

ScienceCloud Project Data

Analytical Type File Registration Guide

Summary: The following information explains how to associate an Analytical Type file with a sample within ScienceCloud.

Covered Topics

Analytical Type File Registration.....	2
Analytical type file information	2
Register Analytical Type Files in Project Documents	2
Analytical Type Reference Lookup.....	3
Upload Analytical Type Files.....	3
Remove Analytical Type Files Associated with a Container ID	5

Analytical Type File Registration

The following information explains how to associate an Analytical Type file with a sample within ScienceCloud.

Analytical Type files can be found when looking at a batch in Singular View in the Analytical section under the "Analytical Type" header.

First Previous Next Last Print Close Window

C O M P O U N D	IDs	SCYX0000902984					
	Tags						
	Exact Mass	379					
	Molecular Weight	312.412994					
	Molecular Formula	C19 H24 N2 O2					
	Type	Compound					
	Status						
	Name	Praziquantel					
	Trivial Name						
	Comments						
	Stereo Designation						
	Status Comment						

O=C1CC2(CCN1C(=O)C3CCCCC3)CC4=CC=CC=C42

SC-CPD-1070383
SC-BAT-635697

IDs	Tags	Salt	Project ID/Batch Group	Scientist	Registered Date Reporting Date	Registered By
SP-0052					26-JUN-2007	
002MPE001AA4B3		1 Hydrochloride (MW: 36.46)	P027/002MPE001A	Bob Jacobs	26-JUN-2007	D E M O
SP-0053					26-JUN-2007	
PRAZIQUANTEL	SP-006	None	P027/STANDARDS	Bob Jacobs	26-JUN-2007	D E M O

Share (9)

Calculated Physchem Properties

Analytical Show Comments (1)

Sample SCID	Container ID	Well	Location	RT	Purity	Quantity	Init Quantity	Conc	MS Result	MS Found	Analytical Type
SC-SMP-2343918	PLT-002	H04		1.3 (min)	100	5.6 (mg)	5.6 (mg)		380	Y	UV MS

Shipping

PK

Biological & ADMET

Analytical file types displayed for a batch in Singular View

Analytical type file information

The two possible methods for associating a file with a sample include:

- [Register Analytical Type files in Project Documents](#)
- [Upload Analytical Type files through Edit | Chemistry](#)

Register Analytical Type Files in Project Documents

To register an Analytical Type file in Project Documents, the file name must be built using the following naming convention:

```
<Team Name, Team ID or Project ID> + "$" + <Batch ID> + "$" + <Analytical Type> + "$" + <Container ID> + "$" + <Well> + "$" + <some name>.<file extension>
```

Naming Convention Examples

Type of File	Naming Convention
Team Name used, Container/Well omitted	BIOVIA\$EX0000031\$HPLC\$MyFile2HPLC.pdf
Project ID used, Container/Well omitted	P027\$EX0000031\$HPLC\$MyFile2HPLC.pdf
Project ID used, Container/Well included	P027\$EX0000031\$NMR\$Plate0001\$A01\$MyFile1NMR.pdf

☑ Tips:

- Container ID and Well are optional for batches that only contain one sample.
- If multiple samples are present for the batch, then Container ID and Well are required in your file naming convention.
- After the file is properly named, it can be submitted like a registration file in a Chemistry Smart Folder in Project Documents.

Analytical Type Reference Lookup

A complete list of all available Analytical Types is available online. This list is team-specific.

To access the list of analytical types online:

1. Select **Project Data** application from dashboard.
2. Select the **New Data Entry** menu.
3. In the section "Register Multiple Analytical Type Files", click **Show Details**.
4. Select **Available Analytical Types**.

The screenshot shows the 'Register Multiple Analytical Type Files' page in the ScienceCloud interface. The page includes a 'Hide Details' button, an 'Instructional Video' icon, and a list of instructions for registering files. A button labeled 'Available Analytical Types' is highlighted with an orange box and a mouse cursor. An inset window shows the 'Available Analytical Types' table with the following data:

Name	Code
CERTIFICATE OF ANALYSIS	COA
DUAL CHANNEL UV	UV
HPLC	HPLC
LCMS	LCMS
NMR Generic	NMR
PD	PD
PK	PK
QUADRAPOLE MS	MS
TRACE FOR ELSD	ELSD
UNKNOWN	UNKNOWN

Upload Analytical Type Files

If your account is activated for Edit permissions, you can load analytical type files on the Single Edit page.

To upload an analytical type file:

1. Perform a search for the batch and/or Container ID to associate with the analytical type file.
2. When the appropriate batch is displayed on the Results tab, select the **corresponding check box** at the left side.
3. From the **Edit** drop-down list, select **Chemistry** to open the Single Edit page.

Search Results

Structure Assay Results

Open in: SAR Table Tasks Export Edit Save Hit List New Query

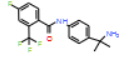
Page 1 of 1 Results: 10 30 50 Biology ounds: 1 1 batches selected Sort By: Relevance View: 1 2

PCCRO16-0215 013RAN02 Melody (ChemServices) (4) ★ 👍 (5)

SCYX0001735507

COMPOUNDS-P028-03 (P028-03)

IC50 = 0.207 ug/mL • enzym1 • Eff-SecA 12-Aug-2011



Edit > Chemistry option for selected batch

- In the **Samples** section at bottom of page, locate the sample **Container ID** to associate with the analytical type file (if there is more than one sample).

Samples Biological Remove all samples Add sample


Container ID	Well	Location	RT	Conc	Conc Unit	Purity	Init Qty	Qty	Unit	MS Result	MS Comment	MS Found	Analytical Type																										
PLT-002	H04	96	1.3			100 UV	5.6	5.6	mg	380	M+H	Y	View [-] [+] [X]																										
<p>Shippings Remove all shippings / Add shipping</p> <table border="1"> <thead> <tr> <th>Container ID</th> <th>Ship Well</th> <th>Qty</th> <th>Unit</th> <th>Ship To</th> <th>External ID</th> <th>Ship Date</th> <th>Ship Track</th> </tr> </thead> <tbody> <tr> <td>SC-SHP-492227</td> <td>SH102</td> <td>29</td> <td>96</td> <td>3.2</td> <td>mg</td> <td>BNARE</td> <td>15-MAR-2007</td> <td>[X]</td> </tr> <tr> <td>SC-SHP-627094</td> <td>SH202</td> <td>30</td> <td>96</td> <td>4</td> <td>mg</td> <td>BSCORNEAUX</td> <td>01-MAY-2007</td> <td>[X]</td> </tr> </tbody> </table>														Container ID	Ship Well	Qty	Unit	Ship To	External ID	Ship Date	Ship Track	SC-SHP-492227	SH102	29	96	3.2	mg	BNARE	15-MAR-2007	[X]	SC-SHP-627094	SH202	30	96	4	mg	BSCORNEAUX	01-MAY-2007	[X]
Container ID	Ship Well	Qty	Unit	Ship To	External ID	Ship Date	Ship Track																																
SC-SHP-492227	SH102	29	96	3.2	mg	BNARE	15-MAR-2007	[X]																															
SC-SHP-627094	SH202	30	96	4	mg	BSCORNEAUX	01-MAY-2007	[X]																															

Single Edit page for selected batch

- The **Analytical Type** column at the right side of the Container ID row displays a View feature for working with analytical type files. To add a file, click the **[+]** icon.

Analytical Type

View [-] [+] [X]



Features to work with analytical type files

- At the dialog box that opens, select the appropriate **Analytical Type** from the drop-down list, and then browse for your analytical type file.

ADD ANALYTICAL TYPE TO CONTAINER ID: CLOUD0001239

Analytical Type **File**

UNKNOWN No file selected.

Browse for and select analytical type files Click OK to upload the file and close the dialog.

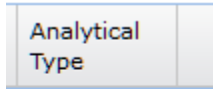
- Click **OK** to save your changes to the batch.

Remove Analytical Type Files Associated with a Container ID

You can remove analytical type files that were previously associated with a Container ID.

To remove a file:

1. From the Analytical Type column at the right side of the Container ID row, click the [-] icon for the View feature.

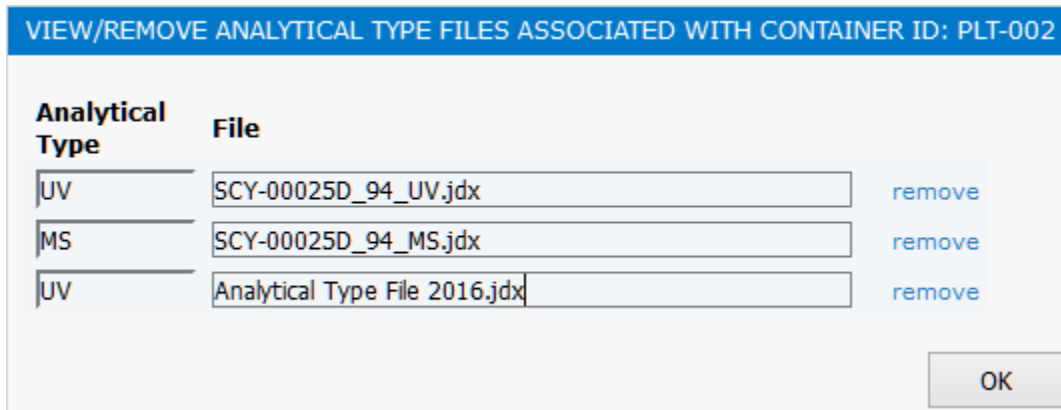


View [-] [+] [X]



Features to work with analytical type files

2. From the dialog that opens, click **Remove** on the line item for the file to remove.
3. At the prompt, click OK to confirm that you want to remove the file.
4. Click **Save** at the top of the page to save changes.



Remove analytical type files