial ID/SOP no	Test Comment	File to Load	File Display Name
									Malaria							
DEACC1234		P. falciparum--K1	% inhibition		98	%					5-May-2015	Bob Nare	SOPMALVT1			
DEACC1235		P. falciparum--K1	EC50	<	0.5	mg/kg	5	mg/kg	24	hour	5-May-2015	Bob Nare	SOPMALVT1	Activity to be confirm	StudyReport.pdf	
DEACC1236		P. falciparum--NF54	EC50		2.5	mg/kg			24	hour	5-May-2015	Bob Nare	SOPMALVT1			
DEACC1237		P. falciparum--NF54	% inhibition		60	%	5	mg/kg			5-May-2015	Bob Nare	SOPMALVT1			
DEACC1238			% inhibition		70	%	5	mg/kg			5-May-2015	Bob Nare	SOPMALVT1			

Assay Info Sheet values

The following information can be reported in the template.

Assay Info Sheet Options

Field Name	Description	Mandatory/ Optional	Example
Batch ID or Container ID/Well	To identify the compound for attaching results, enter the Batch ID or a combination of Container ID and Well. **Note:** When using the External ID option, it works just like the Batch ID column, where the External ID value listed must be unique and will actually be a Batch ID in ScienceCloud. If both a Batch ID and External ID are provided, the Batch ID is used.	M	`DEACC1234`
Three hierarchy levels	Assay will be copied from the Assay Header. Organism and Test Parameter must be chosen from the generated drop-down list.	M	`Malaria, P. falciparum/K1, IC50`
Operator, Value, Value Unit	To keep the value numeric and allow further sorting and filtering within ScienceCloud, separate the Value from the Operator. If an operator is not entered, the Equals operator (=) will be automatically assigned. Value Unit must be chosen from the drop-down list.	M	`<, 0.5, uM`
Dose and Dose Unit	Dose is a numeric value. Dose Unit must be chosen from the drop-down list.	O	`5, mg/kg`
Time Point and Time Unit	Can be used to capture a Time Point relevant to the assay. Both must be chosen from the drop-down list.	O	`24, hour`

Field Name	Description	Mandatory/ Optional	Example
Test Date	Format is dd-mmm-yyyy.	M	`03-JUN-2012`
Tester Name	Must be chose from the drop-down list.	M	`Bob Nare`
Trial ID/SOP	Can be used to capture a SOP or Trial ID (or experiment #). Must be chosen from the drop-down list.	O	`SOPMALVT1`
Test Comment	Free text to provide any additional information (1000 characters maximum).	O	`Activity to be confirmed`
File to Load	Filename of document to load and associate with the value in ScienceCloud.	O	`StudyReport.pdf`

Submit a Template for Registration

To submit a template for registration:

1. From the Apps menu on the ScienceCloud Home page, select **Project Documents**.
    Or from the Project Data page, click the **Project Documents** icon (right side of search box in blue header.)
2. Click on the Biology Smart Folder created for registration (indicated by the icon), and select **Upload** from menu bar.
3. Browse for and select the file, and then select any of the options detailed in the table below.

Template Submission Options

Option	Description
Only verify biological template file(s)	• If selected, email feedback will be provided after the file is validated. The file icons will also change appearance, based on status. See table below for details. • When not selected, validation is done in the background and the file will be registered automatically. Email feedback will be provided after the registration is complete. **Note:** By default, this option is always selected/checked.
Allow loading of duplicate records	• If selected, ScienceCloud will register all values present in the template, even if some would normally be seen as duplicate values because their data is identical. • If not selected, ScienceCloud will report an error for any data points seen as duplicate entries, so they can be corrected.
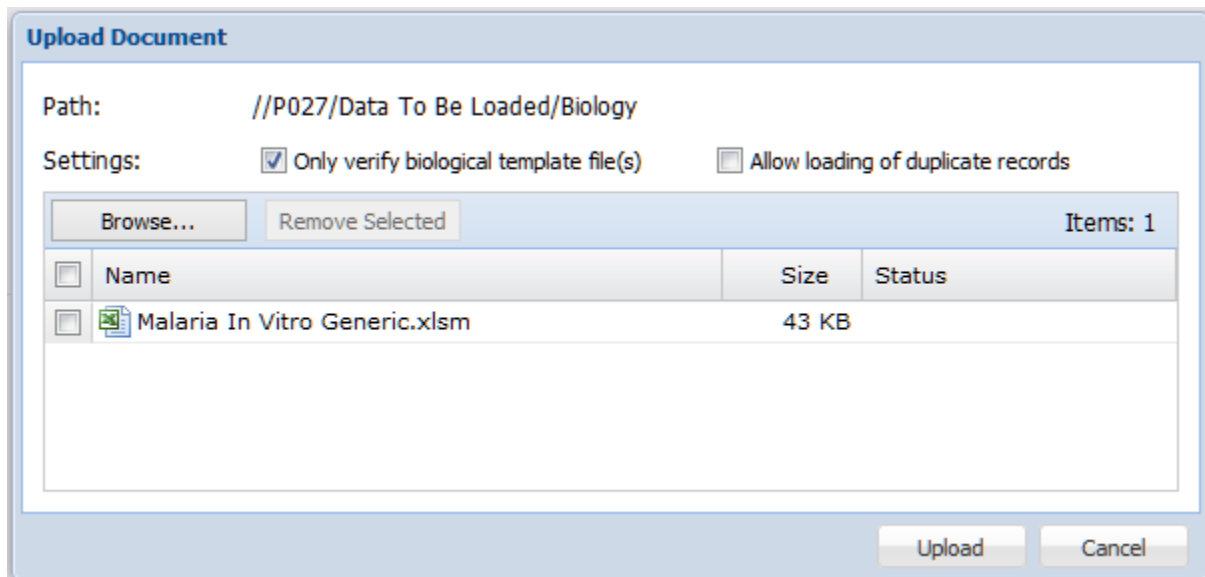
Upload biological template in Project Documents

File Icons

The file icon will change appearance based on the status. The following table provides details about the various icons that can be displayed for this purpose.

File Icon Status Indicators

Option	Description
	Valid – The validation was successful (without errors or warnings) and the file can now be registered.
	Error – A critical error was discovered in the file that must be resolved before it can be used in ScienceCloud.
	Warning – The file contains data that is unfamiliar or unusual. Questionable points were detected, such a text values or a future date. If necessary, resolve these issues before registering.

Resolve Errors

To resolve errors:

1. Click the filename to download the file.
2. Open the file.
3. The content will be modified to guide you to the issue(s).
4. Resolve any issues.
5. Save the file again.
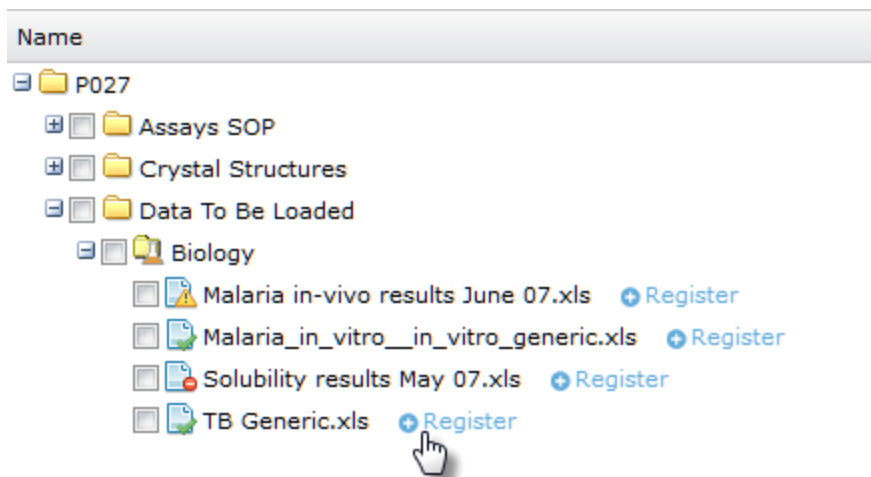6. Import the newest version of the file.

Locating error in file to fix

Register a File

To register the file:

If the file icon is displayed in green or yellow, and you are okay with the warnings, you can register the file.

▸ Click **+ Register** to the right of the filename.

Register a file

Note: You will receive feedback via email when the registration is complete.

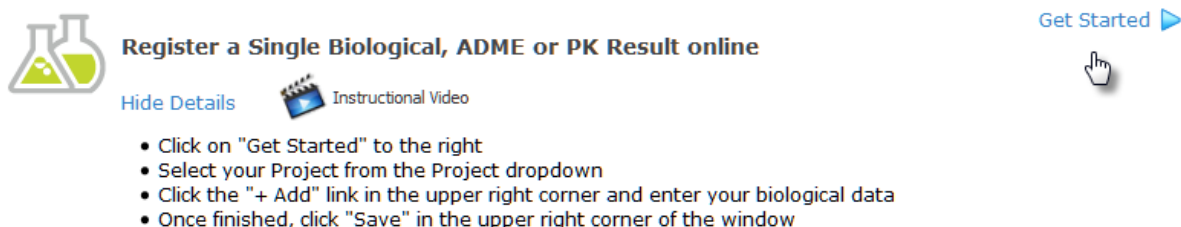# Register Single Biology Data (Single Biology Registration)

Use the New Biological Data page to enter biological data for batches within a project. The following tasks are covered in this section:

- Add New Biological Data
- Upload Additional Background Information for a Record
- Add Multiple Biological Data Records
- Remove Data Records
- Resolve Errors

Add New Biological Data
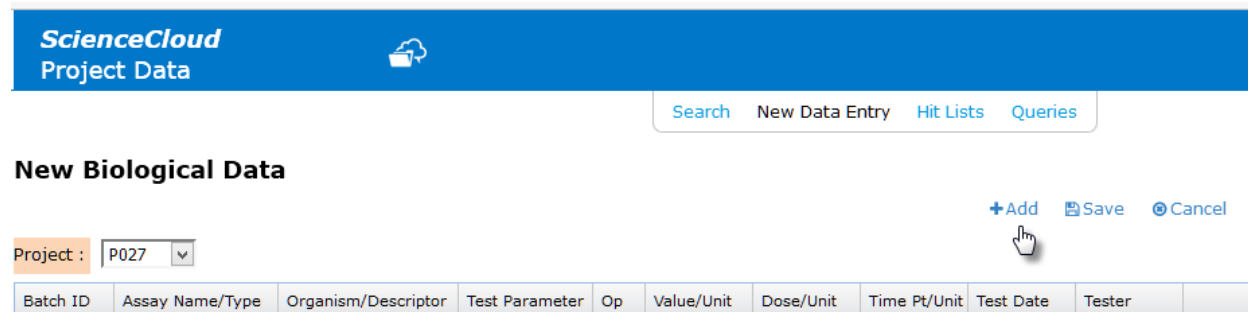
To add new biological data:

1. From the Apps section on the Home page, click **Project Data** to open the Project Data page.
2. From the top menu, select **New Data Entry** to open a getting started navigation page.
3. In Register a Single Biological, ADME or PK Result online, click **Get Started**.

Get Started option

4. The New Biological Data page opens. Select a project from the **Project** drop-down list and then click **Add** to add a new record.

Add new record

5. (Required) Enter the **Batch ID**.
6. Enter information into other fields where applicable (see table below for details).
7. Click **Save** to save the new records and related information.

New Biological Data

Project : P027

Batch ID	Assay Name/Type	Organism/Descriptor	Test Parameter	Op	Value/Unit	Dose/Unit	Time Pt/Unit	Test Date	Tester
JCT01-0002	Chagas in Vitro--IN V	T. cruzi--Tulahuen C4 (	IC50	<	0.5 ug/mL	5 mg/kg	24 hour	05-JUL-2016	HELEN PEARS [+] [X]

New biological data record

New Biological Data Fields

Field	Details	Example
Batch ID	(Required) The existing Batch ID where the new biological data should be registered.	PCUCT01-0002
Assay Name/Type	(Required) Name and type of assay. All available assays for the project are displayed in a drop-down list.	Malaria in Vitro–IN VITRO Solubility-ADME
Organism/Descriptor	(Required) Organism name and descriptor. All available organism names and descriptors are displayed in a drop-down list. (If Descriptor was not entered during creation, "unknown" will be used.)	P. falciparum/K1 P.falciparum/NF54 P.falciparum/GHA P.falciparum/3D7
Test Parameter	(Required) Authorized test parameters. All available test parameters are displayed in a drop-down list.	% inhibition IC50
Op	(Optional) Test value operator. All available operators are displayed in a drop-down list. If an operator is not entered, the Equals operator (=) will be automatically assigned.	<
Value/Unit	(Required) – Value (Optional) – Unit. All available units are displayed in a drop-down list. **Note:** It is important to separate the Value from the Operator to keep the Value numeric and allow further sorting and filtering within ScienceCloud. Value Unit must be selected from the drop-down list.	0.5, uM
Dose/Unit	(Optional) Dose is a numeric value. Select Dose and Unit from a drop-down list. All available units are displayed in a drop-down list. If you enter a Dose, you must also provide a unit.	5, mg/kg
Time Pt/Unit	(Optional) Can be used to capture a Time Point relevant to the assay. All available units are displayed in a drop-down list.	24, hour
Test Date	(Required) This value must be in the format DD-MMM-YYYY and can be manually entered or selected from a calendar picker.	03-JUN-2012

Field	Details	Example
Tester	(Optional) Select a name from the drop-down list. If left blank, the currently logged-in user will be automatically assigned.	`Bob Nare`
[+]	Opens a dialog for uploading a file with additional details for use with the data record (described below).	`SOPMALVT1 StudyReport.pdf` `Activity to be confirmed`

Upload Additional Biological Information for a Record

A file can be attached that contains additional details for use with a biological data record. Use the Biological Details dialog for this purpose.

To upload files:

1. Click **[+]** to open the Biological Details dialog.
2. Enter the following information:

   - **Trial ID:** Text field for entering the name of the trial ID. Useful for capturing a SOP or Trial ID (or experiment number).
   - **Select File:** Click **Choose File or Browse** and select the file to upload and attach to the record.
   - **Test Comment:** Free-form text field for entering information about the biological details.

Uploading a biological file to a record

3. Click **OK** to close the dialog.
4. Click **Save** to save the new records and related information.

Add Multiple Biological Data Records

Multiple data records can be added at the same time

To add another record to the same project:

1. Click **Add**. A copy of the previously entered record will be added, with an empty Batch ID.
2. Enter the Batch ID for the new record and other related information.
3. Repeat until all required records are added.

Notes:

- If the last record entered only contains the Assay Name, then the next record generated will only contain Assay Name as well.
- If the last record was populated and contains a file attachment, the new record generated will also be populated and contain the same attachment.
- When a new record is added, you can select a new assay from the Assay Name/Type drop-down list. (This clears all fields except Op.) Alternately, you can keep the assay copied from the previous record and update other fields individually.

To add new biological data to a different project:

▶ Select the project from the **Project** drop-down list.

All records for the previously selected project will no longer be displayed. The Assay Name drop-down and other fields will provide relevant options for the currently selected project.

☑ **Tips:**

- Open the Biological Details dialog and update the fields (and file attachment) for the new record.
- Be sure to save the new records and related information.

Remove Data Records

To remove a specific record:

▶ Click **[x]**.

To remove all records:

▶ Click **Remove All**.

Resolve Errors

If data is not properly formatted, or if the required information is not entered, an error message will be displayed that indicates there is a problem with the data, and that nothing will be submitted.
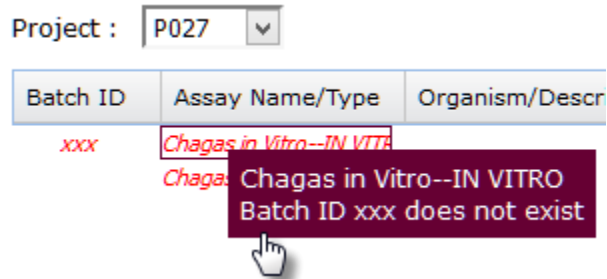

Error message for invalid biological record

To view invalid records (displayed in red onscreen):

▶ Click OK at the prompt.

To get details on the problem with a particular record:

▶ Hover over the record.

Details about an error

Duplicate Records

A duplicate record is defined as a record that contains the same Project ID, Batch ID, Test Conditions, Test Date, and Trial ID as another record that was either submitted previously for the same batch or data set.

A record that is considered a duplicate will generate a dialog (Allow Duplicate) to inform you that the data was already loaded. At the prompt, you can confirm whether or not to load it anyway. Selecting **No** allows the duplicate data to be loaded. A line will be printed in red and a message will be displayed confirming the duplicate state.

To view details:

▶ Hover over the error.

To correct the errors:

1. Modify the data.
2. Click **Save**.

Appendices

Appendix A: Support for Biological Templates

This section provides additional background information to support biological templates for use in ScienceCloud.

- Biological dictionary
- Report data for multiple projects with a single template
- Template layout protection
- Associating documents to a value
- Dose and time point

Biological Dictionary

A biological dictionary is available in ScienceCloud for Team Data Administrators to control the hierarchy levels and units. All dictionary entries must be in the Dictionary Admin and Assay Admin prior to using them on templates. Dictionary entries will not be created on-the-fly with templates.

Note: For further assistance using the biological dictionary, contact your Team admin.

Report Data for Multiple Projects with a Single Template

To use the same template to report results for several projects, enter the ScienceCloud Team ID in the **Project ID** box in the Assay Header sheet. ScienceCloud will then check batch existence in all of the Team's projects.

Template Layout Protection

The template layout is protected because ScienceCloud needs to know where to find the values. However, it is fine to enter values wherever the template supports it.

Associating Documents to a Value

You can load and attach a document to a biological value. To upload the document, enter the filename in the **File to Load** field on the Assay Info sheet. The document can be uploaded at the same time you upload the template for submission.

All documents associated with a biological value listed on the Assay Info Sheet must be uploaded. This document can be found in **Singular View** by searching for the associated data in Project Data.

Dose and Time Point

ScienceCloud uses dose and time point values when it builds the SAR table by creating a separate column for each value. Thus, the SAR table offers five hierarchy levels, three of which you determine, and two (dose and time point) that are determined by ScienceCloud.