ScienceCloud Project Data
Chemical Registration Guide

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

Covered Topics

Getting Started with Chemical Registration

Introduction

Chemical Registration can be completed both in Project Data via Single Registration as well as Project Documents via batch registration.

ScienceCloud supports registration for the following kinds of chemical data:

- Single compound (online via Project Data)
- Multiple compounds (from a file via Project Documents)

Chemical Data Template Registration

The following information explains how to configure and register chemical templates for use within ScienceCloud during batch registration in Project Documents.

File Content

A properly prepared chemical data registration file must contain the fields shown in the table below. Enter these field names exactly as they are shown. If you do not have information for the optional fields for any of the compounds being registered, do not include the field in your file. Optional, less frequently used fields are listed in Appendix A: Registration Fields for Chemical Data.

Required Fields for Chemical Data Registration Templates

Field Name	Description	Mandatory/ Optional/ Good Practice	Format	Example
batch_group_id	Registers the compound to a ScienceCloud project batch group.	M	Char (50 max)	`OXAZOLE`
batch_id	Batch ID for the new batch. Must be unique within your Team in ScienceCloud. **Notes:** • Multiple Batch IDs are allowed per Batch. Use commas to separate multiple IDs. • This field is not required in teams that auto-generate Batch IDs.	M	Char (50 max)	`PCUCT01-0002`
Project_id	Registers the compound to a ScienceCloud project.	M	Char (50max)	`P027`
batch_tag	Adds other IDs to the batch (e.g., Vendor ID, Partner ID). Use commas to separate multiple IDs.	O	Char (50 max)	`PG74`

Field Name	Description	Mandatory/ Optional/ Good Practice	Format	Example
scientist	Assigns the compound to a scientist based on the scientist's ScienceCloud username. If blank, the username of the person registering the file is automatically assigned.	GP	Char (50 max)	BSMITH
quantity	Quantity of the sample.	O	float	3
unit	Unit for the above quantity.	O	Char (10 max)	Mg
purity	Purity of the sample in % as determined by a standard analytical technique (e.g., HPLC/UV, HPLC/MS). Do not include "%" in your numerical entry.	O	float	90
batch_comment	Text field for adding information relevant to the screener.	O	Char (500 max)	Poor solubility
salt_name	Name of the salt. Must be present in the Team's Salt Dictionary prior to registration.	O	Char (60 max)	Hydrochloride
salt_coeff	Number of occurrences of the salt.	O	float (30 max)	2
molecular_weight	Molecular weight of the sample. If a chemical structure is included in the registration, leave the molecular weight field blank, as it will be automatically calculated from the structure.	O	float	234.34
molecular_formula	Molecular Formula of the molecule. If a chemical structure is included in the registration, leave the molecular formula field blank, as it will be automatically calculated from the structure.	O	Char (no limit)	C18H26CIN3
container_id	Identifies the container used to store the compound (e.g., vial number, plate number). If not included, a default container "NA" will be registered.	O	Char (50 max)	PL012301

Field Name	Description	Mandatory/ Optional/ Good Practice	Format	Example
well	Well position in a 96-well plate or other kind of plate. If not applicable for a compound, leave blank. If not included, a default well of "-1" will be registered.	O	Char (5 max)	`A01`

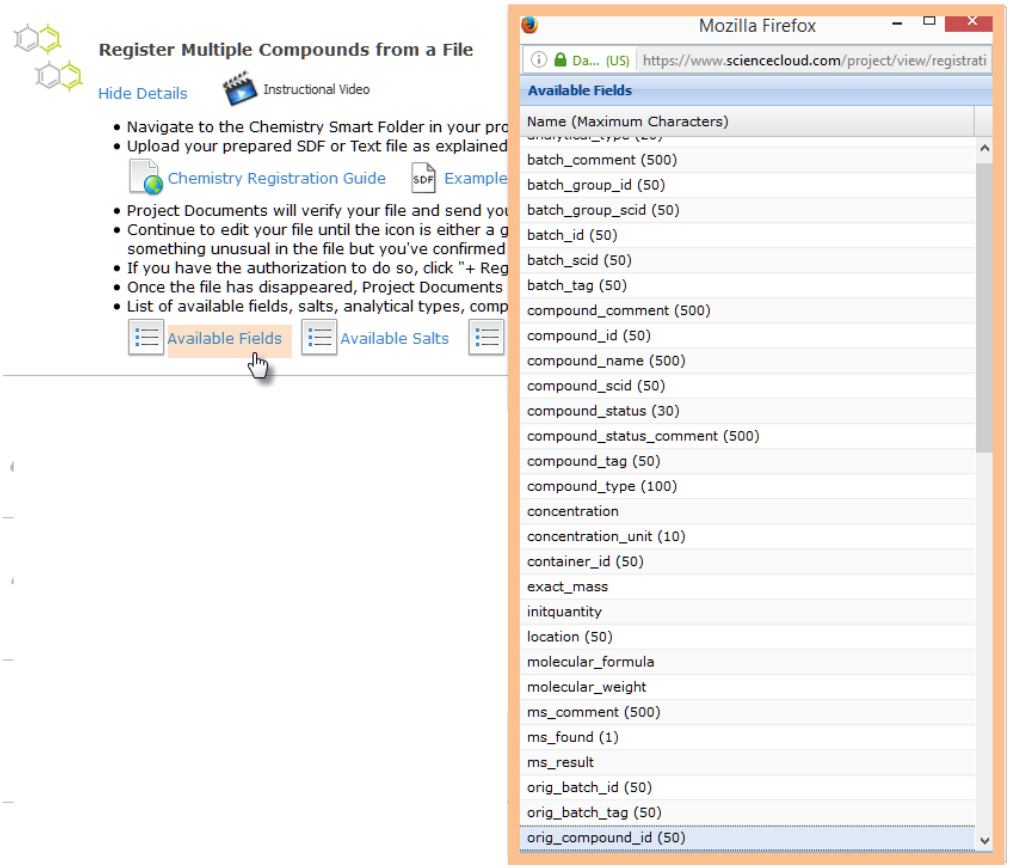
Additional Resources

A complete listing of any of the following can be viewed online:

- Available fields
- Available salts
- Available analytical types
- Available compound types
- Available compound statuses

To view an online list:

1. Open the Project Data application.
2. Select the **New Data Entry** menu option.
3. In Register Multiple Compounds from a File, click **Show Details**.
4. Click an option to open a list. For example, click **Available Fields** to view the list of all available fields online.



Available fields for chemical registration

☑ **Tip:** Example files and instructional videos are also available.

Prerequisites (File Formats)

Before registering chemical structures, prepare one *SD file* containing the structures and the additional information. The field names in the SD file must be the ones specified in the Available Fields list.

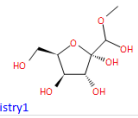
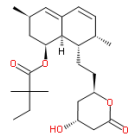
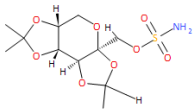
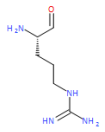
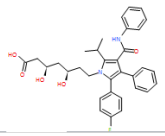
An alternative method is to prepare one *text file in Excel* with the chemical structures represented by their SMILES string in a column labeled "SMILES". However, for a better representation of the stereochemistry, use SD files when possible.

If you do not have any chemical structures to register, prepare a *text file in Excel*. Name each column header with the field name specified in the Available Fields list, fill in the Excel spreadsheet, and then save as a text file (Tab Delimited).

File Examples

The following are examples of chemical registration files in different formats.

SD file created in Insight for Excel:

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	CHEMISTRY	scientist	Project_id	batch_group_id	salt_name	batch_id	salt_coeff	batch_comment	Purity	Quantity	Unit	container_id	well	batch_tag	compound_tag
2	 Chemistry1	SCLOUD	SCDEMO	Partner Compounds	hydrochloride	SCLOUD0001234	1	low solubility	100	7	mg	CLOUD54321	A01	Party1,Party2	CompoundXYZ,CRO-Comp3
3	 Chemistry2	SCLOUD	SCDEMO	Partner Compounds		SCLOUD0001235			90	7	mg	CLOUD54320	A02	CRO2	
4	 Chemistry3	SCLOUD	SCDEMO	Partner Compounds	Acetate	SCLOUD0001236	2		95	4	mg	CLOUD54319	A03	ABC123	
5	 Chemistry4	SCLOUD	SCDEMO	Partner Compounds		SCLOUD0001237			95	14	mg	CLOUD54318	B01		PureCompound9573
															

SD File created in Insight for Excel

Text file created with Excel (chemical structures represented by their SMILES string):

	A	B	C	D	E	F	G	H	I	J	K
1	smiles	project_id	batch_group_id	batch_id	scientist	salt_name	salt_coeff	batch_comment	purity	quantity	unit
2	OC[C@]1(O)O[C@@H]([C@H](O)[C@H]1O)CO)OC	SCDEMO	Partner Compounds	SC0001234	SCLOUD	hydrochloride	1	low solubility	100	7	mg
3	O([C@@H]1[C@@]/2([C@H]([C@H](/C=C\C2=C\[C@@H](C1)C)C)CC[C@H]1OC(=O)C[C@H](O)C1)[H])C(=O)C(CC)(C)C	SCDEMO	Partner Compounds	SC0001235	SCLOUD				90	7	mg
4	S(OC[C@@]12OC[C@]3(OC(O[C@]3([C@@]1(OC(O2)(C[H])C)[H])[H])(C)C)[H])[H])(=O)(=O)N	SCDEMO	Partner Compounds	SC0001236	SCLOUD	Acetate	2		95	4	mg
5	N[C@H](C=O)CCCNC(N)=N	SCDEMO	Partner Compounds	SC0001237	SCLOUD				95	14	mg
6	Fc1ccc(c2n(c(C(C)C)c(c2c2ccccc2)C(=O)Nc2ccccc2)CC[C@@H](O)C[C@@H](O)CC(O)=O)cc1	SCDEMO	Partner Compounds	SC0001238	SCLOUD				90	21	mg
7	Fc1ccc(c2n(c(C(C)C)c(c2c2ccccc2)C(=O)Nc2ccccc2)CC[C@@H](O)C[C@@H](O)CC(O)=O)cc1	SCDEMO	Partner Compounds	SC0001239	SCLOUD				75	45	mg
8											

Text file created with Excel (chemical structures represented by SMILES string)

Text file created with Excel (without structures):

	A	B	C	D	E	F	G	H	I	J	K
1	project_id	batch_group_id	batch_id	scientist	salt_name	salt_coeff	batch_comment	purity	quantity	unit	molecular_weight
2	SCDEMO	Partner Compounds	SC0001234	SCLOUD	hydrochloride	1	low solubility	100	7	mg	210.182
3	SCDEMO	Partner Compounds	SC0001235	SCLOUD				90	7	mg	418.574
4	SCDEMO	Partner Compounds	SC0001236	SCLOUD	Acetate	2		95	4	mg	339.363
5	SCDEMO	Partner Compounds	SC0001237	SCLOUD				95	14	mg	158.205
6	SCDEMO	Partner Compounds	SC0001238	SCLOUD				90	21	mg	558.65
7	SCDEMO	Partner Compounds	SC0001239	SCLOUD				75	45	mg	274.53
8											

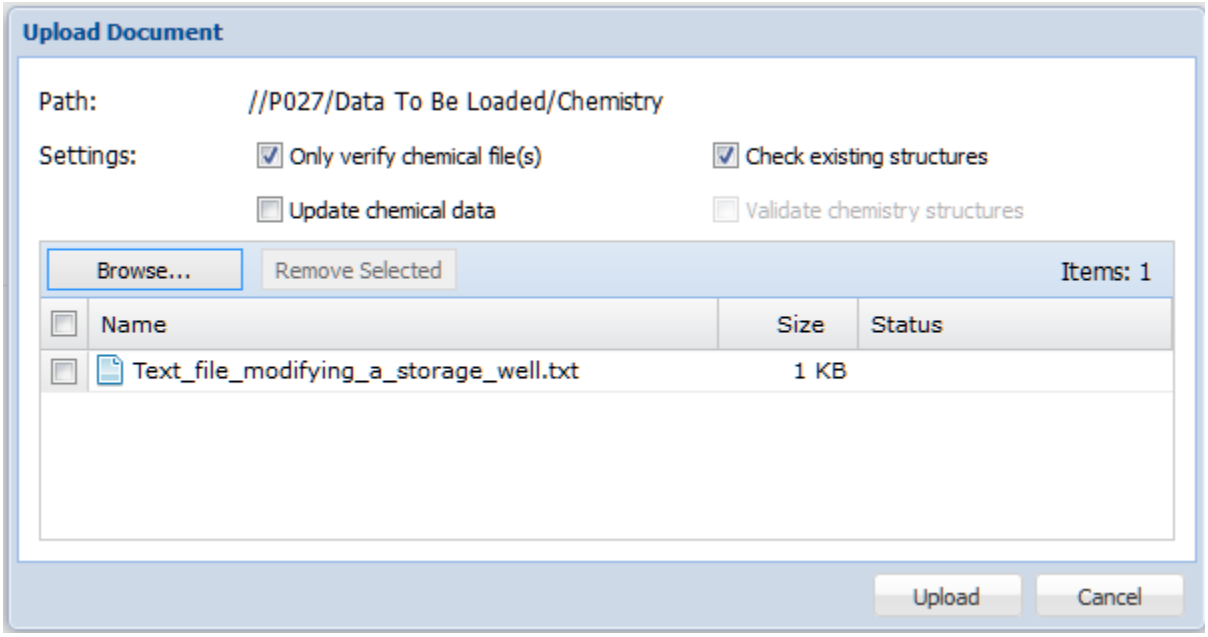
Text file created with Excel (without structures)

Submit a File for Registration

To submit a file for registration:

1. From the ScienceCloud home page, go to **Project Documents**.

   Or from Project Data, click the **Project Documents** icon .
2. Click the **Chemistry Smart Folder** created for registration.
3. Click **Upload** from the toolbar.
4. Use the Upload Document dialog to browse for and select the file to register. Select any of the options described in the table below.



Overview of Project Documents features

Options for Submitting Files for Registration

Setting	Value
Only Verify Chemical File(s)	• If checked, email feedback will be provided after the file is validated. The file icons will also change appearance, based on status. See below for details. Recommended. • When not checked, 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 checked.
Update Chemical Data	Not required for the initial registration. Applicable when adding new information (sample, shipping, etc.) to an existing compound, or when updating existing values to new values. See Modify Chemical Data.

Setting	Value
Check Existing Structures	If checked, ScienceCloud searches for any structure that is the same as the one you are registering both in your file and in ScienceCloud. This is based on the Team setting – tautomer matching can be on the Team level or Project level. **Note:** By default, this option is always checked. Do not enable this feature under the following conditions: • If the compound was not previously registered. • If the compound was previously registered, but you want to register the current information as a brand new compound.
Validate Chemistry Structures	If checked, ScienceCloud will process the structure validation Pipeline Pilot protocol specified in your Team to ensure structures are drawn to your specified standards. **Note:** When a structure does not meet these standards, changes will be made to the structure, and an email will be sent that provides detailed information. • When not checked, chemistry structures are not validated. • This option is greyed out (unavailable) if no validation protocol is associated with the Team.

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

Icon	Status
	**Valid** – The validation was successful (without errors or warnings) and the file can now be registered.
	**Warning** – The file contains data that is unfamiliar or unusual. Questionable points were detected, such as an existing compound, so a subsequent batch will be created. If necessary, resolve these issues before registering.
	**Error** – A critical error was discovered in the file that must be resolved before it can be used in ScienceCloud.

Resolve Errors

To resolve errors:

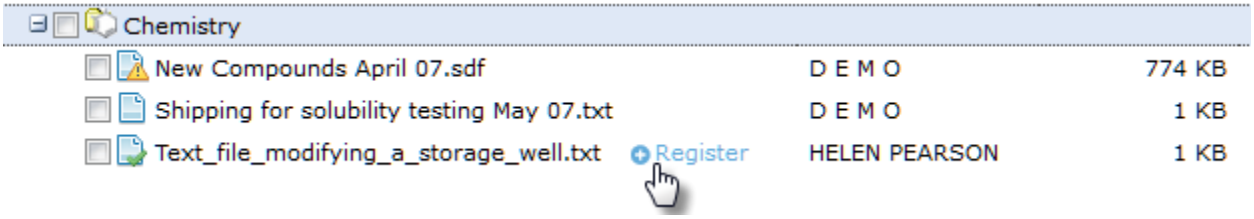
1. Click the filename to download the file.
2. Open the file.
3. The content will be modified to guide you to the issue(s).
4. Resolve any issues.
5. Save the file again.
6. Import the newest version of the file.

Register a File

To register the file:

If the file icon is 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 should receive feedback via email when the registration is complete.

Register Subsequent Batches

To register a subsequent batch using an SD file:

- Reuse the same structure as the one used in the first batch.

To register subsequent batches without using the structure:

- Include the "compound_id" column in your text file, and enter the compound ID that should be associated with the new batch.

The following is an example of a text file for subsequent batch registration.

	A	B	C	D	E	F	G	H	I	J	K
1	project_id	batch_group_id	compound_id	batch_id	scientist	salt_name	salt_coeff	batch_comment	purity	quantity	unit
2	SCDEMO	Partner Compounds	SCT00000001	SC0001234	SCLOUD	hydrochloride	1	low solubility	100	7	mg
3	SCDEMO	Partner Compounds	SCT00000002	SC0001235	SCLOUD				90	7	mg

Text file for subsequent batch registration

Notes:

- The registration fields that affect compound data (molecular_weight, compound_name, etc.) will be ignored if used in a file to create subsequent batches.
- The parent compound must be updated directly.
- Any changes to compound level information (structure, comments, etc.) for one batch will update compound level information for all subsequent batches.

Register Multiple Samples

Multiple samples for one batch can be registered in the same file.

To register multiple samples:

1. Repeat the batch information (e.g., batch_id, project, batch group, etc.) on the following lines.
2. Change the sample information (e.g., purity, quantity, etc.) to reflect the additional samples.

Note: When entering multiple sample information, container_id and well are mandatory.

The following is an example of a text file for multiple samples registration.

	A	B	C	D	E	F	G	H	I
1	project_id	batch_group_id	batch_id	scientist	container_id	well	purity	quantity	unit
2	SCDEMO	Partner Compounds	SC0001234	SCLOUD	Container1	A01	100	7	mg
3	SCDEMO	Partner Compounds	SC0001234	SCLOUD	Container1	A03	90	6	mg
4	SCDEMO	Partner Compounds	SC0001234	SCLOUD	Container1	A05	99	5	mg
5									

Text file for multiple samples registration

Register Multiple Shipments

Multiple shipments for one batch can be registered in the same file.

To register multiple shipments:

1. Repeat the batch and sample information on the following lines.
2. Change the shipping information (e.g., ship_container_id, ship_well, etc.) to reflect the additional shipments.

The following is an example of a text file for multiple shipments registration.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	project_id	batch_group_id	batch_id	scientist	container_id	well	purity	quantity	unit	ship_container_id	ship_well	ship_quantity	ship_unit	
2	SCDEMO	Partner Compounds	SC0001234	SCLOUD	Container1	A01	100	7	mg	Ship_Plate1	B01	2	mg	
3	SCDEMO	Partner Compounds	SC0001234	SCLOUD	Container1	A01	100	7	mg	Ship_Plate2	C01	2	mg	
4	SCDEMO	Partner Compounds	SC0001235	SCLOUD	Container1	A03	90	6	mg	Ship_Plate1	B03	2	mg	
5	SCDEMO	Partner Compounds	SC0001235	SCLOUD	Container1	A03	90	6	mg	Ship_Plate2	C03	1	mg	
6														

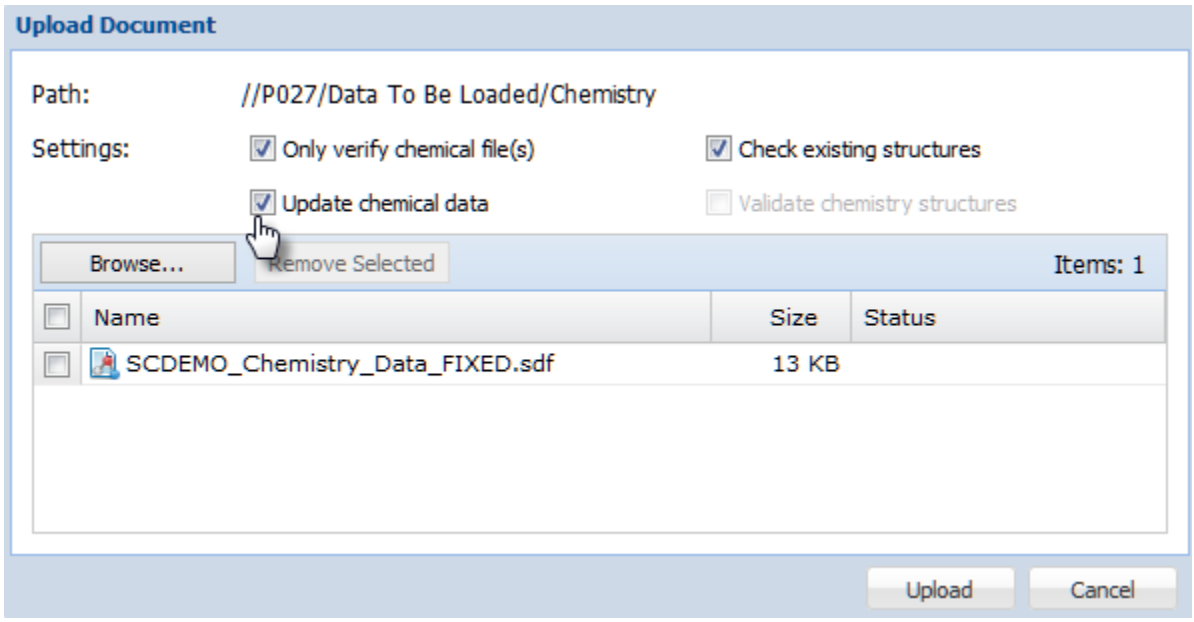
Text file for multiple shipment registration

Modify Chemical Data

You can modify existing chemical information for a set of compounds by preparing the same file format as for registration. The Batch ID field is mandatory because it will be used as the key to identify the compound to modify. The Container ID and Well fields are mandatory when modifying any sample fields (e.g., quantity, location, purity, shipping).

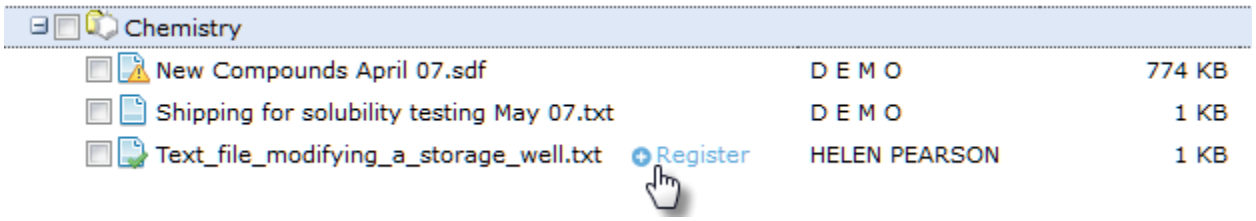
To modify chemical data:

1. When uploading the file, select the **Update Chemical Data** check box in the upload dialog. This is used to add new data (samples, shippings, etc.) to existing batches, and to modify values as described below in Modify Values Using ID Fields.



Update chemical data option selected when uploading chemistry files for registration

2. After validation, click **Update** at the right of the filename to update the data in ScienceCloud. You will receive feedback via email when the update is complete.



Update option for newly uploaded chemistry file

Modify Values Using ID Fields

A special process is required to modify existing values. Both the original (current value) and new values must be included using special fields in the file so that ScienceCloud can correctly match and update with appropriate data. During this process, it is not necessary to include the mandatory fields from the original file registration process. However, additional fields need to be included so ScienceCloud can update the appropriate items.

Use the field names shown in the table below to mention the original value.

ID Fields and Values

Value to Modify	Put Original (Old) Value Here	Put New Value Here	Additional Required Fields for Modification
Compound ID	`orig_compound_id`	`compound_id`	
Batch ID	`orig_batch_id`	`batch_id`	
Compound Tag	`orig_compound_tag`	`compound_tag`	
Batch Tag	`orig_batch_tag`	`batch_tag`	`batch_id`

Value to Modify	Put Original (Old) Value Here	Put New Value Here	Additional Required Fields for Modification
Storage Container ID / Well	`orig_container_id / orig_well`	`container_id / well`	`batch_id`
Shipping Container ID /Well	`orig_ship_container_id / orig_ship_well`	`ship_container_id / ship_well`	`batch_id, container_id, well`

An example of a text file for modifying a storage well is illustrated below.

	A	B	C	D	E
1	batch_id	orig_container_id	orig_well	container_id	well
2	SC0001234	Container1	A01	Container1	B03
3	SC0001235	Container1	A03	Container1	B05
4					

Text file for modifying a storage well

Register Single Compounds (Single Chemistry Registration)

Use the Single Registration page to register a single compound and its associated data without an SD or text file. Structures are optional in Single Registration.

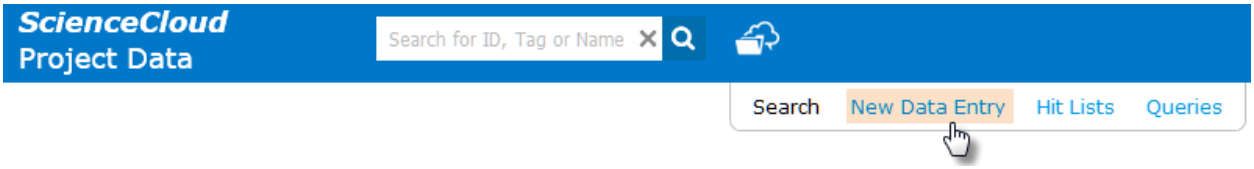
The following tasks are involved in registering single compounds:

1. Start Single Registration
2. Register a Compound (with Structure)
3. Add Sample and Shipping Information
4. Add Biological Data

Start Single Registration

To start Single Registration:

1. From the Apps section on the Home page, click **Project Data** to open the Project Data page.
2. From the top menu bar, select **New Data Entry** to open a getting started option.

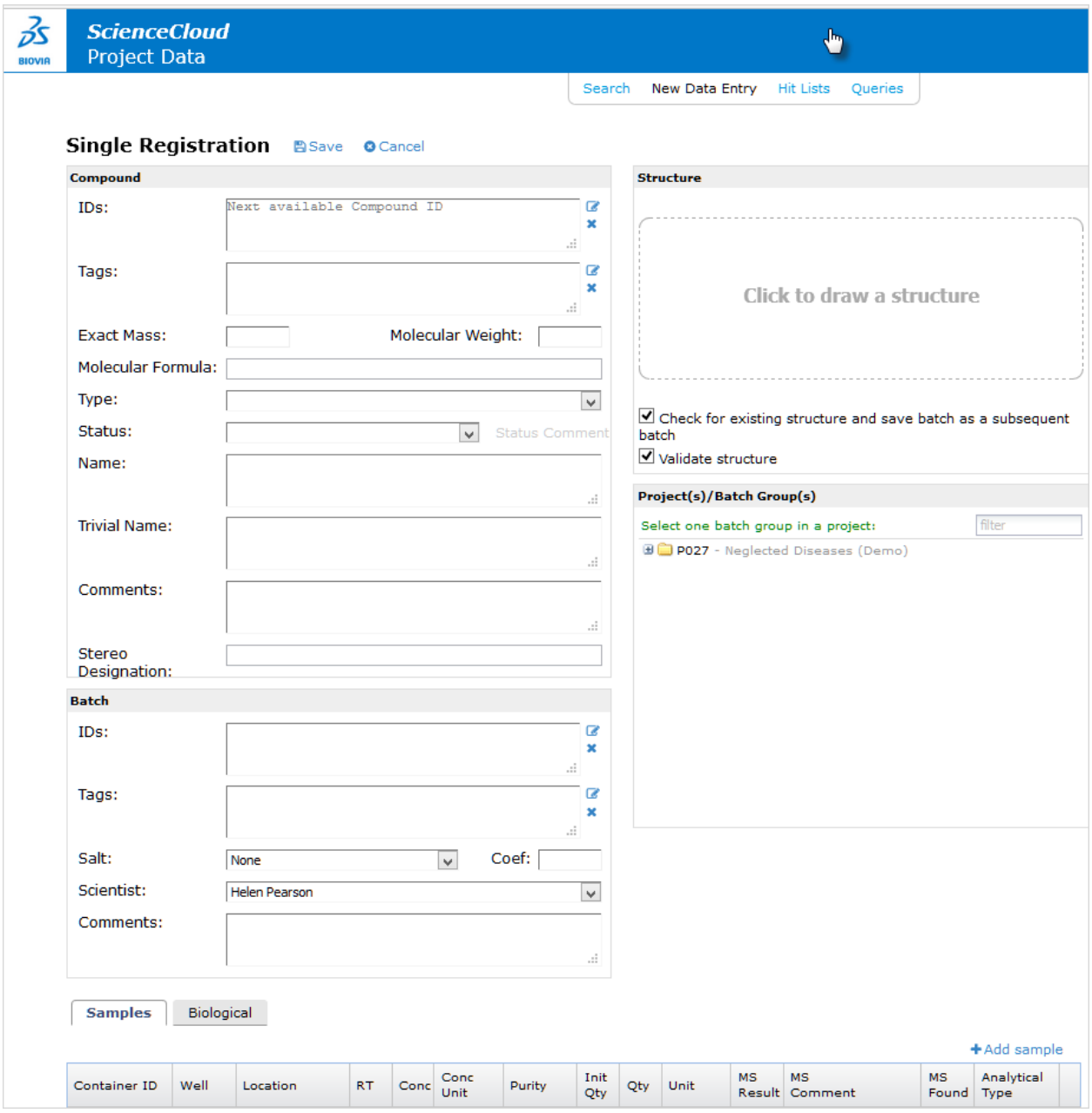


New Data Entry menu option for starting Single Registration

3. In Register a Single Compound online, click **Get Started** to open Single Registration.

Navigation feature to open feature for registering a single compound

The Single Registration page looks like the following when it first opens.



Single Registration page (default view)

Single Registration Features

The Single Registration page includes the following features:

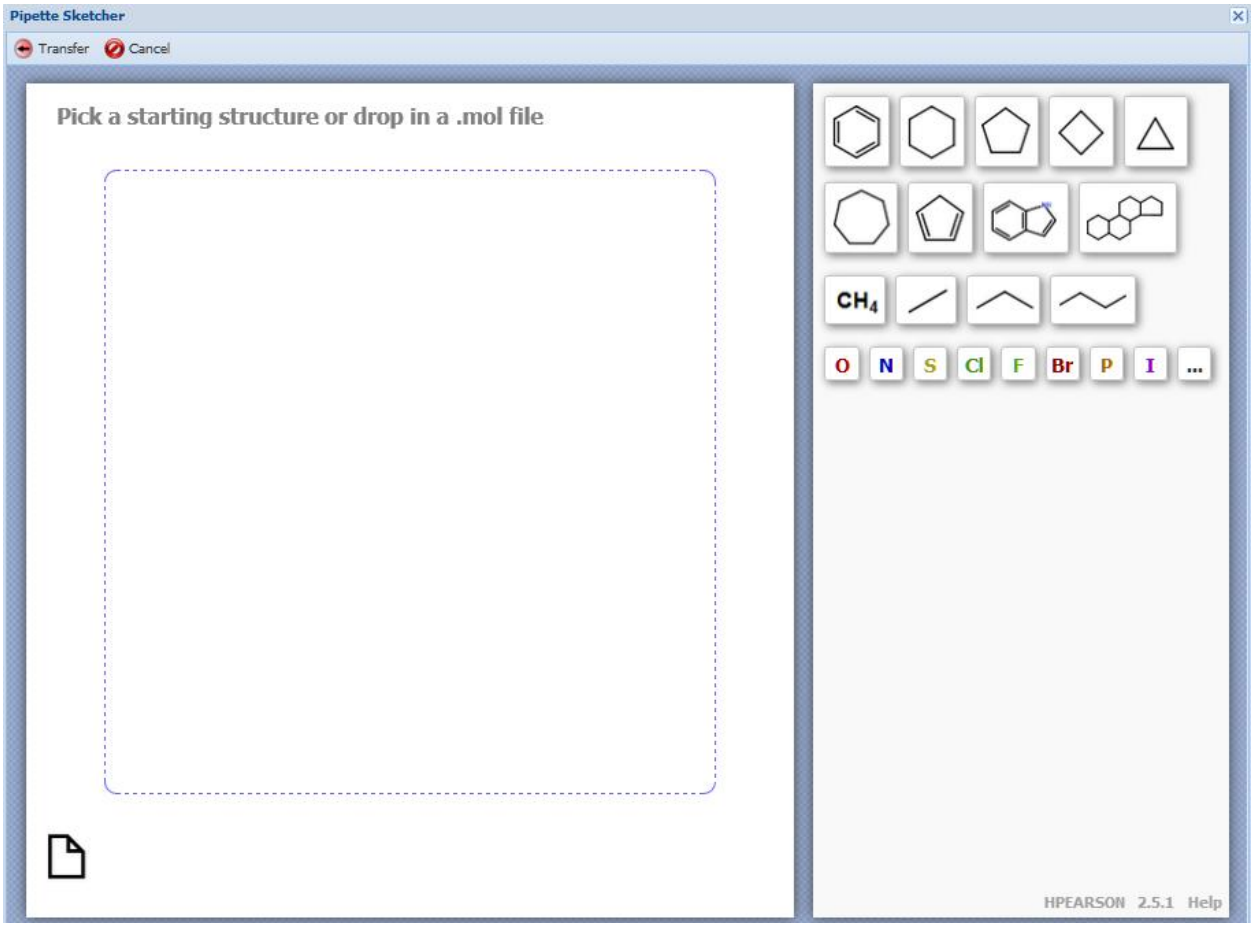
- **Toolbar** – Save and Cancel toolbar buttons. Save will save the new compound. Cancel will return you to the New Data Entry page.
- **Compound** – Text fields for entering information about the compound.
- **Batch** – Text fields for entering information about the batch.
- **Structure** – Opens a drawing program for drawing the compound structure.

- **Projects/Batch Groups** – Lists the projects and batch groups that can be used to register the compound.
- **Samples tab** – Add sample and shipping information in this form.
- **Biological tab** – Add biological data for the compound/batch that is getting registered.

Register a Compound (with Structure)

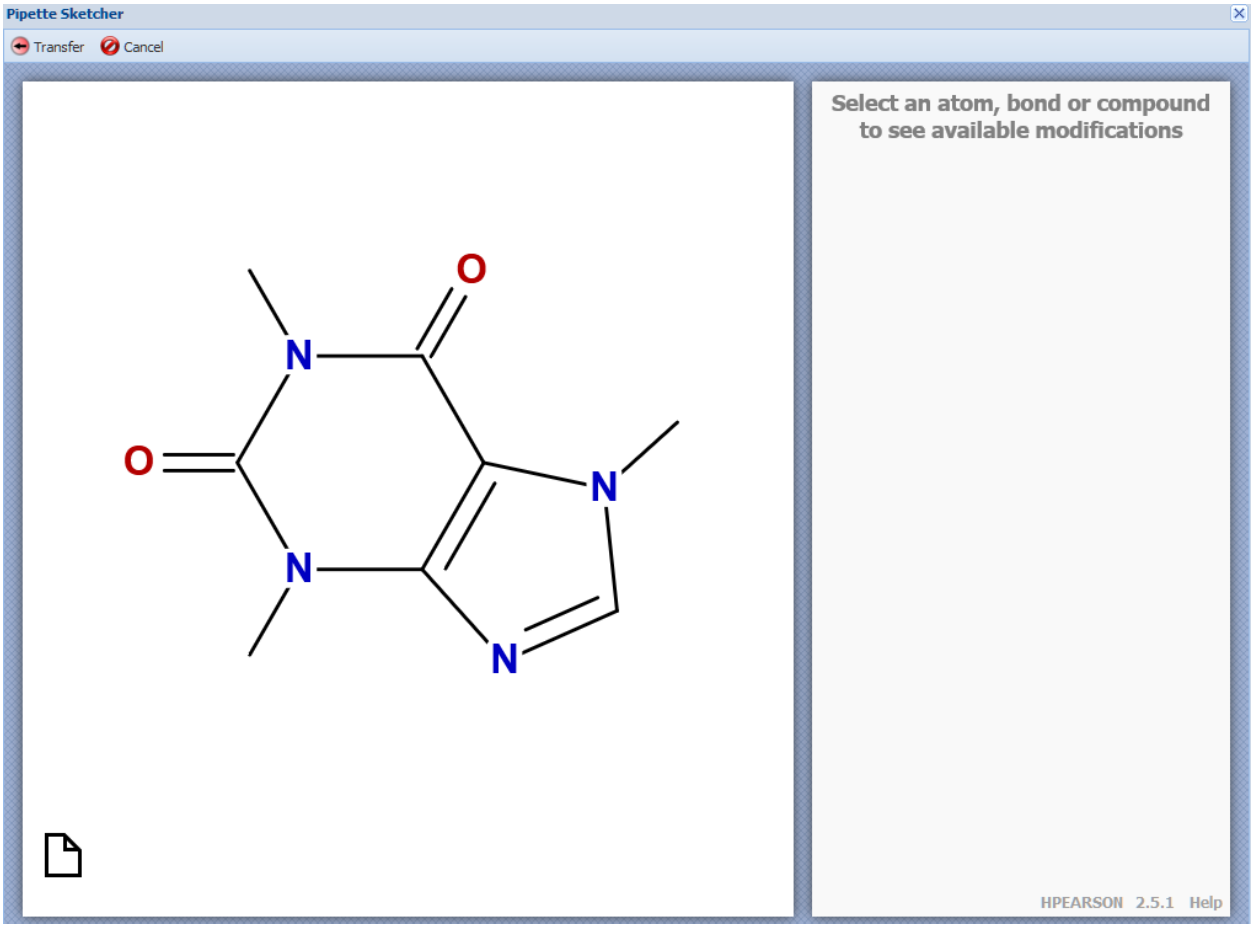
To register a compound with structure:

1. Click the **structure box** to open either Pipette Sketcher or a third-party sketcher tool that is compatible with ScienceCloud, such as BIOVIA Draw.



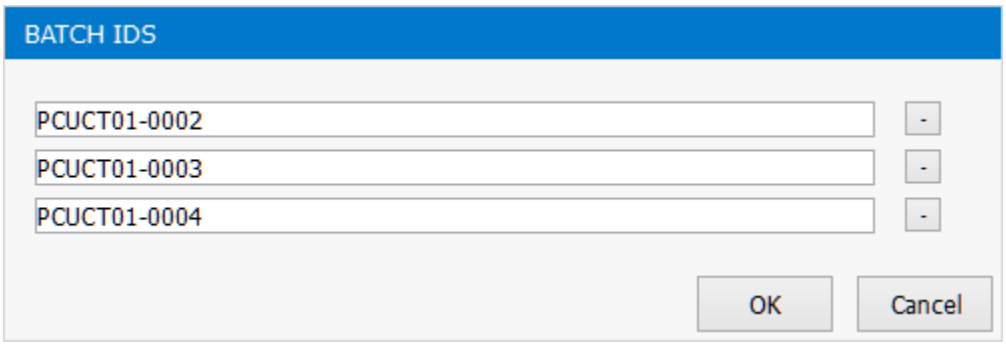
Pipette Sketcher tool

2. Enter a structure by doing one of the following:
   - Drag and drop a previously created .mol file into the sketcher tool.
   - Draw a structure in the sketcher tool.



.mol file dropped into drawing tool

3. Click **Transfer** to return the structure to the Single Registration page.
4. (Required) In **Batch IDs**, enter the batch IDs in the text box that opens. To enter multiple IDs, click [+].

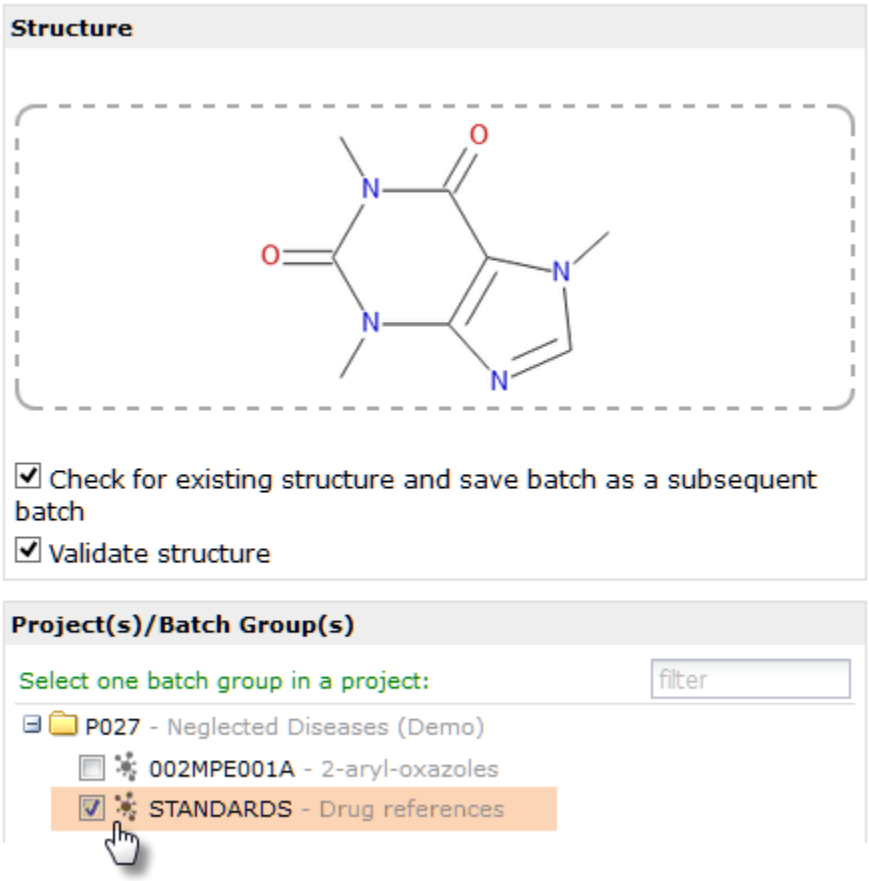


Text box for entering compound IDs

Notes:

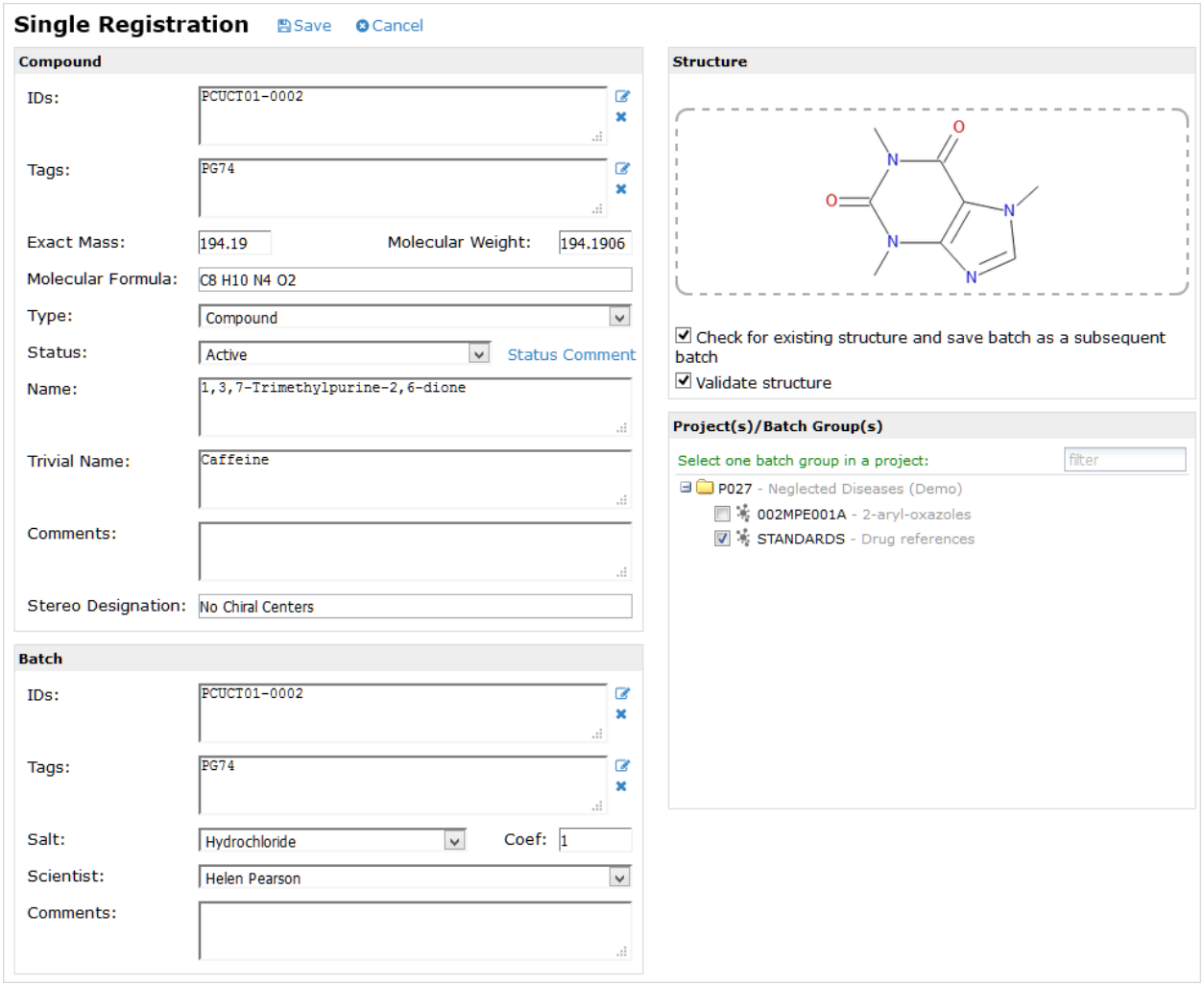
- Batch IDs must be unique to ScienceCloud (50 characters max). For example: `PCUCT01-0002`.
- Some teams auto-generate batch numbers. This field is not required for those teams. Consult your team administrator to confirm batch ID generation.

5. (Required) The projects and batch groups that can be used to register the compound are listed below the structure box. Select from the list one batch group from a project in which to register the new compound.



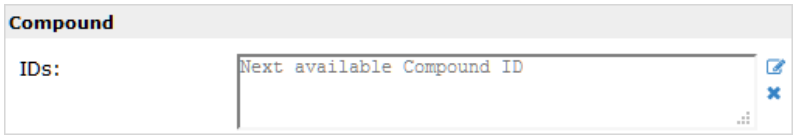
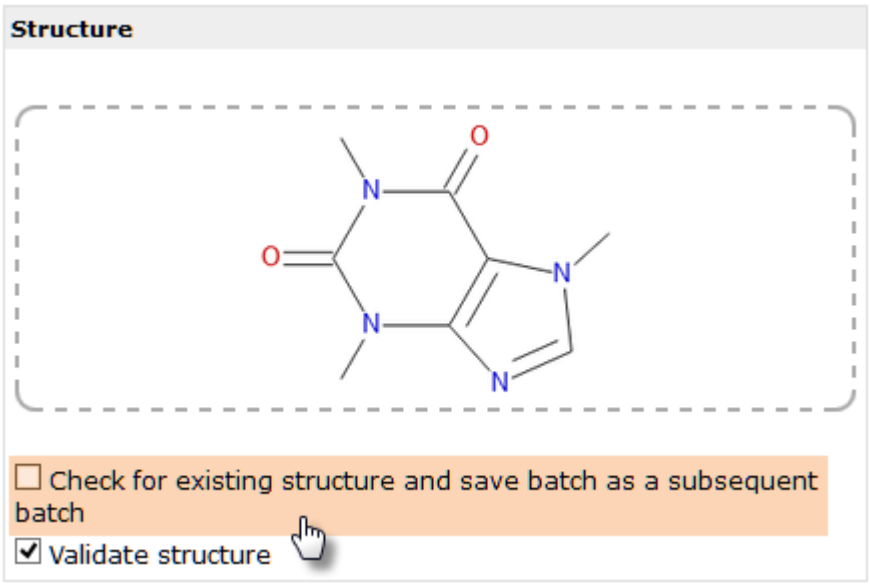
Selected batch group

6. (Optional) Add additional information in the appropriate fields (described in the tables below).
7. Click **Save** to save the single registration settings.



New single registration settings

Single Registration Compound ID Options

To	Do this
Assign a compound ID	In **Compound IDs**, enter the ID numbers.  Compound IDs field ☑ **Tip:** To have a Compound ID automatically assigned, leave this box blank.
Register a new compound	If a compound was previously registered and the current information needs to be registered as a new compound, clear the check box for **Check for existing structure and save batch as a subsequent batch**.  Check box option
Save as a subsequent batch of an existing compound	If the current information should be registered as an additional batch for an existing compound, select the check box for **Check for existing structure and save batch as a subsequent batch**.

Single Registration Fields

Field	Description	Example
Compound IDs	Unique identifier assigned to the compound. For further details, see the previous section "Single Registration Compound ID Options".	SCYX0012344
Compound Tags	Any additional IDs for the compound (e.g. Vendor ID, Partner ID). Compound tags can be non-unique.	PG74

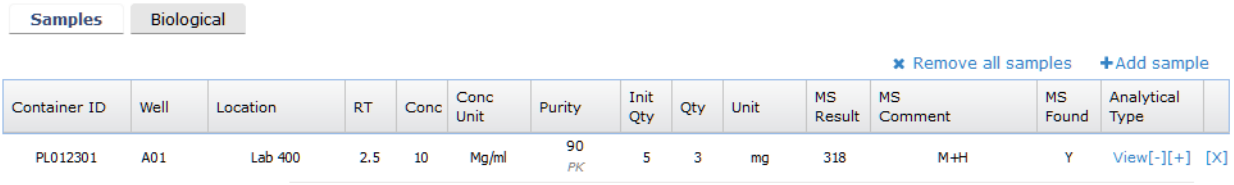
Field	Description	Example
Exact Mass	Exact mass of the compound	`340`
Molecular Weight	Molecular weight of the compound. Not required if a structure is provided during registration.	
Molecular Formula	Molecular formula of the compound. Not required if a structure is provided during registration.	
Compound Type	Compound type; controlled by the Team dictionary. Examples are "C', "S", "LO", or "LG".	`C`
Compound Status	Status of the compound; controlled by the Team dictionary. Examples are Active, Terminated, On Hold, Validated, or Rejected.	`Active`
Compound Status Comment	Textual description of compound status.	
Compound Name	Chemical name of the compound.	`Diethylcarbamazine`
Compound Trivial Name	Trivial name of the compound.	`Diethylcarbamazine citrate,1642-54-2`
Compound Comments	Textual description of the compound.	
Compound Stereo Designation	Textual description on the stereochemistry of the compound.	`R isomer`
Batch IDs	(Required) The batch IDs to be assigned for the new batch. Must be unique in the Team. Multiple IDs are accepted. (50 characters max.) Not required for teams that auto-generate the batch id.	`PCUCT01-0002`
Batch Tags	Any additional IDs for the compound (e.g. Vendor ID, Partner ID). Batch tags can be non-unique.	`PG74`
Salt	Name of the salt. Controlled by the Team dictionary.	`Hydrochloride`
Coef	Number of occurrences of the salt.	`2`
Scientist	The ScienceCloud user to which the compound should be assigned. By default, the logged in user is selected.	`Bob Smith`
Batch Comments	Textual description on the batch.	

Add Sample and Shipping Information

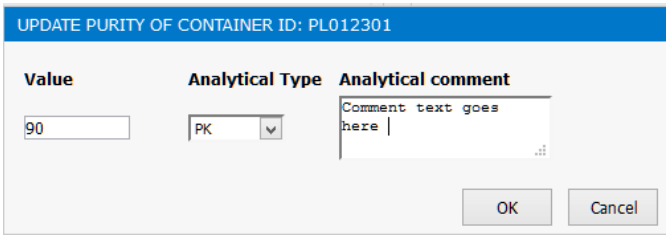
Use the Samples tab to add sample and shipping information.

To add sample information:

1. Click the **Samples** tab located below the Single Registration fields.
2. Click **Add Sample**. A new sample line is added in the Samples section at the bottom of the samples list.
3. (Optional) Enter information in **Container ID**.
4. (Optional) Enter information in the other fields where necessary (described in the table below).
5. Multiple new samples can be added. Click **Add Sample** and repeat the above steps.
6. Click **Save** to save the single registration entry.



Sample information for a single registration file **Samples Tab Fields**

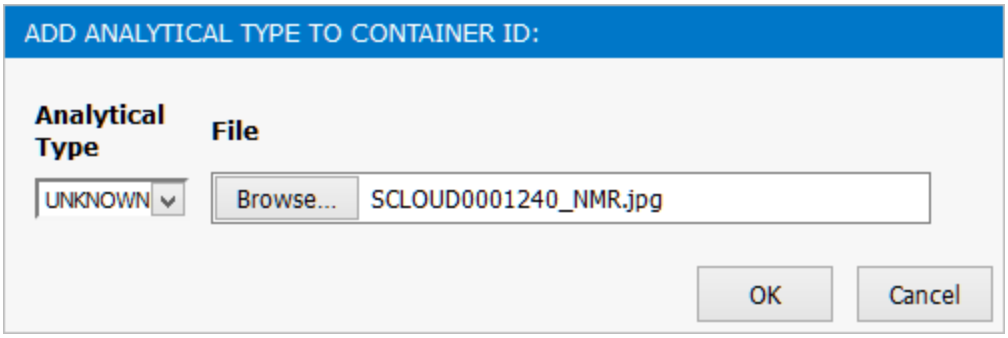
Field	Details	Example
Container ID	Identifier of the container that is used to store the compound (for example, vial number, plate number).	`PL012301`
Well	Well position in a 96-well plate or other kind of plate. If not applicable for a compound, leave blank. Plate size can be adjusted by clicking the "96".	`A01`
Location	Location of a sample.	`Lab 400`
RT	Retention time (in minutes).	`2.5`
Conc	Concentration of the batch.	`10`
Conc Unit	Unit for the above concentration quantity.	`Mg/ml`
Purity	Purity of the sample in % as determined by a standard analytical technique (HPLC/UV or HPLC/MS for example). Enter information in the dialog that opens and click OK to save it. Do not include "%" in your value entry.  Dialog for entering purity information for container ID	`90`
Init Qty	The initial quantity of the sample contained in the well.	`5`
Qty	Current quantity of the sample contained in the well.	`3`

Field	Details	Example
Unit	Unit for the above quantity.	mg
MS Result	The mass observed by the analytical instrument (Mass Spec.).	318
MS Comment	Free text comment that can be used to list adduct(s), protonation, and other MS related comments.	M+H
MS Found	Was the mass of the molecule found by the analytical instrument? (Y/N)	Y
Analytical Type	Type of analytical technique used to detect the purity. A file may also be uploaded to be associated with the sample.	UV

Add Analytical Type Information

To add analytical type information:

1. In the Analytical Type field, click **[+]**.
2. Select an **Analytical Type** from the drop-down list.
3. Click **Choose File or Browse** and browse for an analytical file to attach to the sample.
4. Click **OK** to exit the dialog.
5. Click **Save** to save the single registration entry.

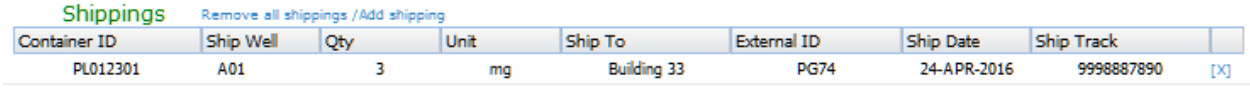


Dialog for entering analytical type information to a container ID

Add Shipping Information

To add shipping information:

1. Click **Add Shipping** beneath the appropriate sample.
2. (Optional) Enter required information in **Container ID**.
3. (Optional) Enter information into other fields if necessary (described in the table below).
4. Multiple lines of shipping information for a sample can be added. Click **Add Shipping** and repeat the above steps.
5. Click **Save** to save the single registration settings.



Shipping information for a single registration

Shipping Fields

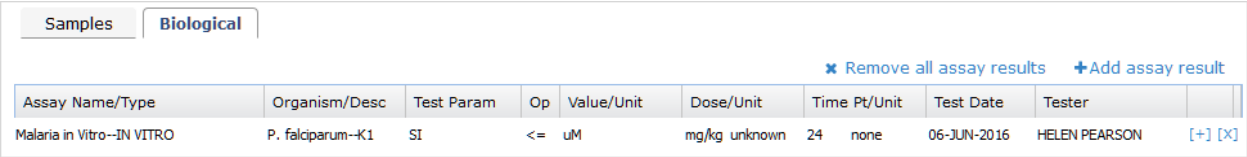
Field	Details	Example
Container ID	Identifier of the container that is used to store the compound in (for example, vial number, plate number).	PL012301
Ship Well	Well position in a 96-well plate or other kind of plate. If not applicable for a compound, leave blank. Plate size can be adjusted by clicking the "96".	A01
Qty	Quantity of the sample.	3
Unit	Unit for the above quantity.	mg
Ship To	Free text field to indicate where the sample was shipped.	Lab 400
External ID	Any additional IDs for the shipping (e.g. Vendor ID, Partner ID). If entering more than one, separate with commas.	PG74
Ship Date	Shipping date (format: DD/MMM/YYYY).	03/DEC/2010
Ship Track	Tracking number of the carrier (e.g. FedEx tracking number).	1234578900

Add Biological Data

Use the Biological tab to add biological data for the compound/batch that is getting registered.

To add biological data:

1. Click the **Biological** tab located below the Single Registration fields.
2. Click **Add assay result**. A new record is added in the Biological tab.
3. Enter biological data for the record in the fields (described in the table below).
4. Multiple new records can be added. Click **Add assay result** and repeat the above steps.
5. Click **Save** to save the single registration settings.

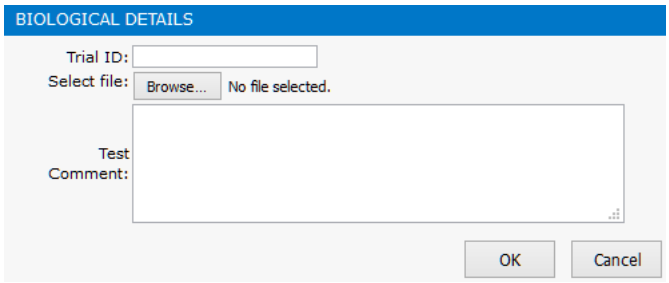


New biological data for the record

New Biological Data Fields

Field	Details	Example
Assay Name/Type	Name and type of assay. All available assays for the project are displayed in a drop-down list.	Malaria--In vitro
Organism/Desc	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

Field	Details	Example
Test Param	Authorized test parameters. All available test parameters are displayed in a drop-down list.	`% inhibition` `IC50`
Op	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. If a Unit is not selected, "none" will be automatically assigned. **Note:** It is important to separate the Value from the Operator to keep the Value numeric and allow further sorting and filtering within ScienceCloud.	`0.5, uM`
Dose/Unit	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	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`
Tester	(Optional) Select a name from the drop-down list. If left blank, a value of "Unknown Unknown" will be automatically assigned.	`Bob Nare`

[+]	Opens a dialog for uploading a Trial ID, file associated with the test value data point, and a Test Comment (described below).
	 
	
	Dialog to upload a file
		`SOPMALVT1`
		`StudyReport.pdf`
		`Activity to be confirmed`

Appendices

Appendix A: Registration Fields for Chemical Data

The following table provides information about all fields used by chemical data registration files.

Chemical Data Registration Fields

Field Name	Description	Format	Example
analytical_type	Type of analytical technique used to detect the purity; controlled by the Team dictionary	Char (20 max)	`UV`
batch_comment	Text field for adding information relevant to the screener.	Char (500 max)	`Poor solubility`
batch_group_id	Registers the compound to a ScienceCloud project batch group.	Char (35 max)	`OXAZOLE`
batch_id	Batch ID for the new batch. Must be unique within your Team in ScienceCloud. **Notes:** • Multiple Batch IDs are allowed per Batch. Use commas to separate multiple Batch IDs. • This field is not required with projects that auto-generate Batch IDs.	Char (50 max)	`PCUCT01-0002`
batch_tag	Adds other IDs to the batch (e.g., Vendor ID, Partner ID). Use commas to separate multiple batch tags.	Char (50 max)	`PG74`
compound_comment	Textual description of the compound.	Char (500 max)	
compound_id	Compound ID. If this field is present, ScienceCloud uses it instead of	Char (50 max)	`SCYX0012344`

Field Name	Description	Format	Example
	automatically generating the compound ID. It must be unique in the system.		
compound_name	Chemical name of the compound.	Char (500 max)	`Diethylcarbamazine`
compound_status	Status of the compound; controlled by the Team dictionary.	Char (50 max)	`Active`
compound_status_comment	Textual description of compound status.	Char (500 max)	
compound_tag	Any other IDs to be associated with the compound (e.g., Vendor ID, Partner ID). Use commas to separate multiple compound tags.	Char (50 max)	`XYZ980`
compound_type	Compound type (C, S, LO, or LG); controlled by the Team dictionary	Char (100 max)	`C`
Concentration	Concentration of the batch.	float	`10`
concentration_unit	Unit for the above concentration quantity.	Char (10 max)	`mg/ml`
container_id	Identifies the container used to store the compound (e.g., vial number, plate number).	Char (50 max)	`PL012301`
exact_mass	Exact mass of the compound.	float	`340`
initquantity	The initial quantity of the material contained in a vial or well.	float	`7.5`

Field Name	Description	Format	Example
location	Location of a sample.	Char (50 max)	`Lab 400`
molecular_formula	Molecular Formula of the molecule. If a chemical structure is included in the registration, leave the molecular formula field blank and it will be automatically calculated from the structure.	Char (no limit)	`C18H26CIN3`
molecular_weight	Molecular weight of the sample. If a chemical structure is included in the registration, leave the molecular weight field blank and it will be automatically calculated from the structure.	float	`234.34`
ms_comment	Text field that can be used to list adduct(s), protonation, and other MS-related comments.	Char (500 max)	`M+H`
ms_found	Was the mass of the molecule found by the analytical instrument? (Y/N)	Char (1 max)	`Y`
ms_result	The mass observed by the analytical instrument (Mass Spec.).	float	`318`
plate_format	Format of the plate the sample is stored.	Char (5 max)	`144`
Project_id	Registers the compound to a ScienceCloud project.	Char (50 max)	`P027`
purity	Purity of the sample in % as determined by	float	`90`

Field Name	Description	Format	Example
	a standard analytical technique (e.g., HPLC/UV, HPLC/MS).		
purity_comment	Text field that can be used to enter an analytical comment.	Char (500 max)	`Purity by NMR`
quantity	Quantity of the sample.	float	`3`
regis_date	Uses batch registration date, instead of data registration date within ScienceCloud.	date	`03/12/2010`
rt	Retention time (in minutes).	float	`2.5`
salt_coeff	Number of occurrences of the salt.	Char (30 max)	`2`
salt_name	Name of the salt. Must be present in the Team's Salt Dictionary prior to registration.	Char (60 max)	`Hydrochloride`
scientist	Assigns the compound to a scientist based on the scientist's ScienceCloud username. If blank, the username of the person registering the file is automatically assigned.	Char (50 max)	`BSMITH`
ship_container_id	Shipping Container ID.	Char (50 max)	`SHPLATE01`
ship_date	Shipping date (MM/DD/YYYY).	date	`03/12/2010`
ship_external_id	Shipping External ID.	Char (100 max)	`XID12`

Field Name	Description	Format	Example
ship_plate_format	Format of the plate the shipped sample is stored.	Char (5 max)	`144`
ship_quantity	Shipping quantity.	Float	`4.5`
ship_to	The name of the shipping recipient. This must be a valid ScienceCloud login username.	Char (50 max)	`JGRANT`
ship_track_no	Tracking number of the carrier (e.g., FedEx tracking number).	Char (35 max)	`1234578900`
ship_unit	Shipping quantity unit.	Char (10 max)	`mg`
ship_well	Well position in a shipping plate. If not applicable, leave blank.	Char (5 max)	`A01`
smiles	Smile string structure. This field is only used for text files.	Char	`CH4`
stereo_designation	Text field for comments about compound stereochemistry.	Char (100 max)	`R isomer`
trivial_name	Trivial name of the compound.	Char (500 max)	`Diethylcarbamazine citrate,1642-54-2`
unit	Unit for the above quantity.	Char (10 max)	`Mg`
well	Well position in a 96-well plate or other kind of plate. If not applicable for a compound, leave blank.	Char (5 max)	`A01`