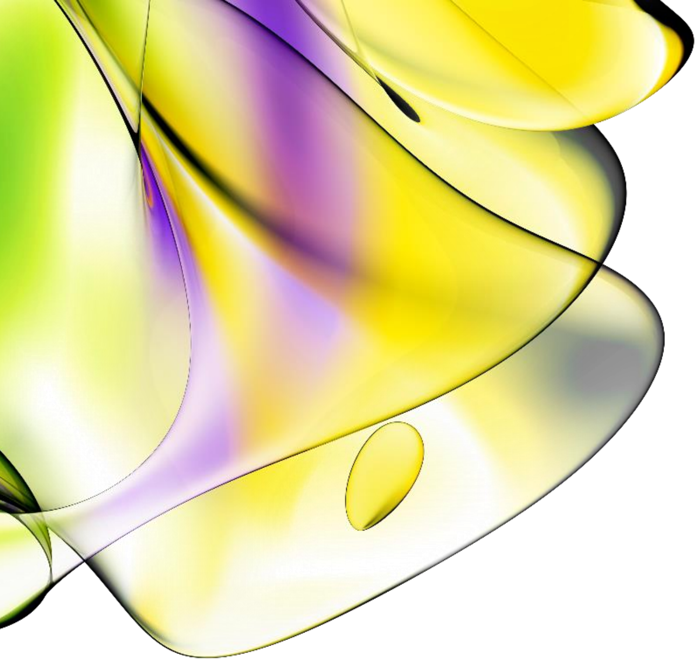


Revvity Signals Inventa^{TM} 3.5.1

User Guide

Powered by Spotfire®

Last Updated: April 12, 2024

Table of Contents

1 Introduction

Signals Inventa^{TM} powered by the Signals Data Factory and Spotfire® empowers scientific professionals to readily access the scientific data the need to discover better drugs faster. Through Revvity Signals proprietary Signals Data Factory, structured and unstructured scientific data are normalized and contextualized such that it can be discovered by Signals Inventa^{TM} scientists in an intuitive and efficient workflow. Through Spotfire, those data are automatically presented in a well-organized SAR workflow that encourages data exploration and drug candidate assessment.

Moreover, Signals Inventa^{TM} includes features to drive the full life-cycle of data. Data Generators (scientists who are actively performing assays and publishing the processed results of those assays) can more easily publish their data with the confidence that those data will be discovered and re-used by the project teams. Data consumers (scientist, project lead, med chemist who need to analyze aggregated data across assays) can dedicate their time to understanding the science rather than painstakingly assembling data.

For Data Generators Signals Inventa^{TM} enables:

- Definition of how their data should be captured and represented.
- Upload data from flat files and Spotfire or integrate data from existing data sources.
- Definition of reusable data mappings such that data from regular protocols upload easily.
- Data verification and validation.
- Fine-grained data set management.

For Data Consumers Signals Inventa^{TM} enables:

- Point-and-click data discovery.
- Real-time feedback of what structures and data matches the defined query criteria.
- Direct integration between search and analysis in all versions of Spotfire® (Spotfire Analyst, Business Analyst and Consumer).
- Create complex nested queries and interrogate any subset of the stored data of interest.
- Query over Structure, any compound attribute, and any assay or measurement, and query over an expanded set of comparison operators.
- Control system performance directly by choosing estimated vs. precise query result counts at different levels of precision.
- Save queries for easy re-use. Saved queries can be public or private.

Note: Configurable entity names (e.g. Compound/Batch, Antibody/Lot) allow Signals Inventa assets/instances to be more meaningful. The model is configured by the System Administrator during system configuration. Only one name pair per Signals Inventa instance. Refer to the Signals Inventa Installation Guide for more information.

For the purpose of screenshots, the Compound/Batch model is depicted throughout this User Guide.

1.1 Out-of-the-Box (OotB) Dashboards

Signals Inventa is a flexible and powerful tool for decision analytics. Analytics dashboards and their underlying data schema are highly configurable by users. **Out-of-the-Box (OotB) Example Data** is provided which can be used to recreate the pre-configured **OotB Dashboards**. The Quick Start Guides will take users step-by-step through generating an example dashboard containing the most-frequently used visualizations. To follow the Quick Start

Guides, ensure that the example data is loaded. The guides and the example data can be downloaded from the Signals Inventa Online Help (Example Data Tutorials Quick Link).

The Quick Start Guide is divided into 3 main sections: Beginner, Intermediate, Advanced, with each building on details of the previous sections. The guide can be followed chronologically, or users can skip specifically to those sections most relevant to their workflows. Some tutorials can be completed in under 5 minutes. Previous knowledge of Spotfire or Signals Inventa is not required, so even brand-new users should feel enabled to follow topics in the Advanced section.

Beginner Dashboard (~15 mins)

- This Beginner Dashboard will teach users to query data using Global Search, generate a SAR table, generate a dose response curve for a reported IC50, and analyze the correlation between two related inhibition assays. The inhibition data in this dashboard was produced using the OotB 4P Dose-Response IC50 Assay Workflow from Signals VitroVivo. The following topics and common questions are addressed:

Loading the OotB Example Data with Global Search
 How can I query all assay data related to any of my compounds so I can generate a SAR table?
Creating a SAR Analysis with the OotB Example Data
 How can I customize a SAR table to only show certain assays, and have it update with the latest data?
Building Well Level Details using OotB Example Data
 How can I build a visualization that represents IC50 data and its corresponding dose response curve data?
Building Assay Correlations using the OotB Example Data
 How can I plot the performance of two related assays and calculate the ratio between them?

Intermediate Dashboard (~25 minutes)

- This Intermediate Dashboard builds upon the beginner dashboard and expands it by teaching users how to configure SAR table and Measurement table views, as well as leverage common Chemistry tools such as substructure searching, scaffold extraction, and R-group decomposition. The following topics and common questions are addressed:

Customizing the SAR Analysis for OotB Example Data
 How can I view data in the SAR table based on Batches instead of Compounds?
 How can I color code assay results in the SAR table so I can quickly identify actives?
 How can I view the individual assay values alongside aggregated value sin my SAR table?
Customizing Well Level Details using the OotB Example Data
 How can I use my own values to generate a dose response curve rather than using Spotfire automatic curve fit?
Chemistry Calculations using the OotB Example Data
 How can I calculate physical properties of my compounds?
 How do I perform a structure or substructure search on an existing data table?
 How can I identify compounds in a series by extracting a common scaffold?
 How can I compare properties and activities of compounds that are related by a conserved core?

Advanced Dashboard (~35 minutes)

- This Advanced Dashboard is designed to teach data stewards how to define entity and measurement data schemas, and to teach assay scientists how to load and standardize their assay results. The visualizations in this dashboard build upon the intermediate dashboard and expand upon it by introducing powerful, but less-frequently used configurations. The following topics and common questions are addressed:

Loading Entity Data into Signals Data Factory (Data Administrators only)

  - *How can I define my own entity and data schema in Signals Inventa (via Signals Data Factory)?*
- Loading Results Data into Signals Inventa
  - *How can I load my own experiment assay data into Signals Inventa?*
- Building a Global Search Query
  - *How can I use Global Search's unified interface to query my newly added entity and measurement data?*
- Customizing the SAR Analysis for the OotB Example Data - Advanced
  - *How can I modify which experimental variables are aggregated in my SAR table?*
  - *How can I add a compound or batch property to my SAR table while limiting the number of columns that are created?*
  - *How can I include standard deviation, count, and other metrics to a SAR table endpoint cell?*
  - *How can I create collections of compounds so I can easily filter to that set and see relationships between sets of compounds?*

Optional Guide: Related Entities (~20 minutes)

- This optional dashboard will teach data administrators how to configure related entities and enable scientists to leverage the relationships with core entities within the Global Search. Refer to the section Search by Related Entity for more information.

Optional Styling Guide (~30 minutes)

- This optional guide will build upon the Advanced Dashboard to add additional flair to visualizations including custom color schemes, text formatting, and gallery form configurations.

OotB Dashboards	Description	Download Supporting Files
Inventa Beginner Dashboard Inventa Intermediate Dashboard Inventa Advanced Dashboard Related Entities Optional Styling Guide	**Out-of-the-Box (OotB) Example Data** is provided which can be used to recreate the pre-configured **OotB Dashboards**.	⤓

If there are additional OotB dashboards or visualizations you would like to see in future releases, please submit them to Revvity Signals Software Ideas Portal for consideration: https://revvitysignals.com/ideas-portal

2 Setting Preferences

Preferences for Signals Inventa can be set to define default values through the Spotfire Administration Manager.

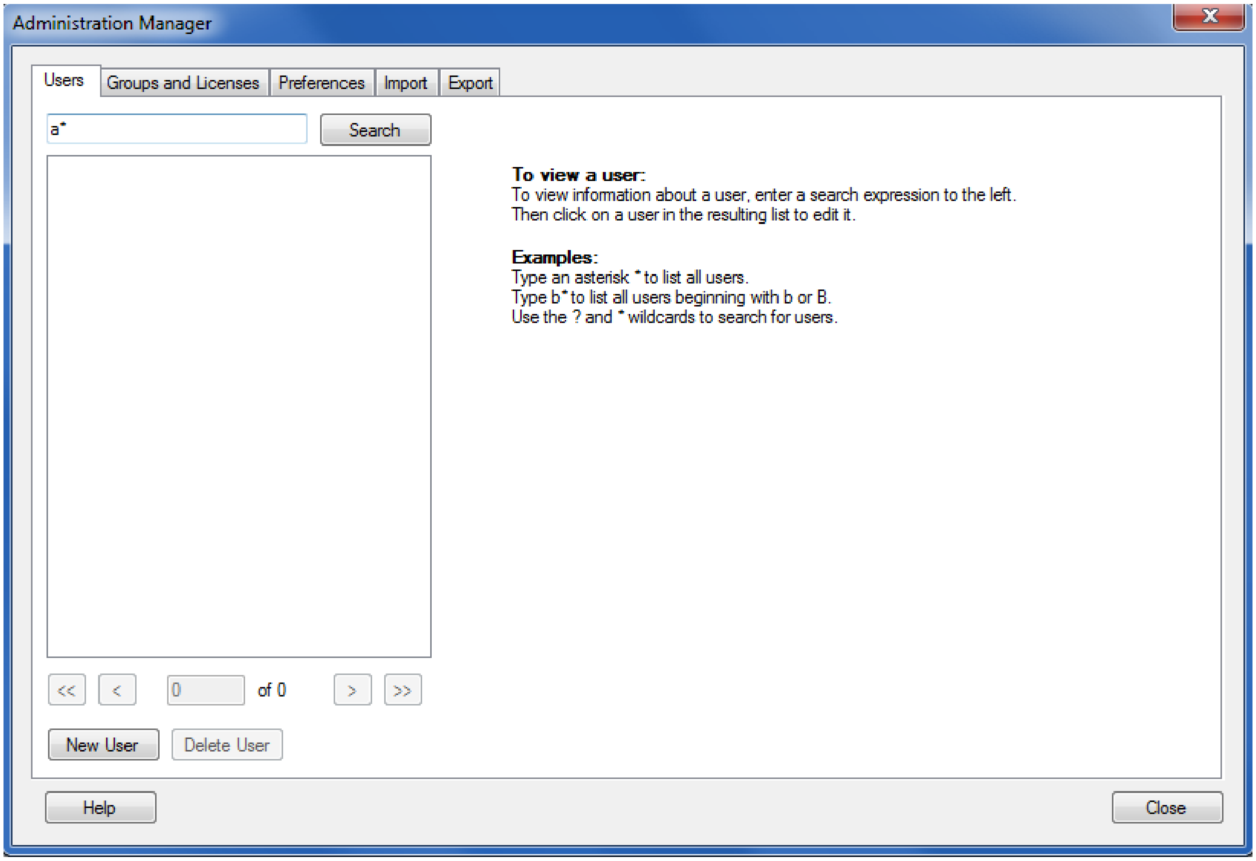
You will need to ensure that the SDF Base URL and Signals Data Factory project name is set as Spotfire preference.

2.1 Accessing the Signals Inventa Preferences

To access the Signals Inventa preferences:

1. Open the Spotfire client, and logon as a Spotfire Administrator. From the **Tools** menu, select the **Administration Manager** sub-menu item. The Administration Manager is only enabled if you logon connected to the Spotfire Server.

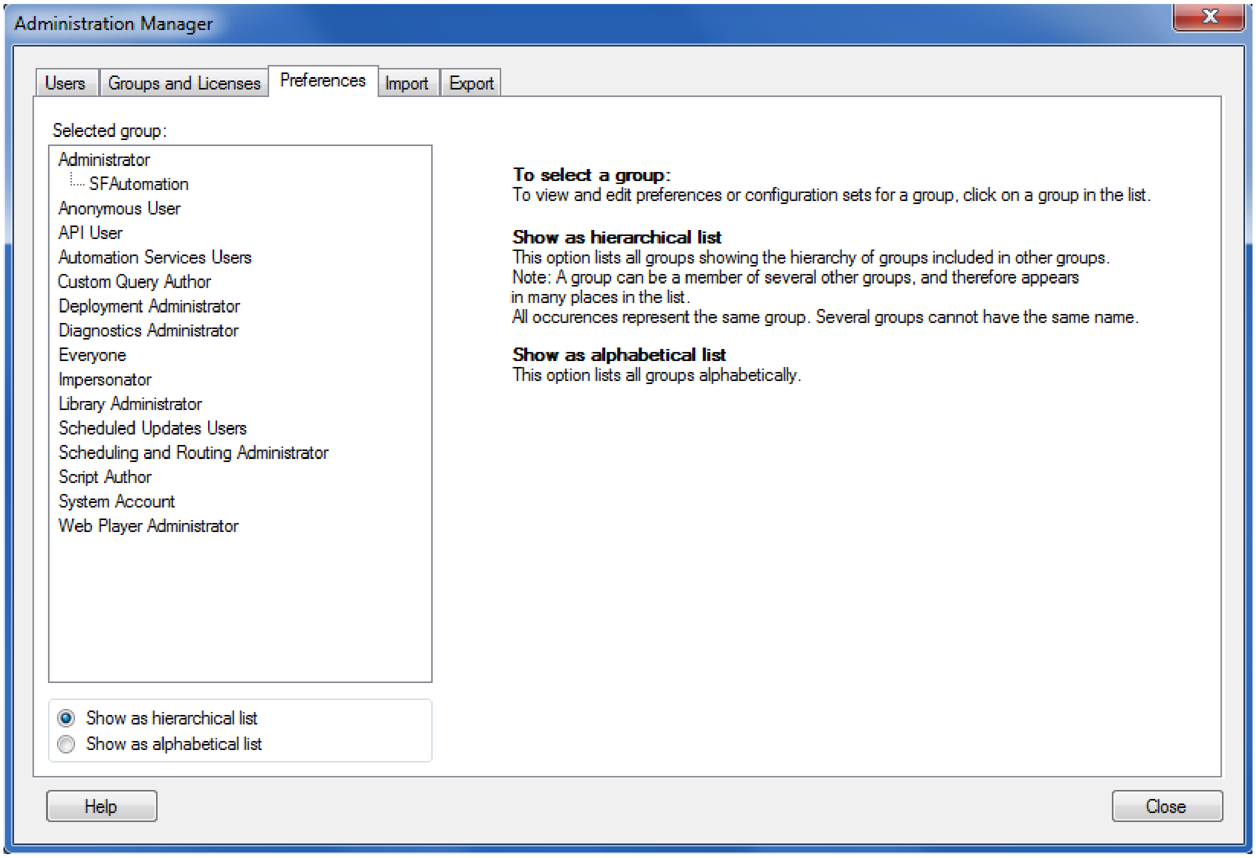
The **Administration Manager** window opens.



To view a user:
To view information about a user, enter a search expression to the left.
Then click on a user in the resulting list to edit it.

Examples:
Type an asterisk * to list all users.
Type b* to list all users beginning with b or B.
Use the ? and * wildcards to search for users.

2. Click on the **Preferences** tab.



Selected group:

- Administrator
  - SFAutomation
- Anonymous User
- API User
- Automation Services Users
- Custom Query Author
- Deployment Administrator
- Diagnostics Administrator
- Everyone
- Impersonator
- Library Administrator
- Scheduled Updates Users
- Scheduling and Routing Administrator
- Script Author
- System Account
- Web Player Administrator

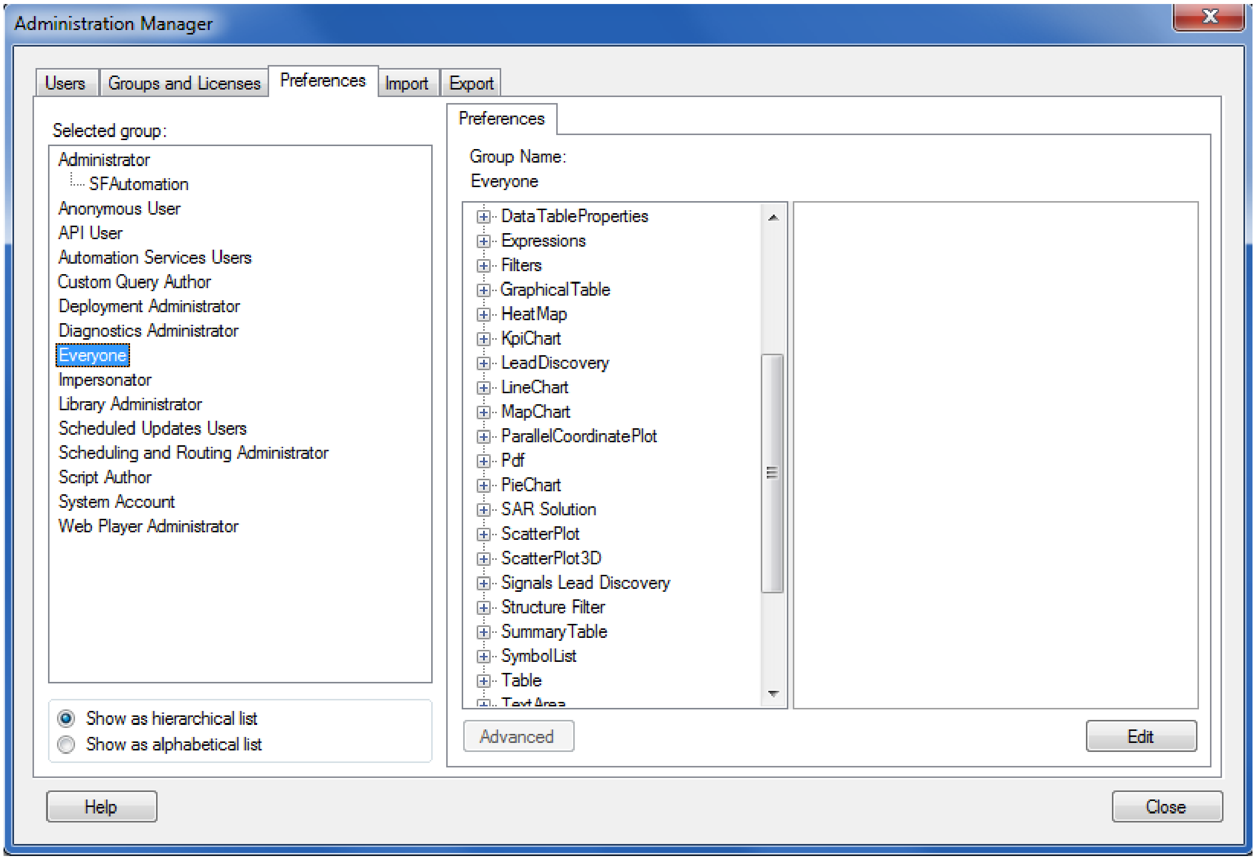
● Show as hierarchical list
○ Show as alphabetical list

To select a group:
To view and edit preferences or configuration sets for a group, click on a group in the list.

Show as hierarchical list
This option lists all groups showing the hierarchy of groups included in other groups.
Note: A group can be a member of several other groups, and therefore appears
in many places in the list.
All occurences represent the same group. Several groups cannot have the same name.

Show as alphabetical list
This option lists all groups alphabetically.

3. Select the Group Name to which the preferences should be applied.



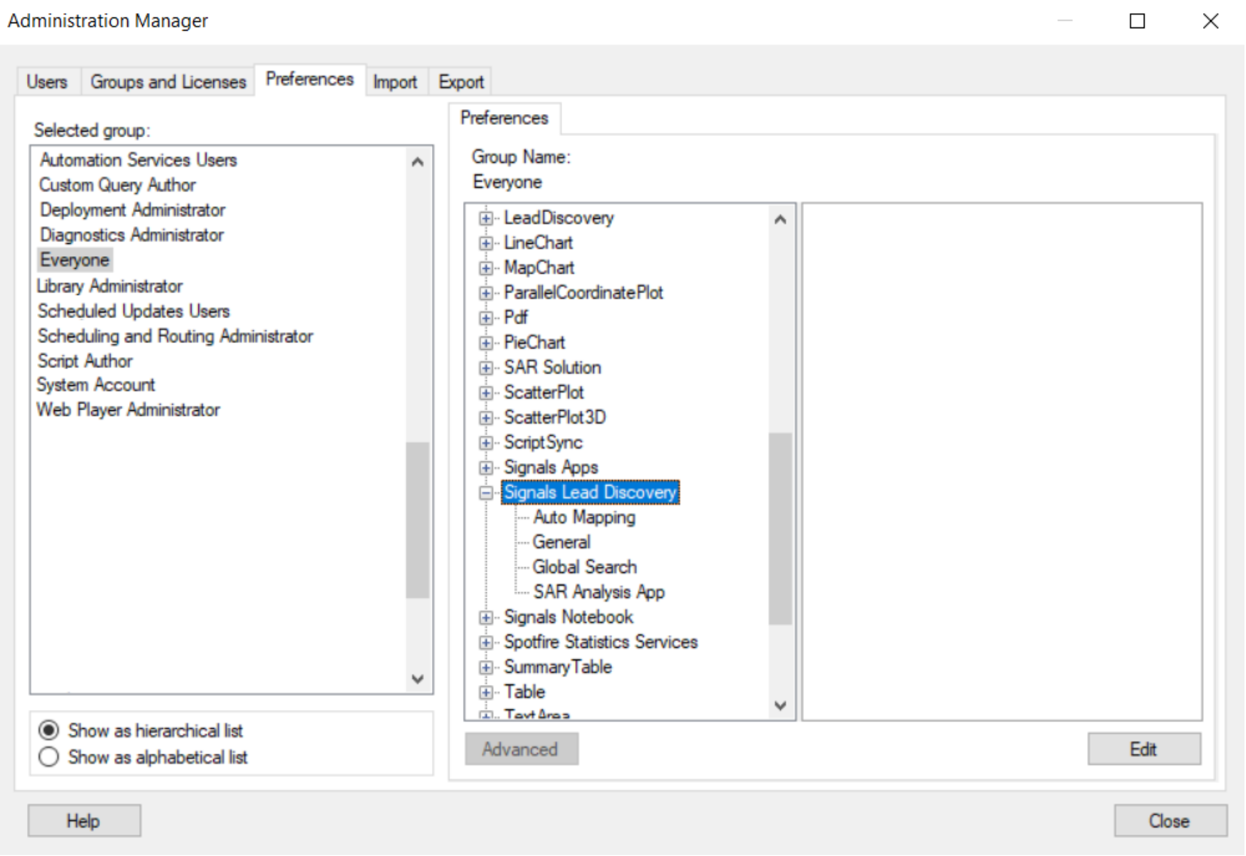
Selected group: Everyone

● Show as hierarchical list

Group Name: Everyone

4. Expand Signals Lead Discovery

Note: For the Signals Inventa 3.5.1 release, the Spotfire preference category name will remain as Signals Lead Discovery.



Group Name:
Everyone

● Show as hierarchical list
○ Show as alphabetical list

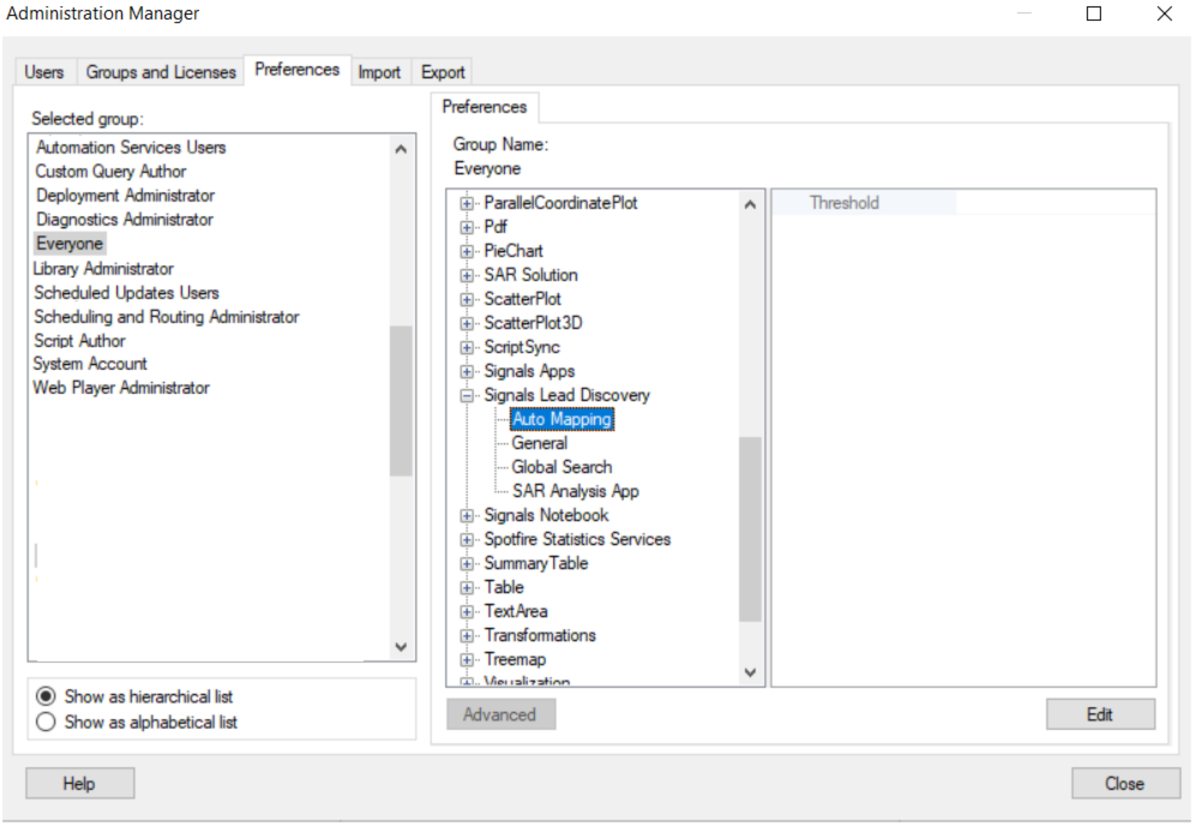
2.2 Setting the Auto Mapping Threshold

The algorithm used in **Auto Mapping** feature of the Publish Measurements tool is dependent on a threshold value to adjust the accuracy of the mapping result. The default value for Auto Mapping is 0.4. If you find that the automapping behavior is too fuzzy or not fuzzy enough, you can modify the threshold for the comparison algorithm in the Spotfire preferences.

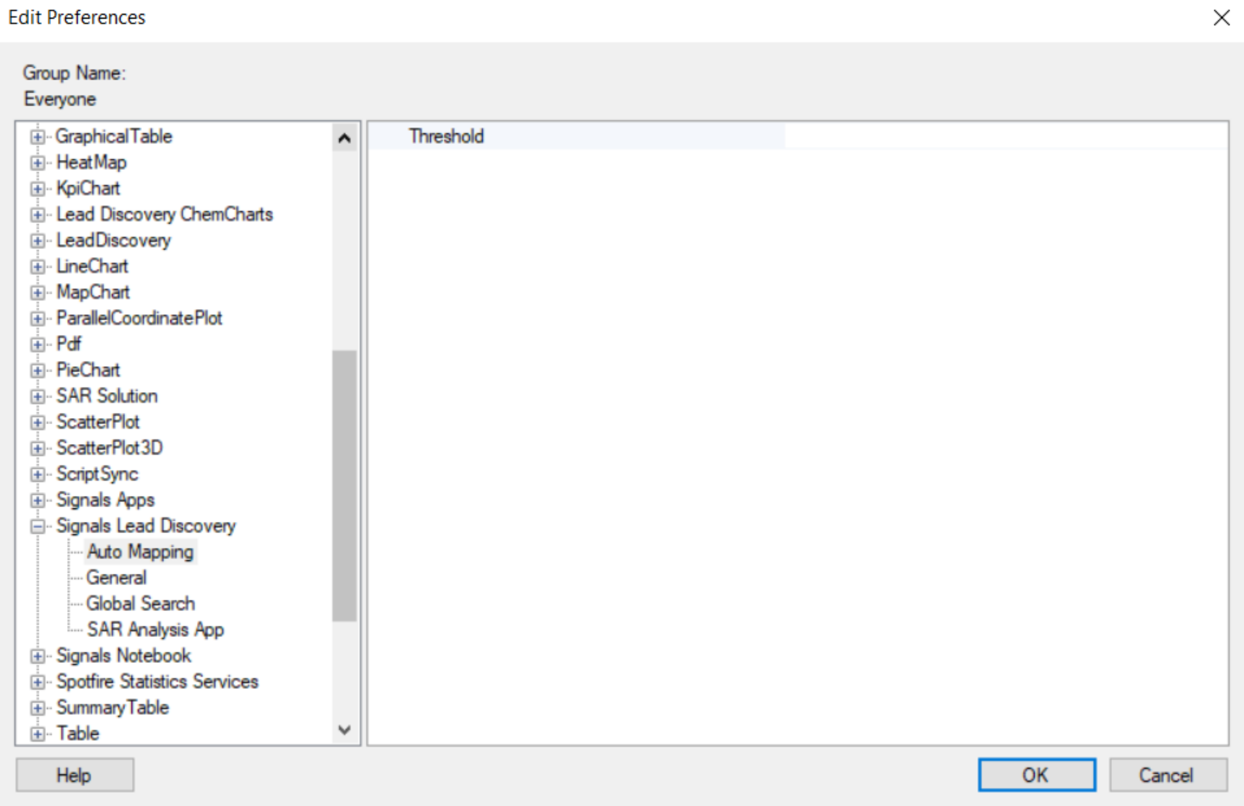
Refer to the section Automapping for information on this feature.

To set the Auto Mapping preference:

1. Access the Signals Inventa preferences via the Administration Manager (refer to Steps 1-4 above - Accessing the Signals Inventa Preferences section).
2. Select **Auto Mapping**.



3. Click on the **Edit** button to open the **Edit Preferences** dialog.



Note: The default value for Auto Mapping is 0.4. However, Spotfire does not display the default value, and therefore the field appears blank.

4. Enter a decimal value to indicate the threshold of string comparison when doing the auto mapping between Measurement Type attributes and Spotfire data table columns. This value should be between 0 (inclusive) and 1 (inclusive), where 0 represents no match and 1 indicates a full match.

5. Click **OK**.

Note: It is recommended that you restart the Spotfire Client in order for the new Preference settings to take effect.

Note: If the Web Player is open, it is necessary to log out and log in again in order for the new Preference settings to take effect.

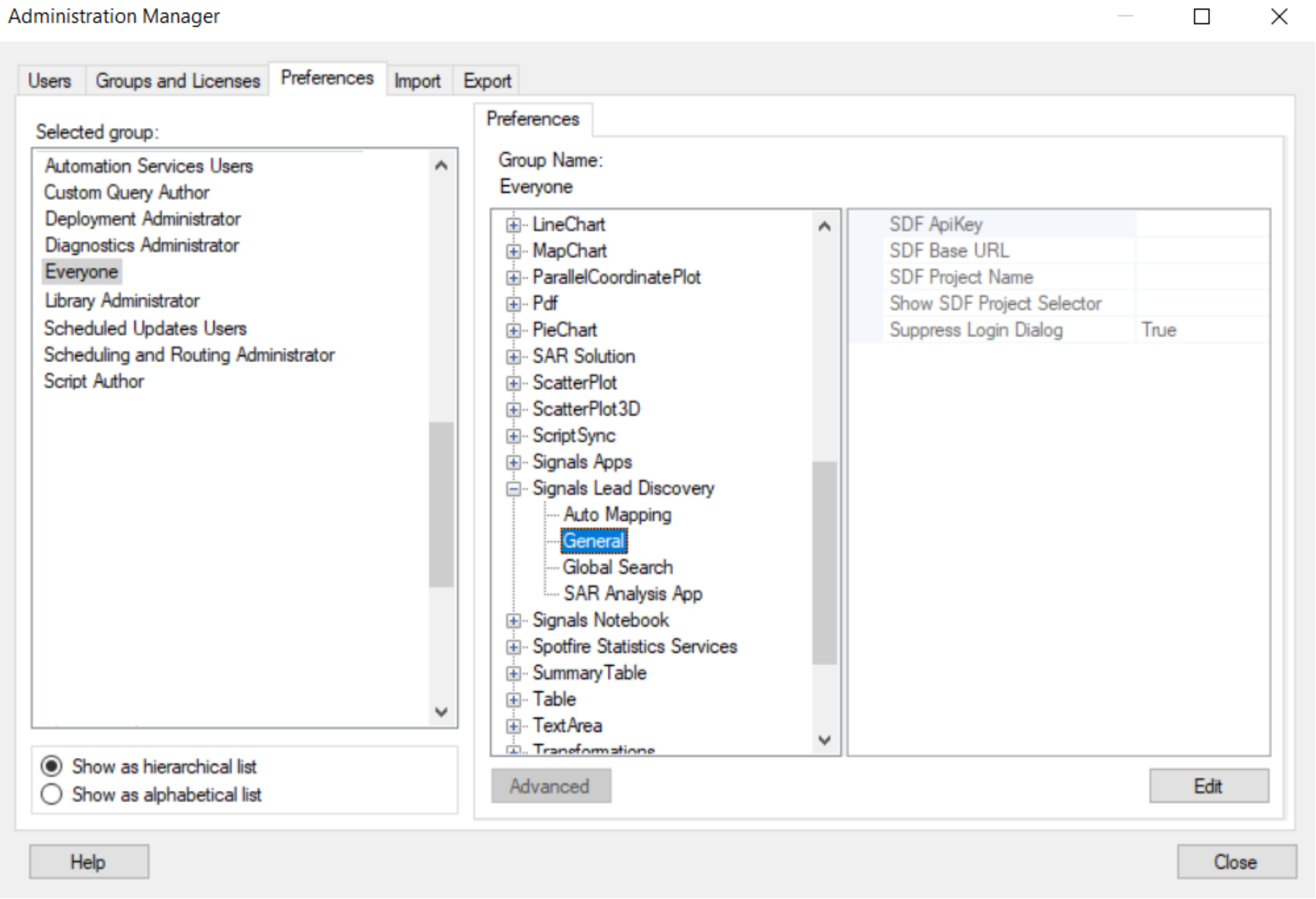
2.3 Setting the SDF ApiKey

Once the **SDF ApiKey** preference is set correctly, users are able to suppress the login dialog by setting the **Suppress Login Dialog** preference to True, so that the API key will be used for authentication and users don't need to provide username and password when using Signals Inventa apps.

Note: Refer to the Manage Users (API Keys) section for information on how to create an API key for a given user.

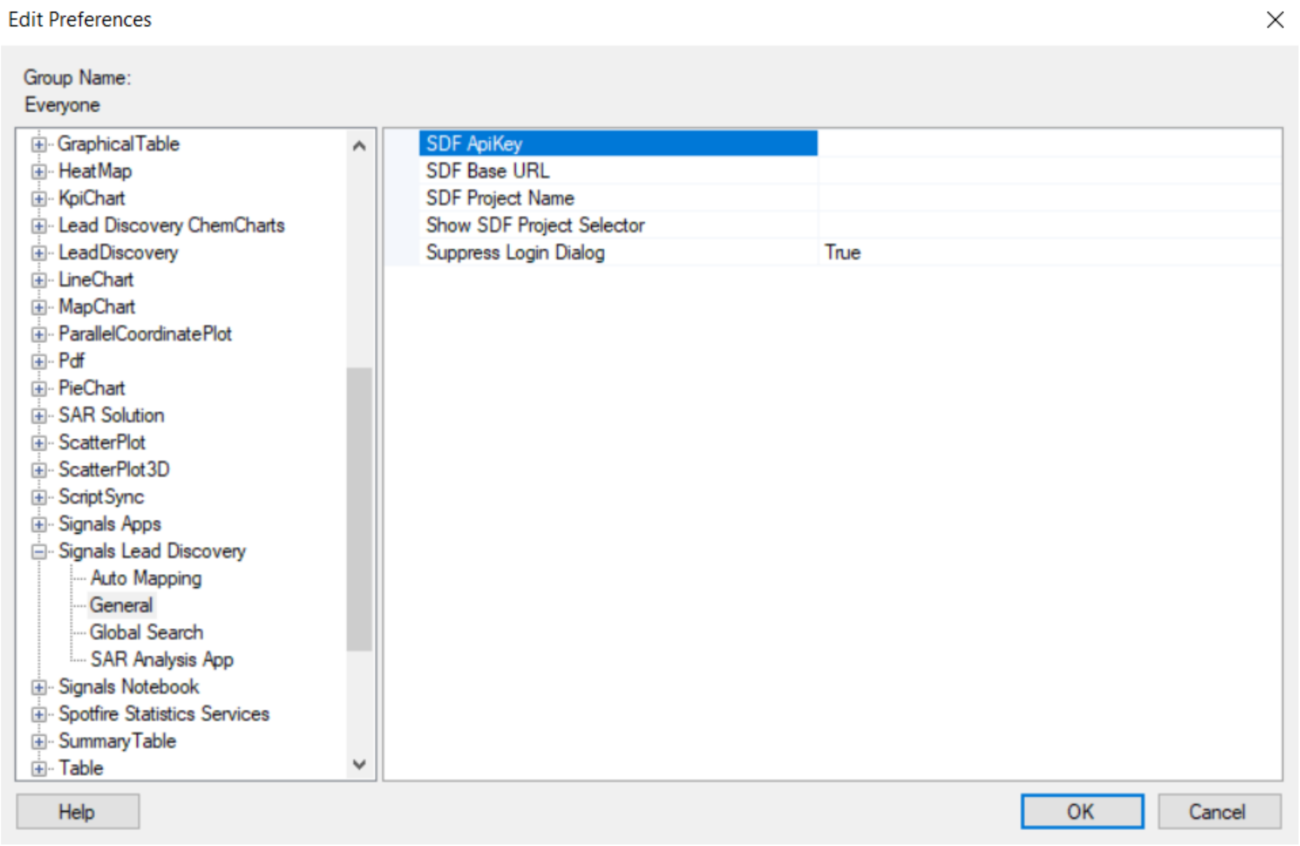
To set the SDF ApiKey preference:

1. Access the Signals Inventa preferences via the Administration Manager (refer to Steps 1-4 above – Accessing the Signals Inventa Preferences section).
2. Select **General**.



SDF ApiKey	
SDF Base URL	
SDF Project Name	
Show SDF Project Selector	
Suppress Login Dialog	True

3. Click on the **Edit** button to open the **Edit Preferences** dialog.



Edit Preferences

Group Name:
Everyone

SDF ApiKey	
SDF Base URL	
SDF Project Name	
Show SDF Project Selector	
Suppress Login Dialog	True

Note: The default value for SDF ApiKey is blank. This option enables Signals Data Factory authentication.

4. Enter the SDF ApiKey for the user.

5. Click **OK**.

Note: It is recommended that you restart the Spotfire Client in order for the new Preference settings to take effect.

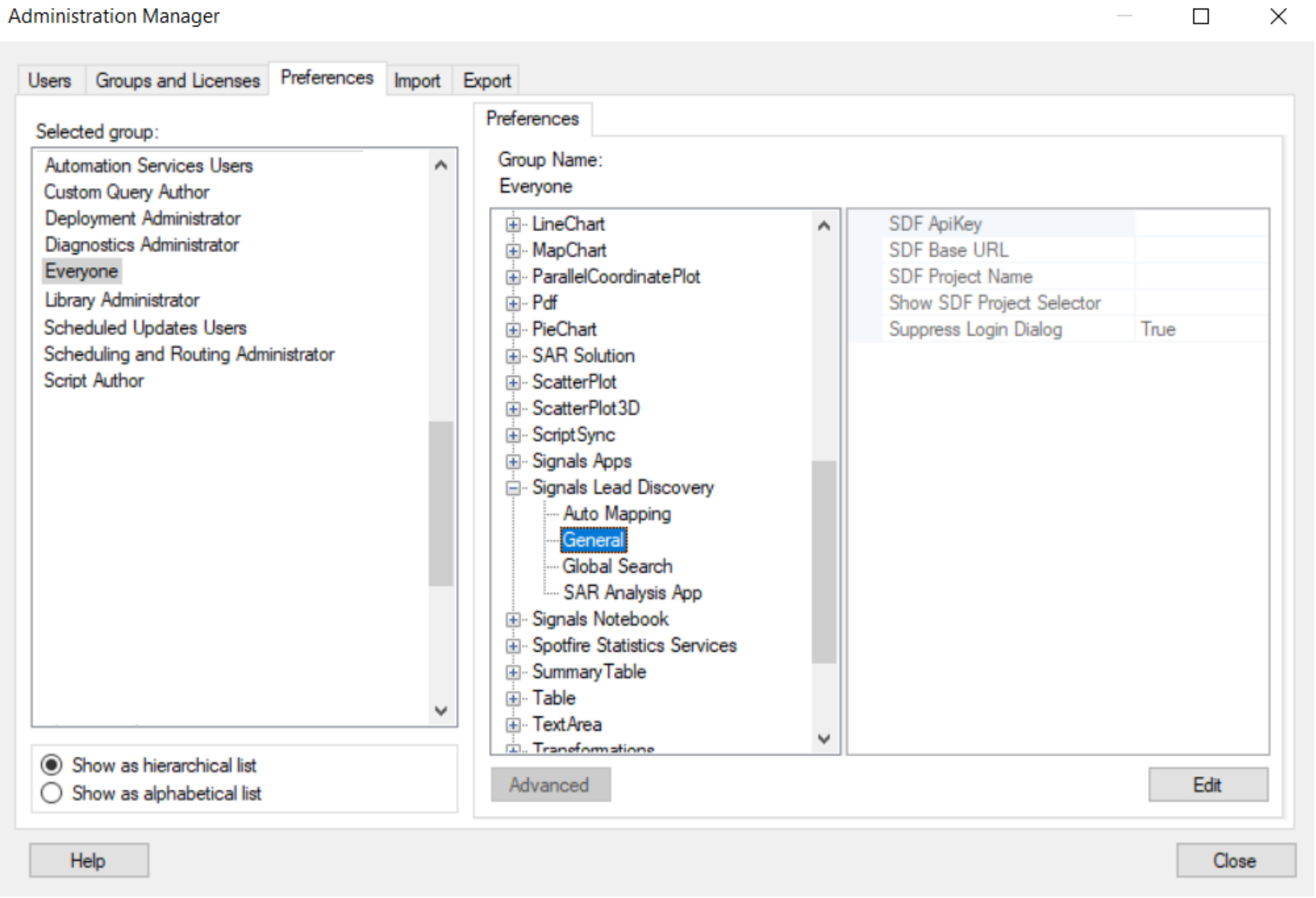
Note: If the Web Player is open, it is necessary to log out and log in again in order for the new Preference settings to take effect.

2.4 Setting the SDF Base URL

To set the SDF Base URL preference:

1. Access the Signals Inventa preferences via the Administration Manager (refer to Steps 1-4 above – Accessing the Signals Inventa Preferences section).

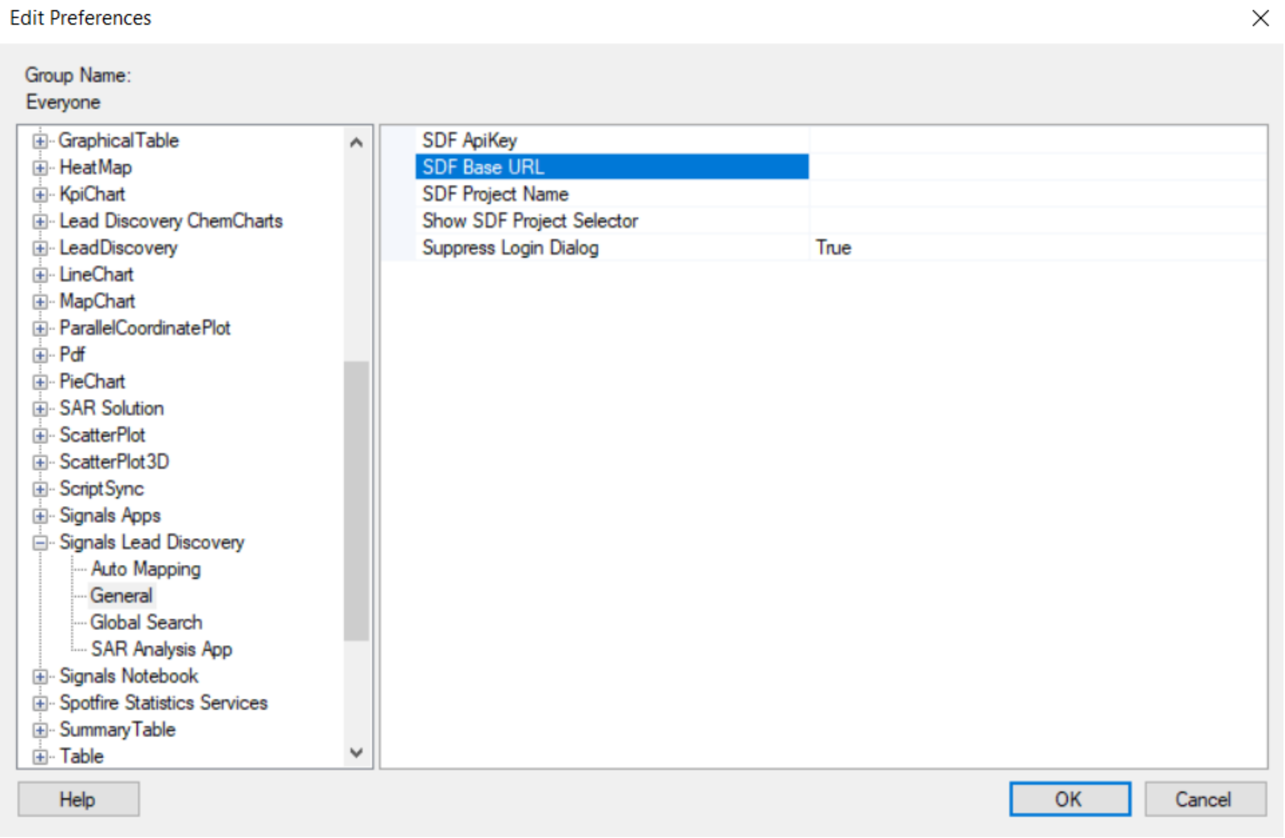
2. Select **General**.



Group Name:
Everyone

SDF ApiKey	
SDF Base URL	
SDF Project Name	
Show SDF Project Selector	
Suppress Login Dialog	True

3. Click on the **Edit** button to open the Edit Preferences dialog.



Group Name:
Everyone

SDF ApiKey	
SDF Base URL	
SDF Project Name	
Show SDF Project Selector	
Suppress Login Dialog	True

Note: The default value for SDF Base URL is “http://localhost ”. However, Spotfire does not display the default value, and therefore the field appears blank.

4. Enter the SDF Base URL.

5. Click **OK**.

Note: The SDF Base URL must begin with “http” or “https”. A host name, an FQDN or an IP address is not a valid setting for this preference.

Note: It is recommended that you restart the Spotfire Client in order for the new Preference settings to take effect.

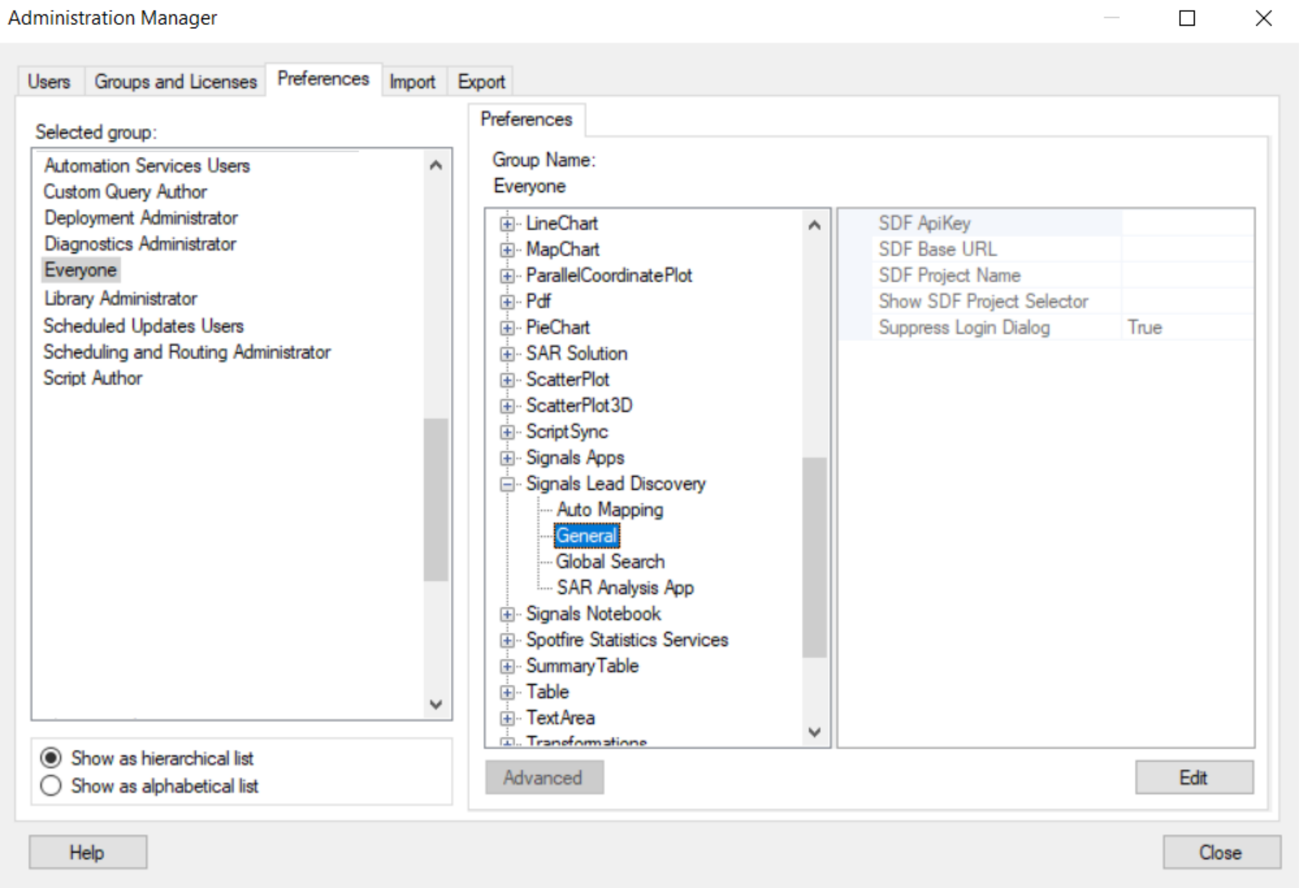
Note: If the Web Player is open, it is necessary to log out and log in again in order for the new Preference settings to take effect.

2.5 Setting the SDF Project Name

To set the SDF Project Name

1. Access the Signals Inventa preferences via the Administration Manager (refer to Steps 1-4 above – Accessing the Signals Inventa Preferences section).

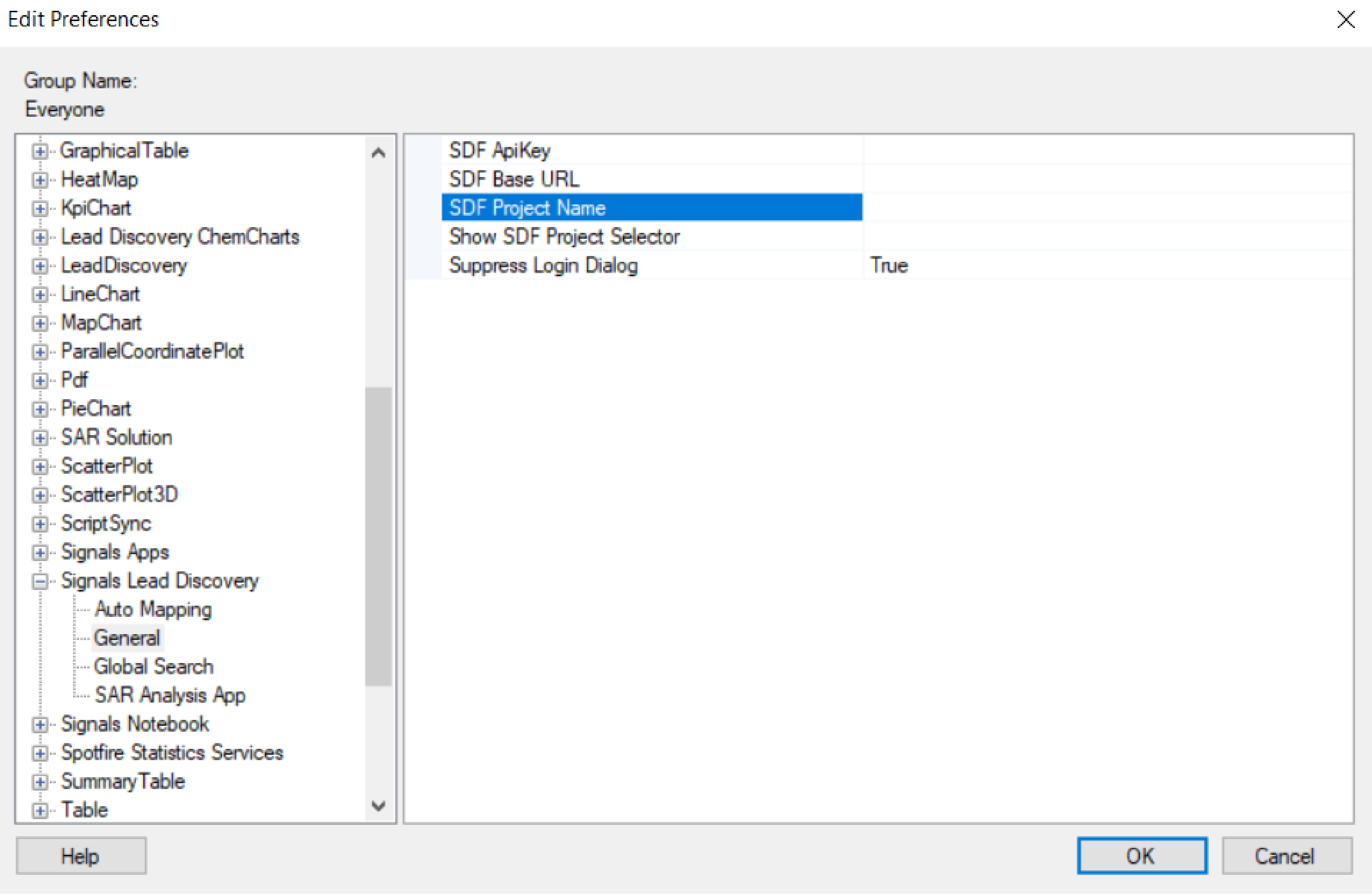
2. Select **General**.



Group Name:
Everyone

SDF ApiKey	
SDF Base URL	
SDF Project Name	
Show SDF Project Selector	
Suppress Login Dialog	True

3. Click on the **Edit** button to open the **Edit Preferences** dialog.



Group Name:
Everyone

SDF ApiKey	
SDF Base URL	
SDF Project Name	
Show SDF Project Selector	
Suppress Login Dialog	True

4. Enter the SDF Project Name to which Signals Inventa will point to. The SDF Project Name is the name of the project that you previously created in Signals Data Factory specifically to be used by Signals Inventa. For more information about the Signals Data Factory projects, please refer to the section "Configuring the Signals Data Factory".
5. Click OK.

Note: It is recommended that you restart the Spotfire Client in order for the new Preference settings to take effect.

Note: If the Web Player is open, it is necessary to log out and log in again in order for the new Preference settings to take effect.

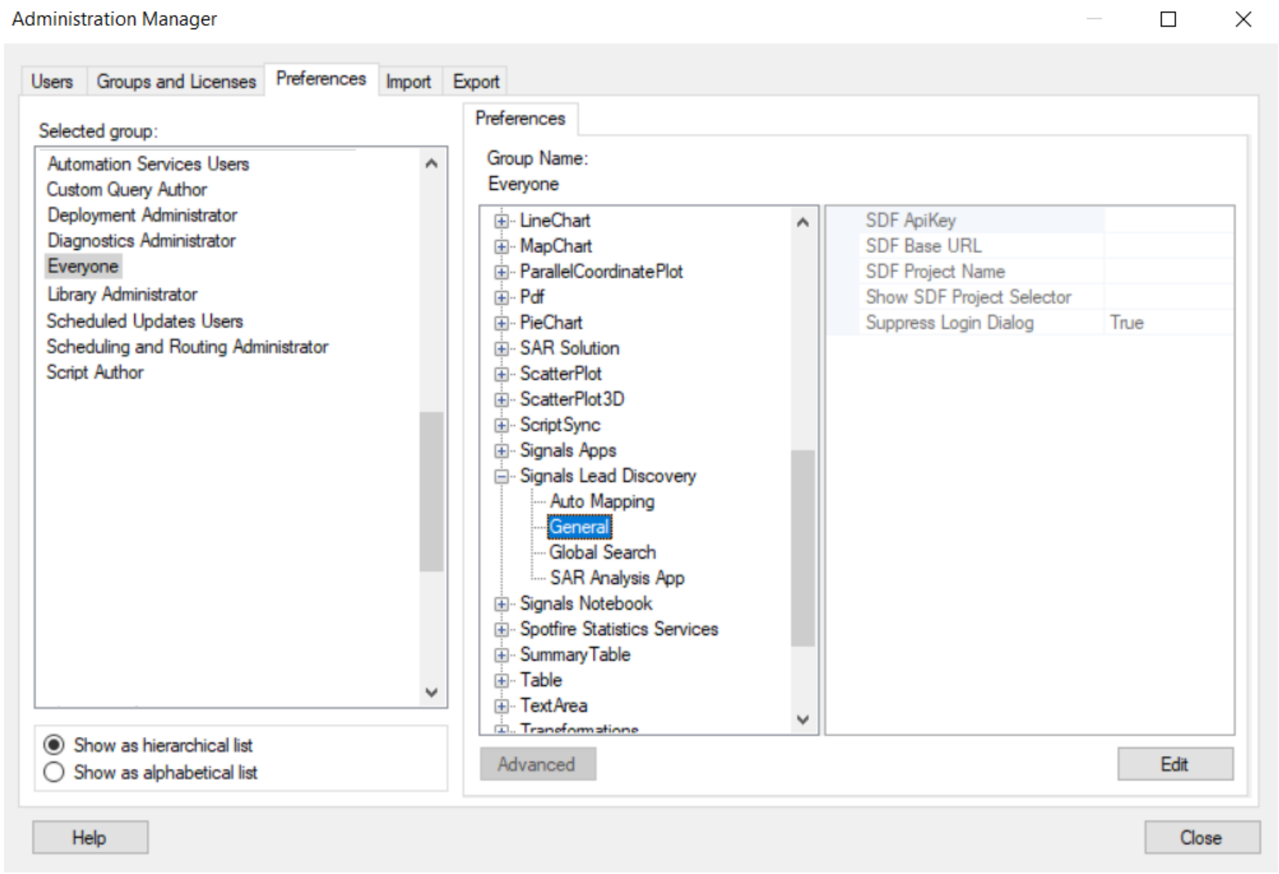
2.6 Setting the Show SDF Project Selector

A preference can be set to show the SDF Project Selector in the Global Search, Publish Measurements and Assay Details visualization interfaces.

To set the Show SDF Project Selector preference:

1. Access the Signals Inventa preferences via the Administration Manager (refer to Steps 1-4 above – Accessing the Signals Inventa Preferences section).

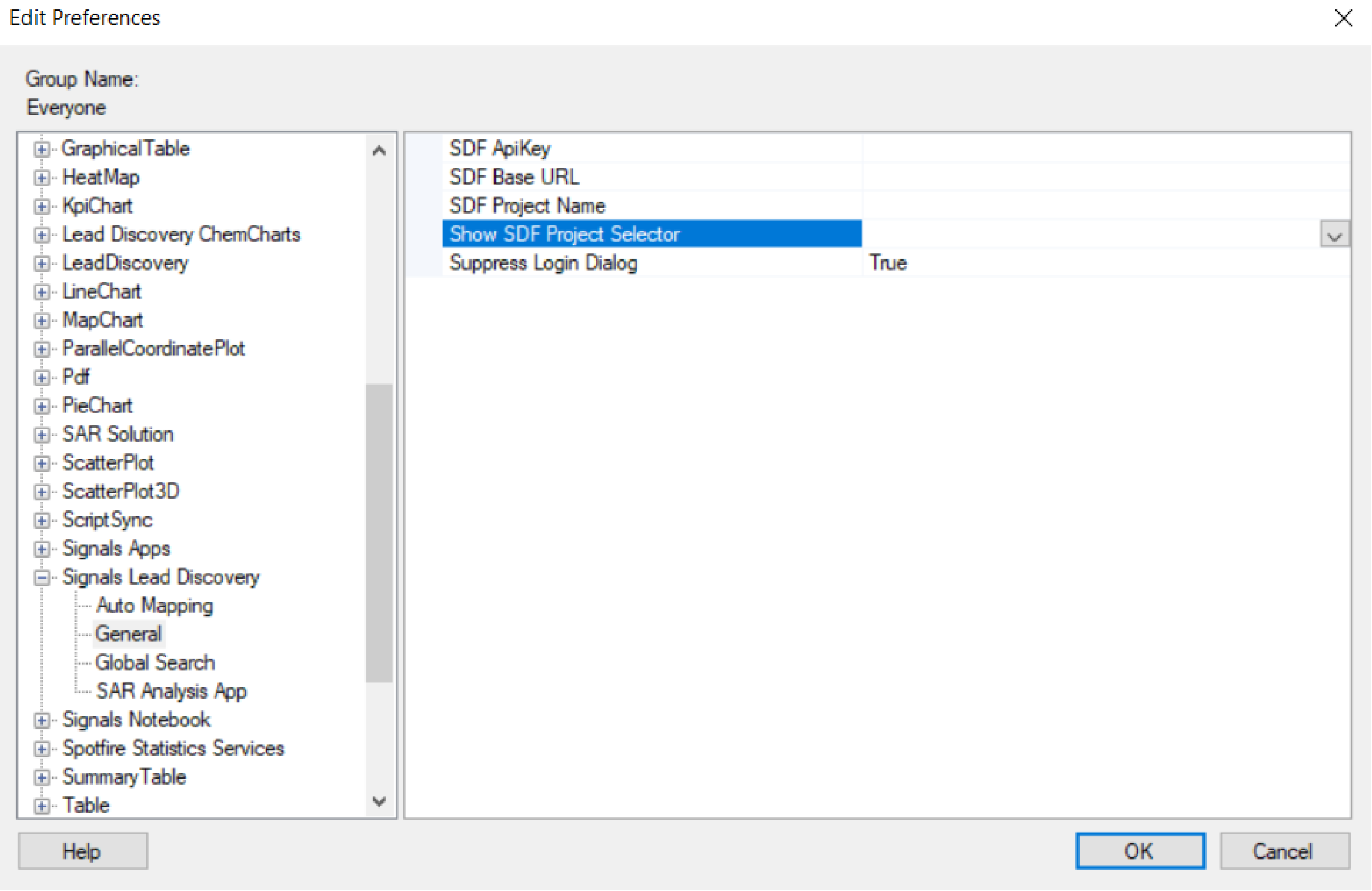
2. Select **General**.



Group Name:
Everyone

SDF ApiKey	
SDF Base URL	
SDF Project Name	
Show SDF Project Selector	
Suppress Login Dialog	True

3. Click on the **Edit** button to open the **Edit Preferences** dialog.



Group Name:
Everyone

SDF ApiKey	
SDF Base URL	
SDF Project Name	
Show SDF Project Selector	
Suppress Login Dialog	True

Note: The default value for Show SDF Project Selector is False. However, Spotfire does not display the default value, and therefore the field appears blank.

4. From the Show SDF Project Selector preference drop down list, select True to show the Project Selector on the Global Search and Publish Measurements interfaces.

5. Click **OK**.

Note: It is recommended that you restart the Spotfire Client in order for the new Preference settings to take effect.

Note: If the Web Player is open, it is necessary to log out and log in again in order for the new Preference settings to take effect.

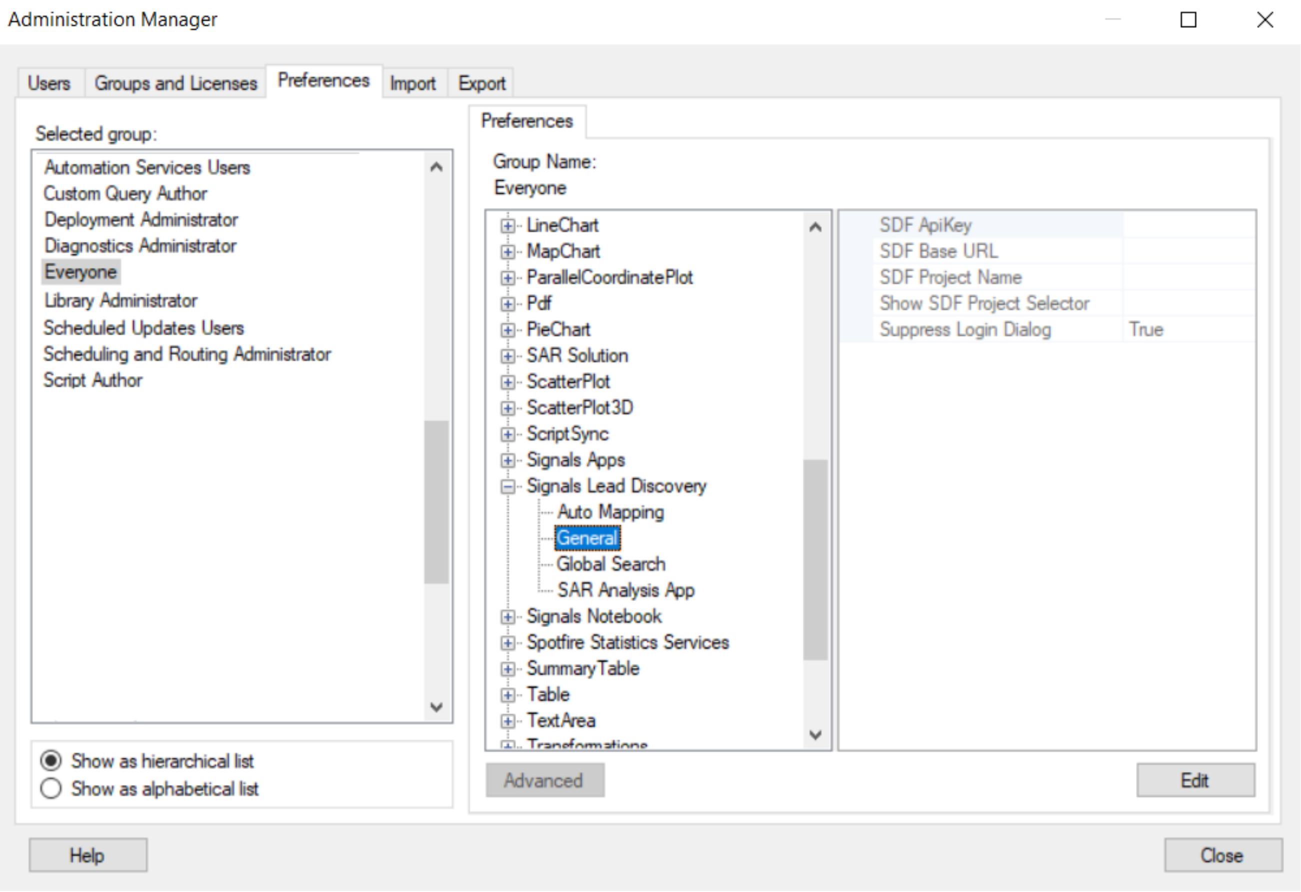
2.7 Setting the Suppress Login Dialog

A preference can be set to suppress the Login Dialog for Global Search and Publish Measurements Tool.

To set the Suppress Login Dialog preference:

1. Access the Signals Inventa preferences via the Administration Manager (refer to Steps 1-4 above – Accessing the Signals Inventa Preferences section).

2. Select **General**.

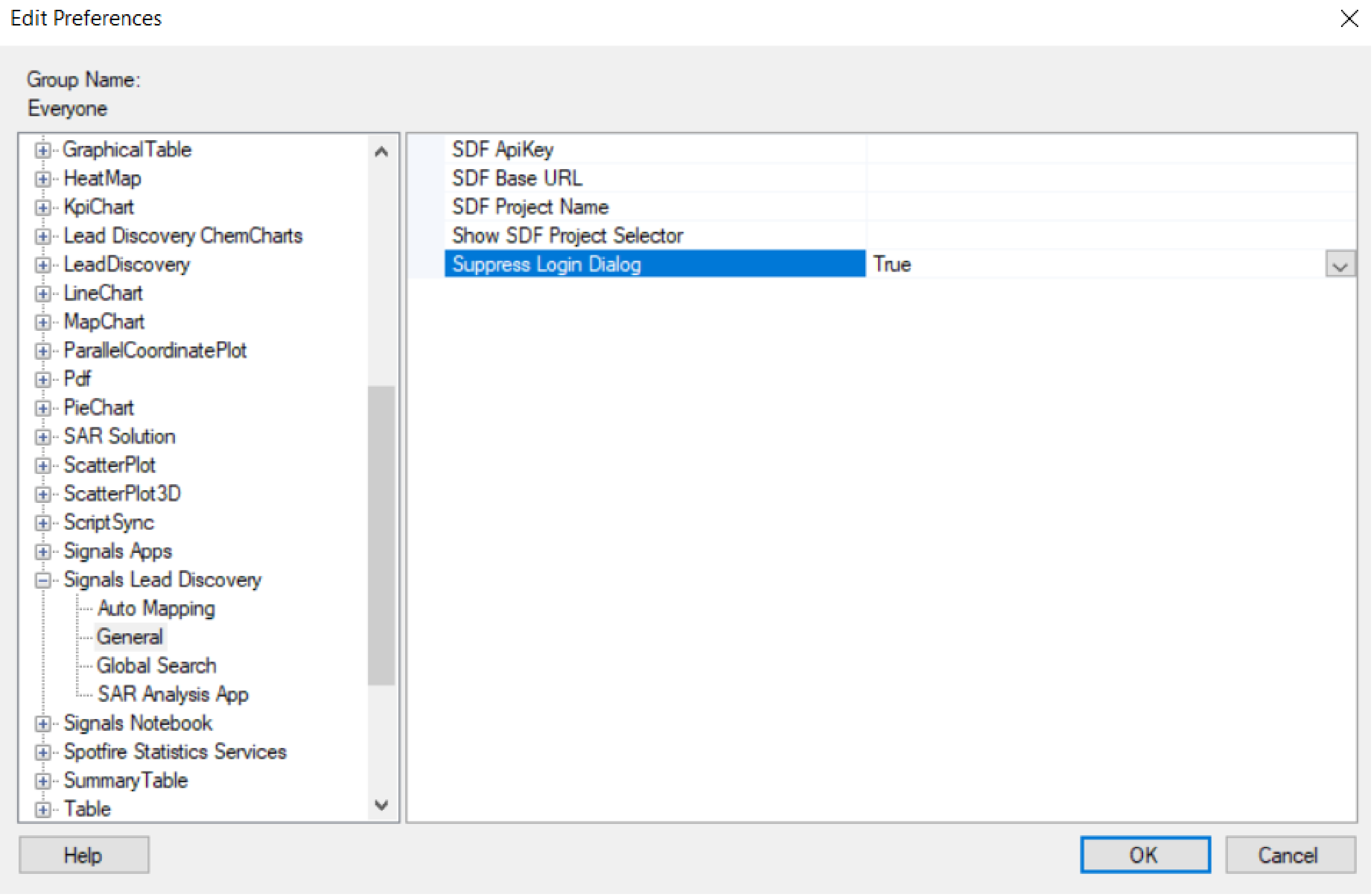


● Show as hierarchical list
○ Show as alphabetical list

Group Name:
Everyone

SDF ApiKey	
SDF Base URL	
SDF Project Name	
Show SDF Project Selector	
Suppress Login Dialog	True

3. Click on the **Edit** button to open the **Edit Preferences** dialog.



SDF ApiKey
SDF Base URL
SDF Project Name
Show SDF Project Selector
Suppress Login Dialog: True

Note: The default value for Suppress Login Dialog is False. However, Spotfire does not display the default value, and therefore the field appears blank.

4. Select True to suppress the login dialog . Users will be logged in directly if the SDF ApiKey has been set up correctly. Refer to Setting the SDF ApiKey section.

5. Click **OK**.

Note: It is recommended that you restart the Spotfire Client in order for the new Preference settings to take effect.

Note: If the Web Player is open, it is necessary to log out and log in again in order for the new Preference settings to take effect.

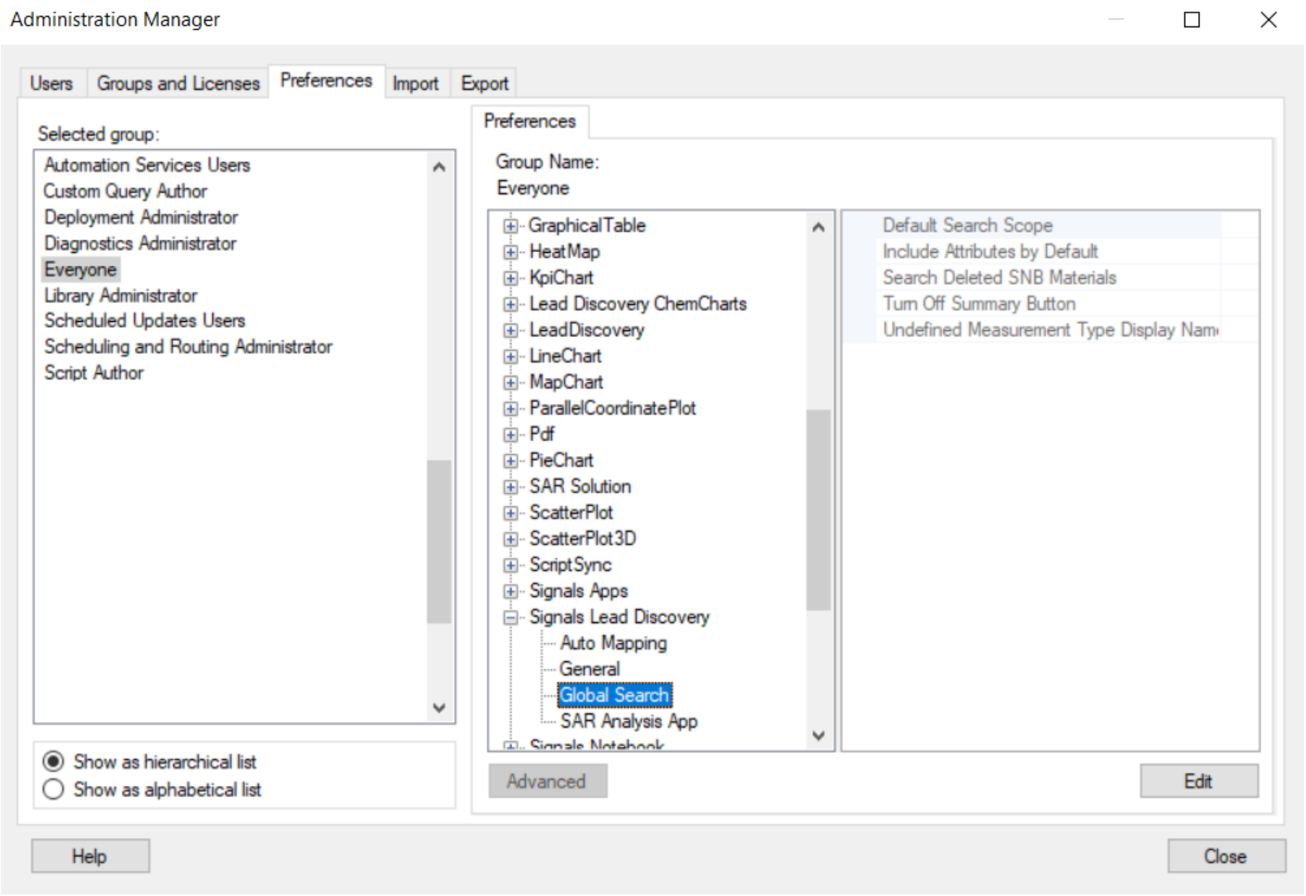
2.8 Setting the Default Search Scope in Global Search

A preference can be set to define the default search scope in Global Search when it is first opened. The preference can be set to Compounds, Batches or Measurements.

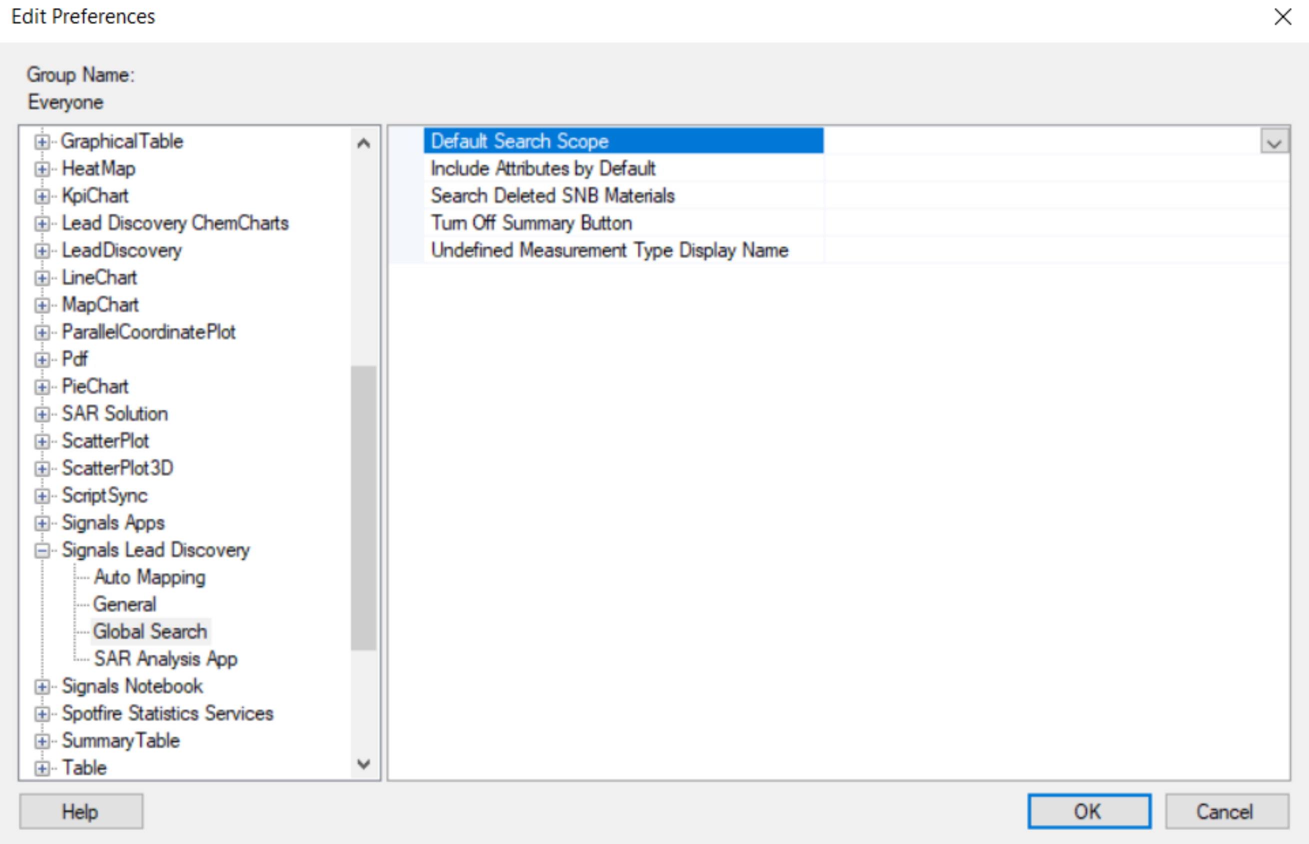
To set the Default Search Scope in Global Search:

1. Access the Signals Inventa preferences via the Administration Manager (refer to Steps 1-4 above – Accessing the Signals Inventa Preferences section).

2. Select **Global Search**.



3. Click on the **Edit** button to open the **Edit Preferences** dialog.



Note: The default value for Default Search Scope is **HierarchicalEntityLevel2**. However, Spotfire does not display the default value, and therefore the field appears blank.

4. From the Default Search Scope preference drop down list, select the default search scope (HierarchicalEntityLevel1, HierarchicalEntityLevel2 or Measurements) to be used by Global Search when it is opened.

Note: HiearchicalEntityLevel1 refers to the first level hierarchical entity, and HierarchicalEntityLevel2 refers to the second level hierarchical entity. If the user has configured the hierarchy to use “Compound/Batch” for example, HiearchicalEntityLevel1 corresponds to Compounds, whereas HiearchicalEntityLevel2 corresponds to Batches. If the user has configured the hierarchy to use “Antibody/Lot”, as another example, HiearchicalEntityLevel1 corresponds to Antibody, whereas HiearchicalEntityLevel2 corresponds to Lot.

5. Click **OK**.

Note: It is recommended that you restart the Spotfire Client in order for the new Preference settings to take effect.

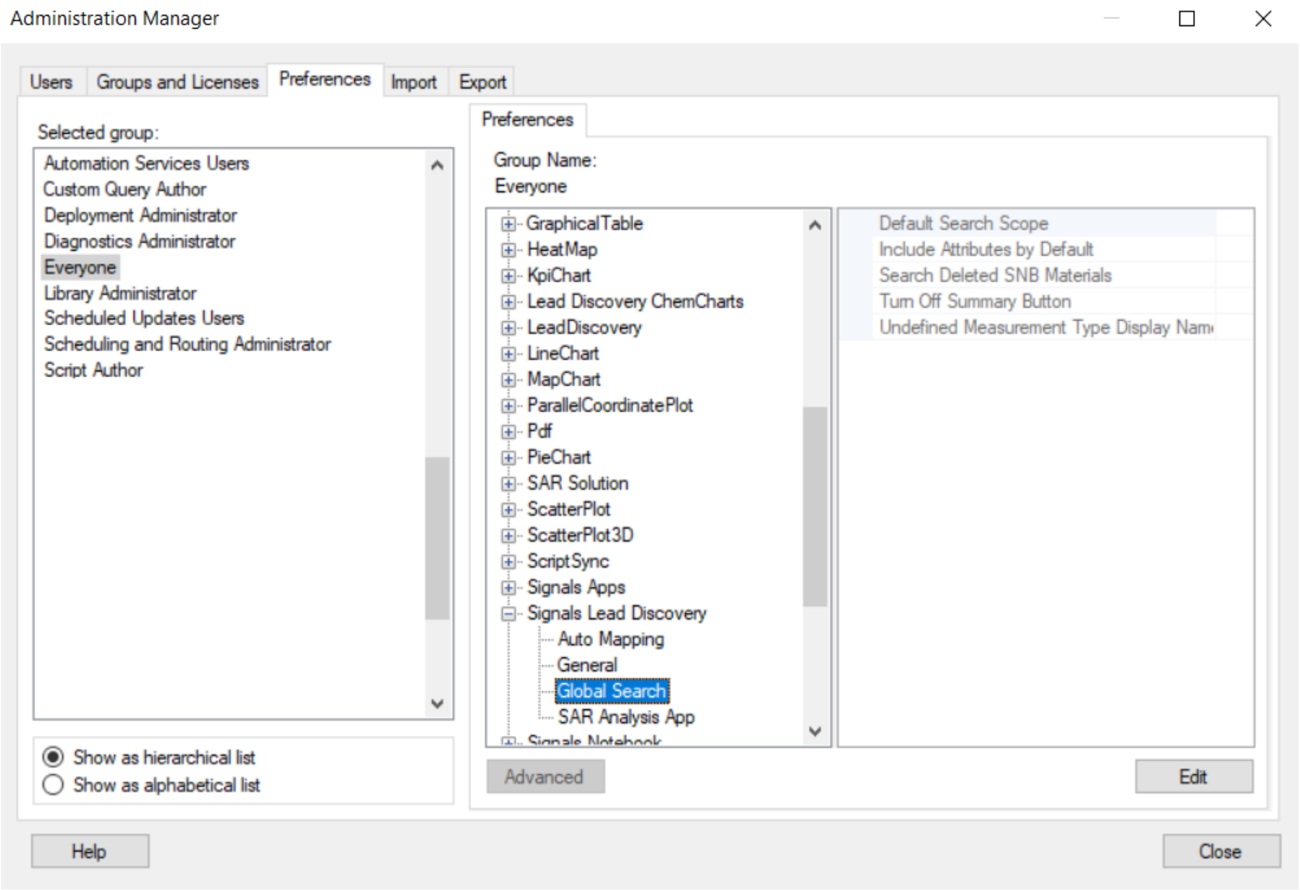
Note: If the Web Player is open, it is necessary to log out and log in again in order for the new Preference settings to take effect.

2.9 Setting the Include Attributes by Default in Global Search

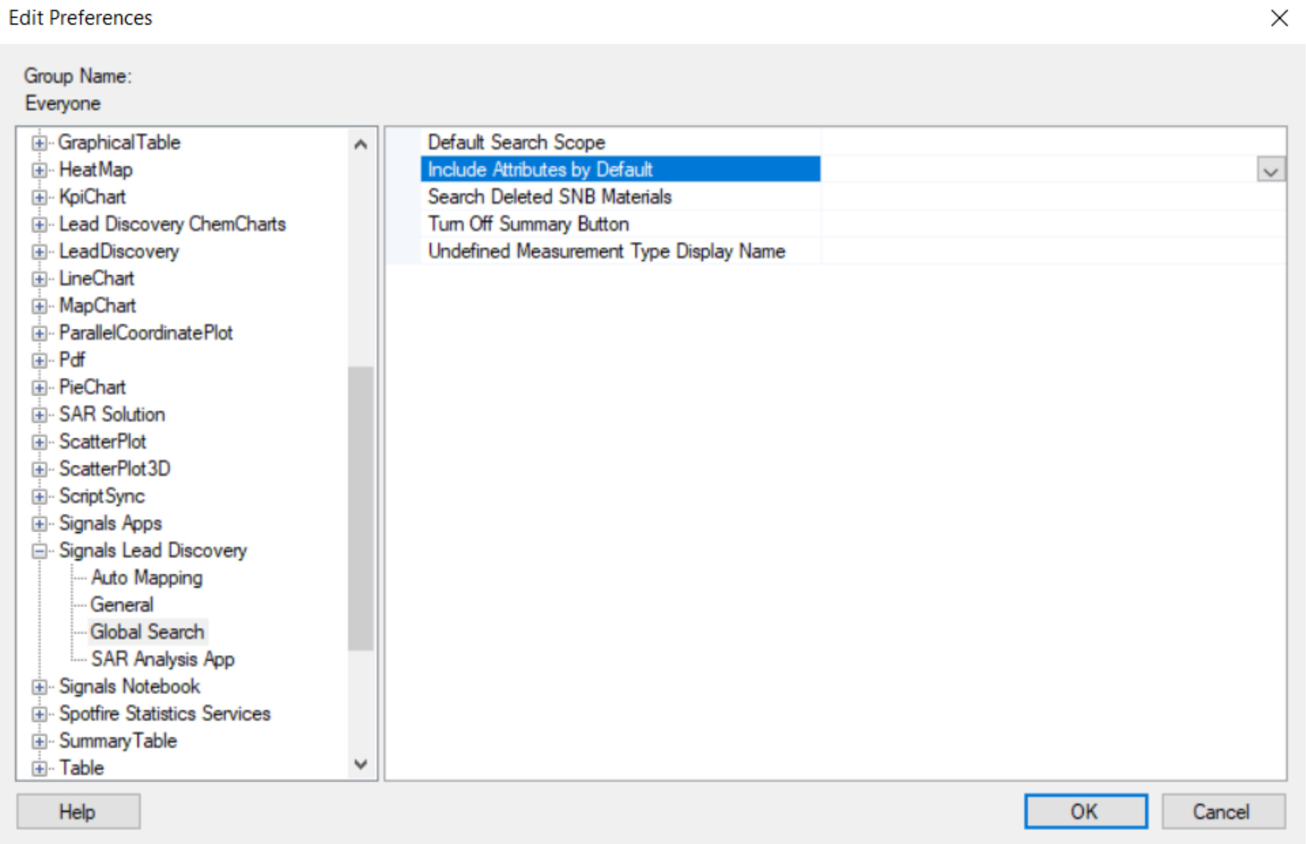
A preference can be set to include measurement attributes by default when downloading results from Global Search into Spotfire.

To set the Include Attributes By Default preference:

1. Access the Signals Inventa preferences via the Administration Manager (refer to Steps 1-4 above – Accessing the Signals Inventa Preferences section).
2. Select **Global Search**.



3. Click on the **Edit** button to open the **Edit Preferences** dialog.



Group Name:
Everyone

Note: The default value for Include Attributes by Default is True. However, Spotfire does not display the default value, and therefore the field appears blank.

4. From the Include Attributes by Default preference drop down list, select False to exclude the attributes by default when downloading results from Global Search into Spotfire.

5. Click **OK**.

Note: It is recommended that you restart the Spotfire Client in order for the new Preference settings to take effect.

Note: If the Web Player is open, it is necessary to log out and log in again in order for the new Preference settings to take effect.

2.10 Setting the Search Deleted Signals Notebook (SNB) Materials

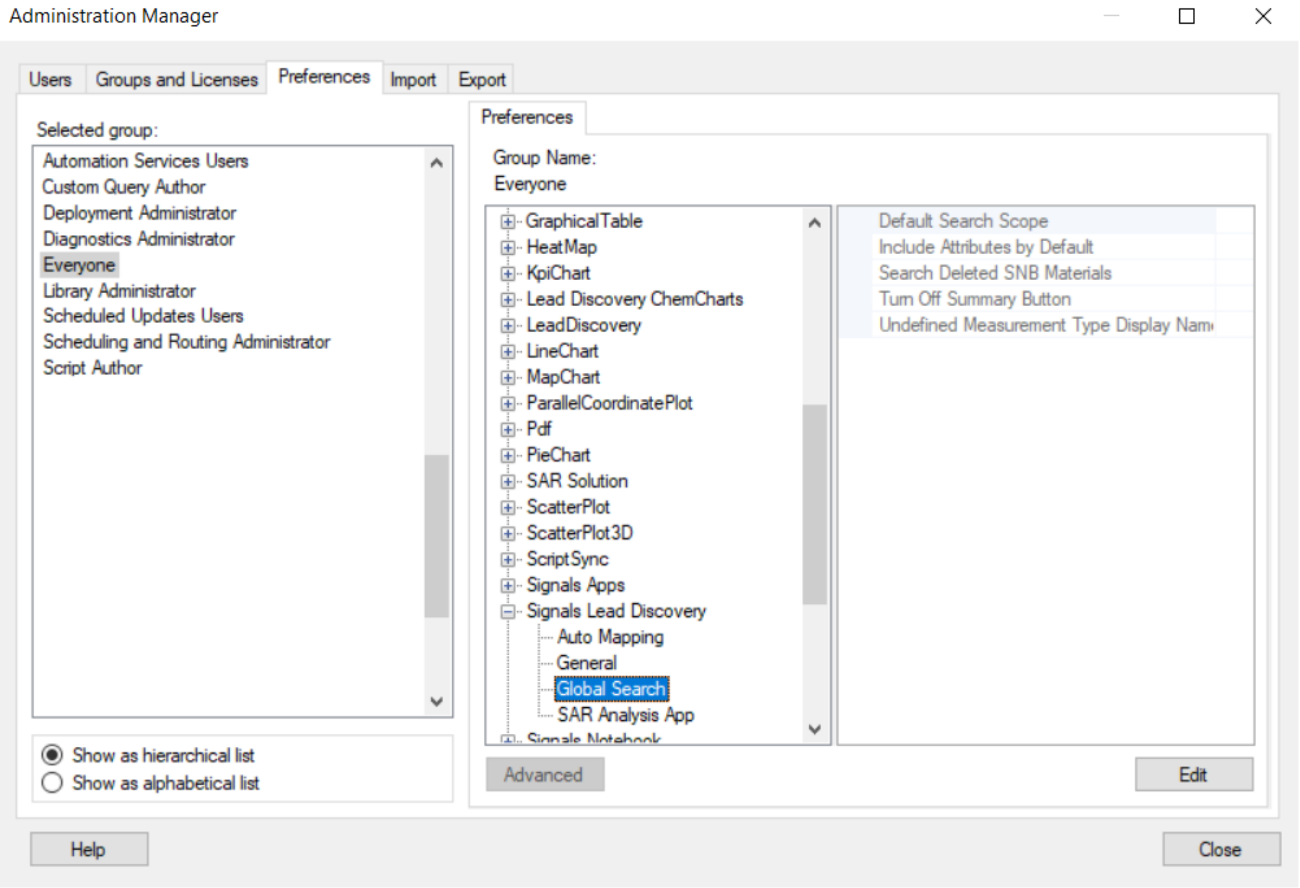
In the case where you are sending materials from Signals Notebook to Signals Inventa, you can indicate if materials that have been deleted from Signals Notebook but still exist because of associated measurements are searchable in Global Search.

Refer to Appendix E: Signals Notebook Integration for more information on Signals Notebook Materials Synchronization.

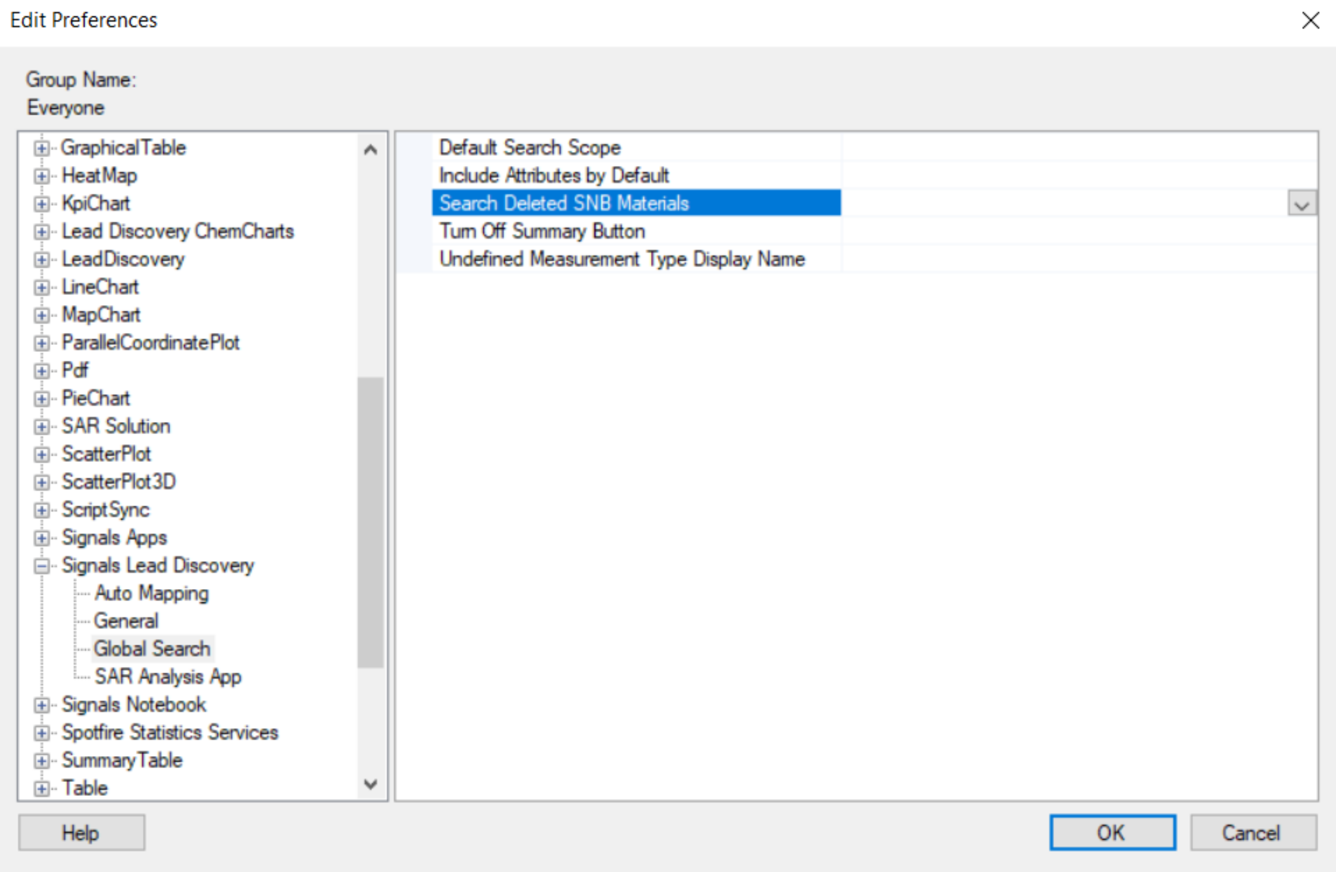
To set the Search Deleted SNB Materials preference:

1. Access the Signals Inventa preferences via the Administration Manager (refer to Steps 1-4 above – Accessing the Signals Inventa Preferences section).

2. Select **Global Search**.

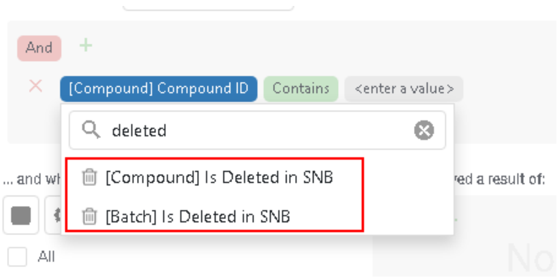


3. Click on the **Edit** button to open the **Edit Preferences** dialog.



Note: The default value for Search Deleted SNB Materials is False. However, Spotfire does not display the default value, and therefore the field appears blank.

4. From the Search Deleted SNB Materials preference drop down list, select True to include deleted Signals Notebook materials in the Global Search. In this case, two additional attributes will be added for a user to create conditions for searching for the deleted Signals Notebook materials.



5. Click **OK**.

Note: It is recommended that you restart the Spotfire Client for the new Preference settings to take effect.

Note: If the Web Player is open, it is necessary to log out and log in again for the new Preference settings to take effect.

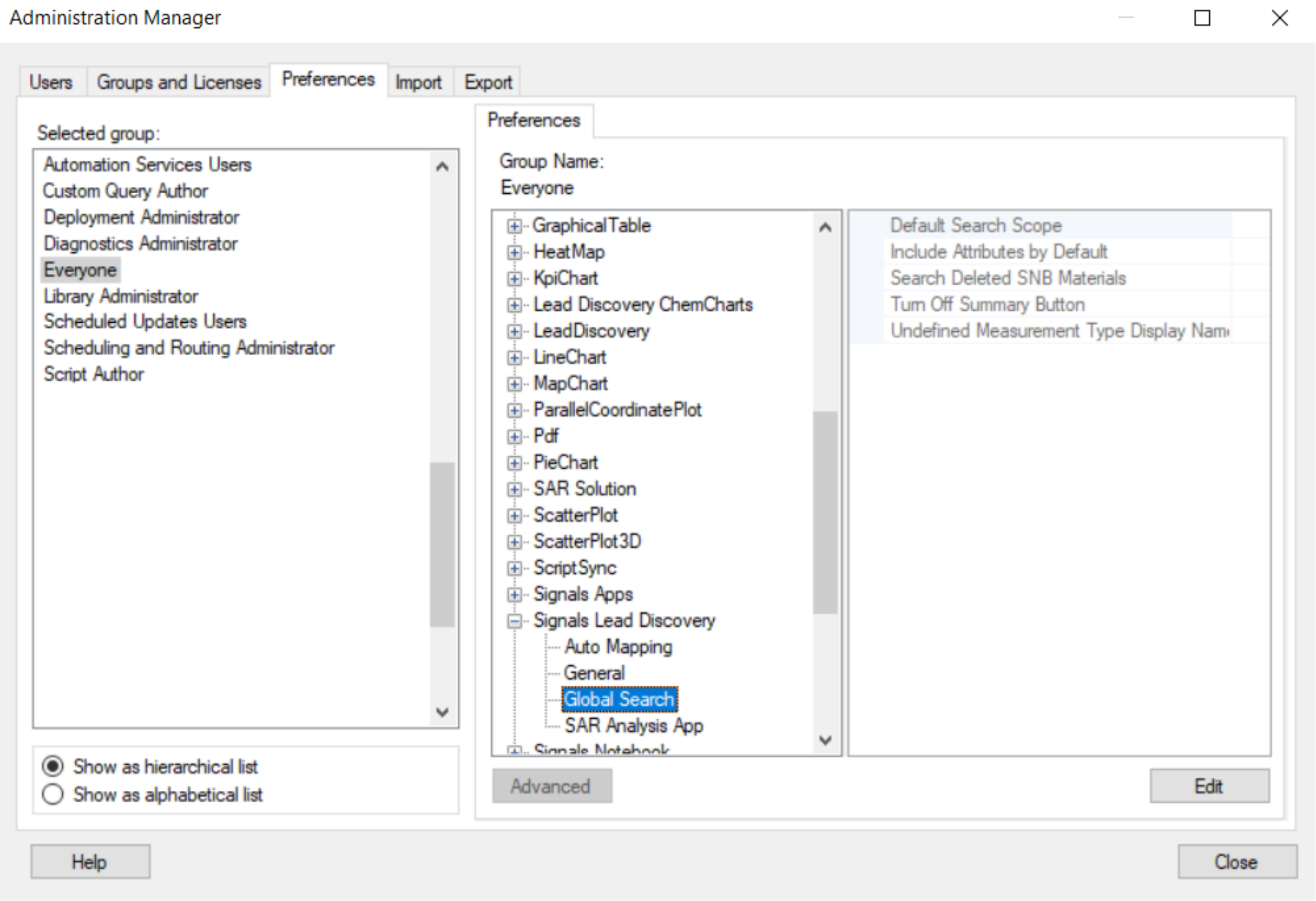
2.11 Setting the Turn Off Summary Button In Global Search

In the case where you want to load the assay summary results automatically, there is the option to hide the **Show me the summary** button on the Summary search panel in Global Search.

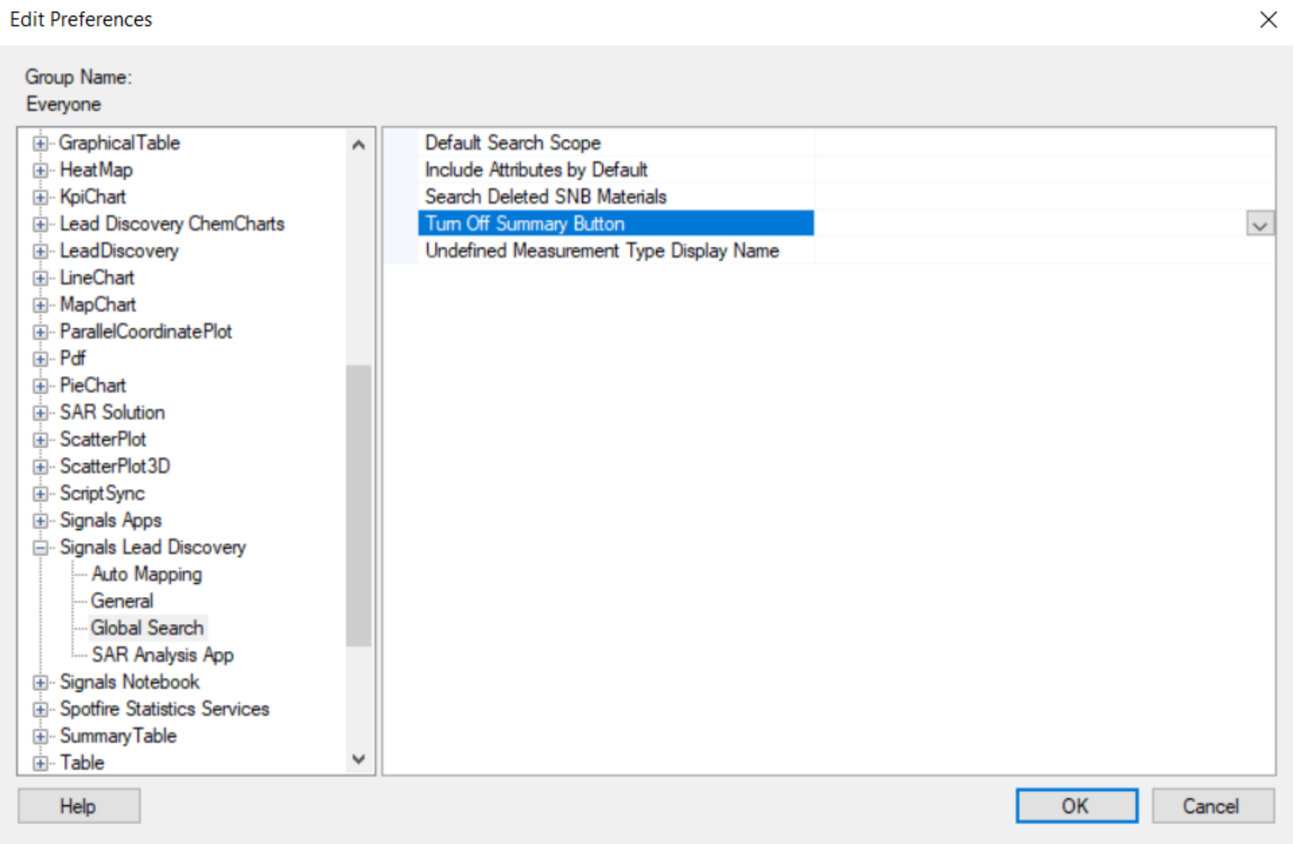
Refer to the section Getting the Summary of the Query to be performed for more information.

To set the Turn Off Summary Button preference:

1. Access the Signals Inventa preferences via the Administration Manager (refer to Steps 1-4 above – Accessing the Signals Inventa Preferences section).
2. Select **Global Search**.



3. Click on the **Edit** button to open the **Edit Preferences** dialog.



Note: The default value for Turn Off Summary Button is False. However, Spotfire does not display the default value, and therefore the field appears blank.

4. From the **Turn Off Summary Button** preference drop down list, select **True to hide the Show me the summary** button on the Search summary panel.

5. Click **OK**.

Note: It is recommended that you restart the Spotfire Client in order for the new Preference settings to take effect.

Note: If the Web Player is open, it is necessary to log out and log in again in order for the new Preference settings to take effect.

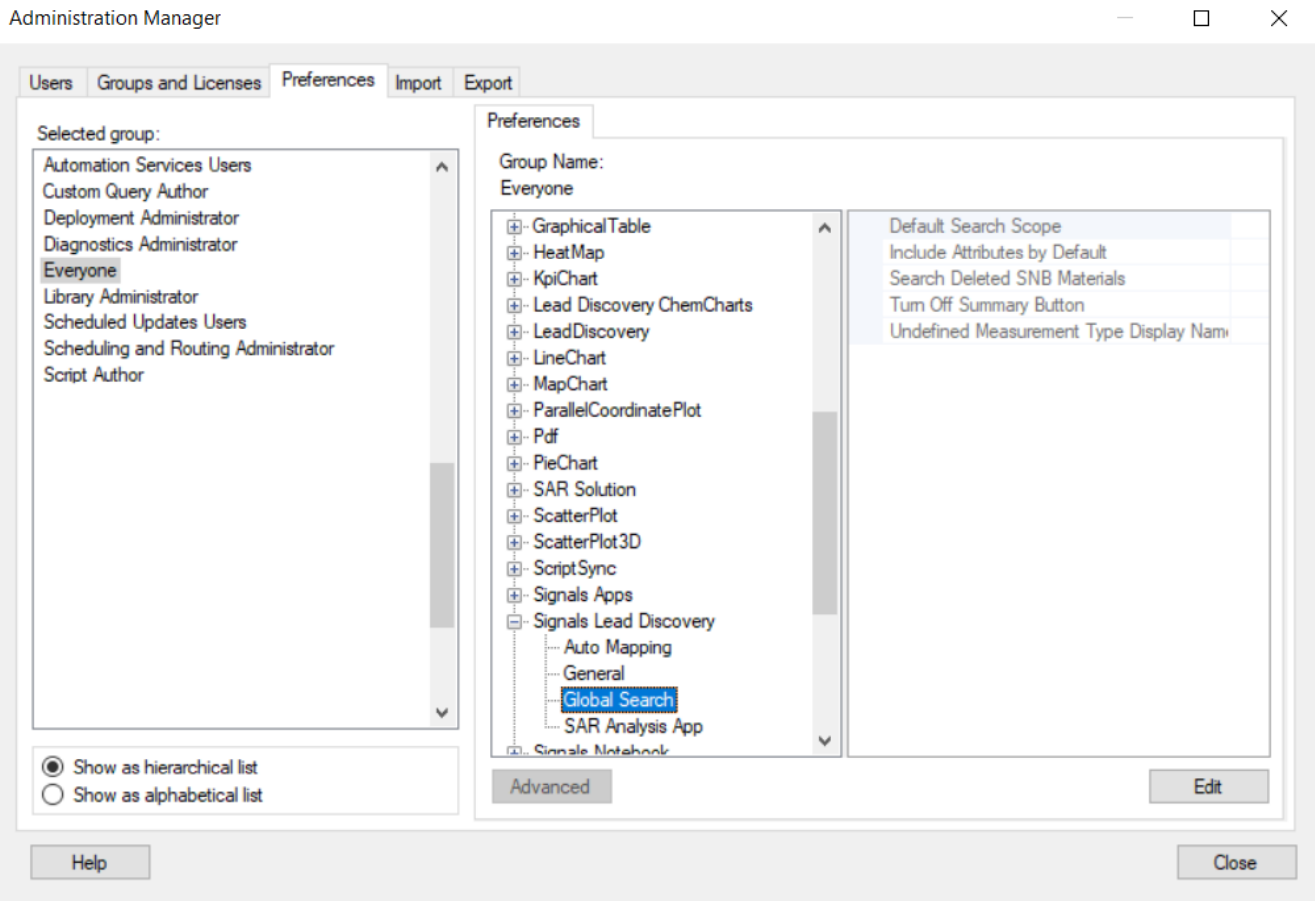
2.12 Setting the Undefined Measurement Type Display Name

In the case where data is loaded directly into the Assay Endpoints Results table and measurement types are not defined, the resulting node in the assay hierachal tree is labelled ‘Endpoints’ by default. The Undefined Measurement Type Display Name preference allows you to specify a display name if you choose not to use the default name.

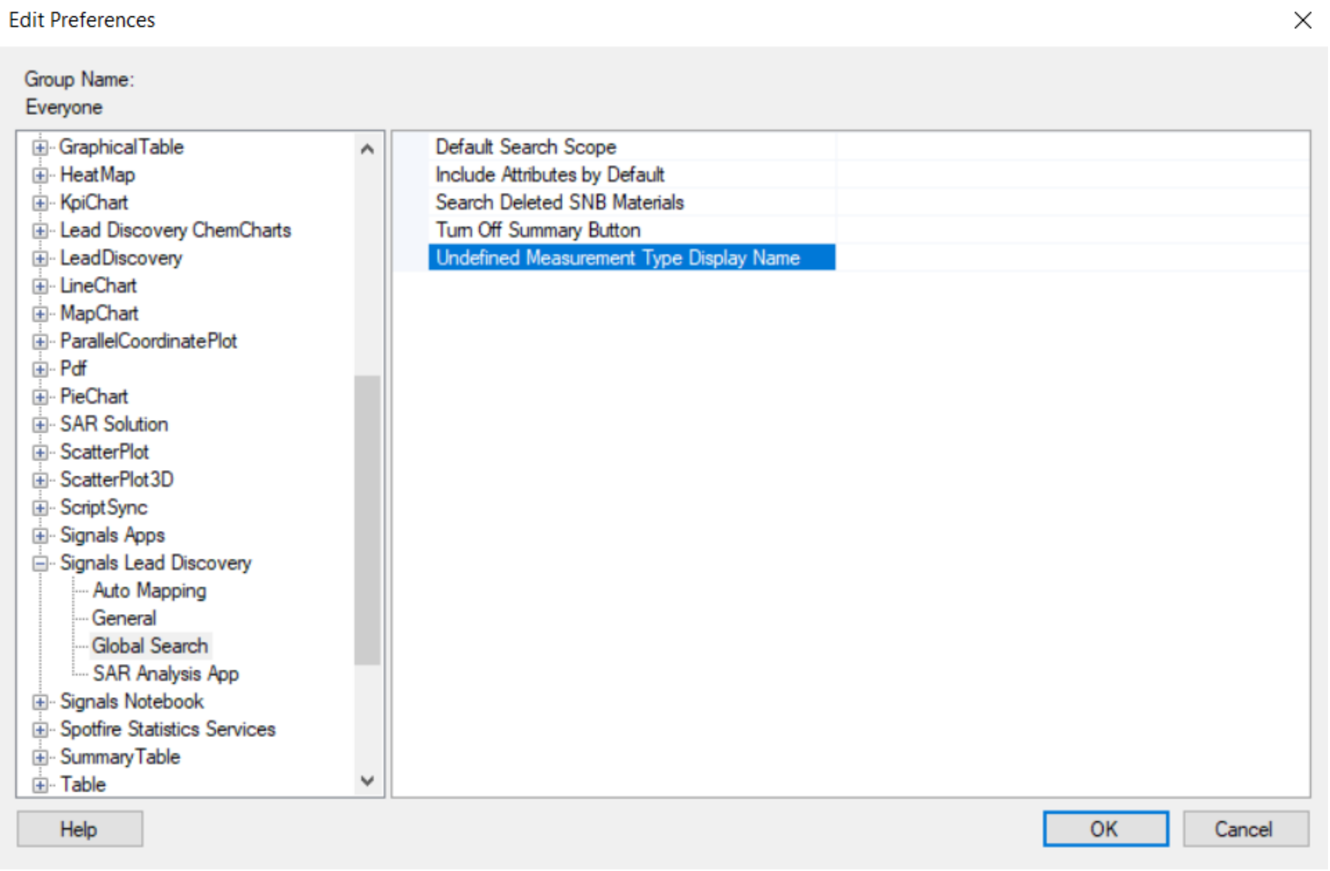
In the case, where there is a mix of some and no measurement types, the resulting node in the assay hierarchal tree is labelled ‘Other Endpoints’ by default. The Undefined Measurement Type Display Name preference allows you to specify a display name if you choose not to use the default name of Endpoints. For example, the node will be labelled “Other {preference value}”.

To set the Undefined Measurement Type Display Name preference:

1. Access the Signals Inventa preferences via the Administration Manager (refer to Steps 1-4 above – Accessing the Signals Inventa Preferences section).
2. Select **Global Search**.



3. Click on the **Edit** button to open the **Edit Preferences** dialog.



Note: The default value for Undefined Measurement Type Display Name is Endpoint. However, Spotfire does not display the default value, and therefore the field appears blank.

4. Enter a display name for the undefined measurement type.
5. Click **OK**.

Note: It is recommended that you restart the Spotfire Client in order for the new Preference settings to take effect.

Note: If the Web Player is open, it is necessary to log out and log in again in order for the new Preference settings to take effect.

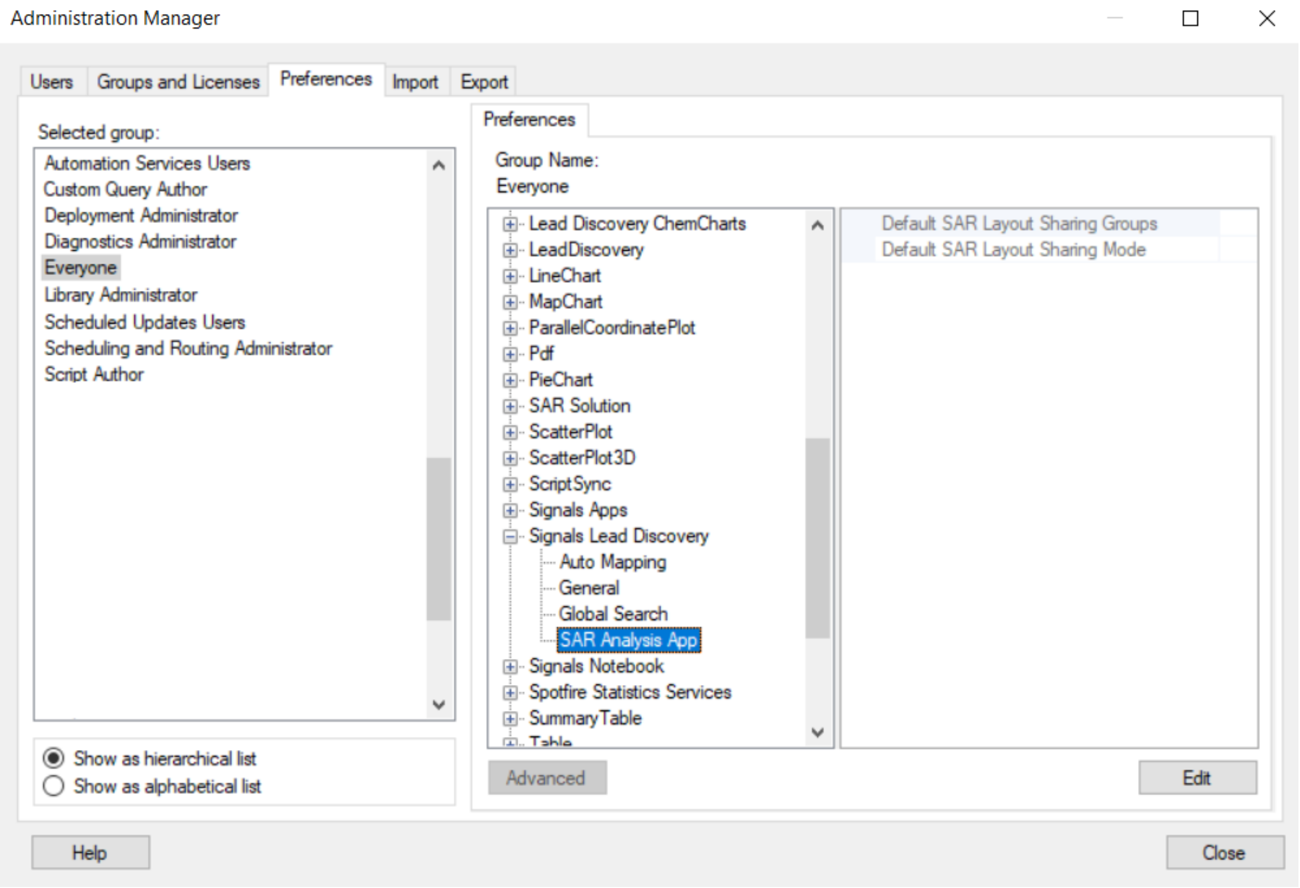
2.13 Setting the Default SAR Layout Sharing Groups in SAR Analysis App

A preference can be set to define the default SAR Layout Sharing Groups in SAR Analysis App. The preference can be set to Compounds, Batches or Measurements.

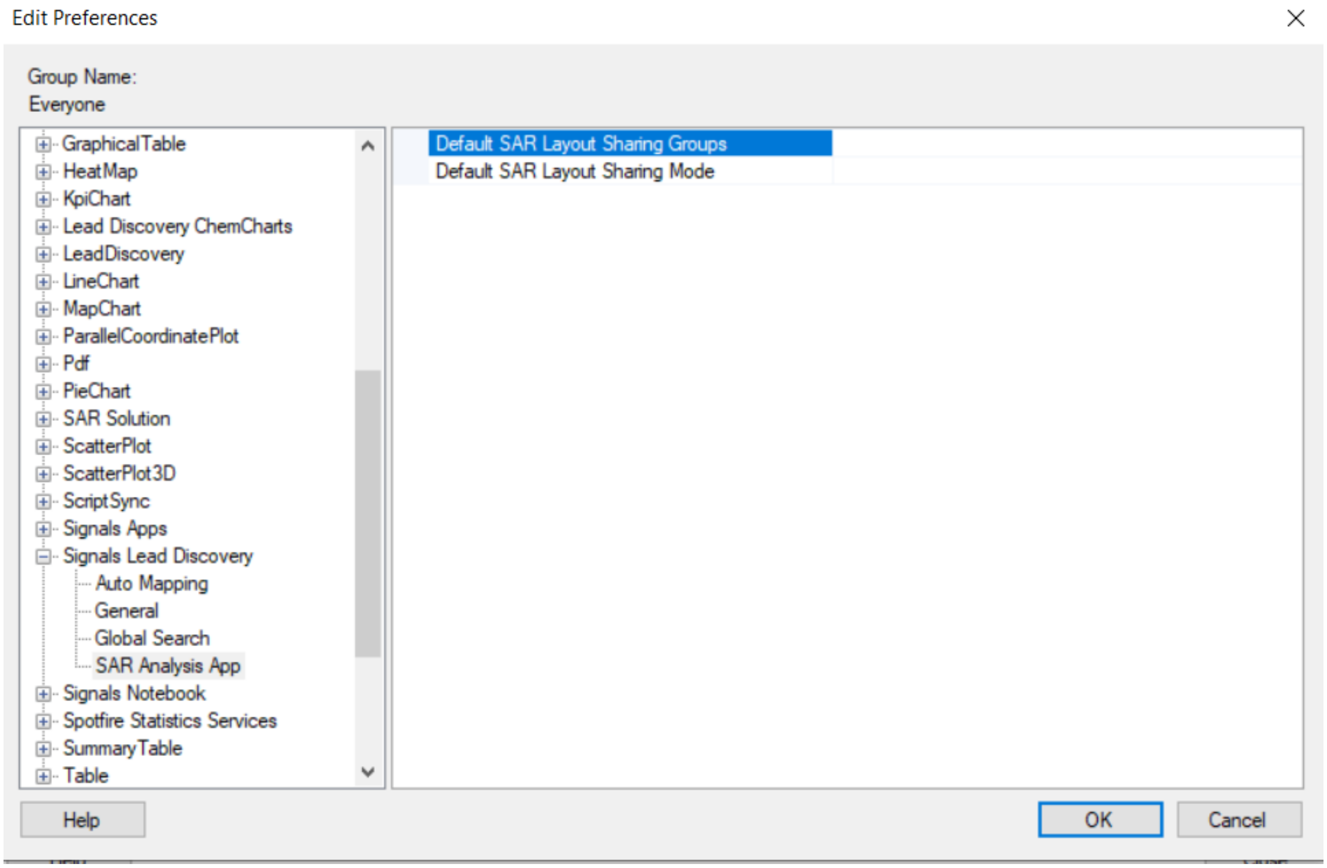
To set the Default SAR Layout Sharing Groups in SAR Analysis App:

1. Access the Signals Inventa preferences via the Administration Manager (refer to Steps 1-4 above – Accessing the Signals Inventa Preferences section).

2. Select **SAR Analysis App**.



3. Click on the **Edit** button to open the **Edit Preferences** dialog.



Note: The default value for Default SAR Layout Sharing Groups is Empty. However, Spotfire does not display the default value, and therefore the field appears blank.

4. Enter default sharing groups for the group sharing mode; separated by commas. If this preference is set, the Groups drop down list when defining SAR layout permissions will automatically populate the group names specified here.

5. Click **OK**.

Note: It is recommended that you restart the Spotfire Client in order for the new Preference settings to take effect.

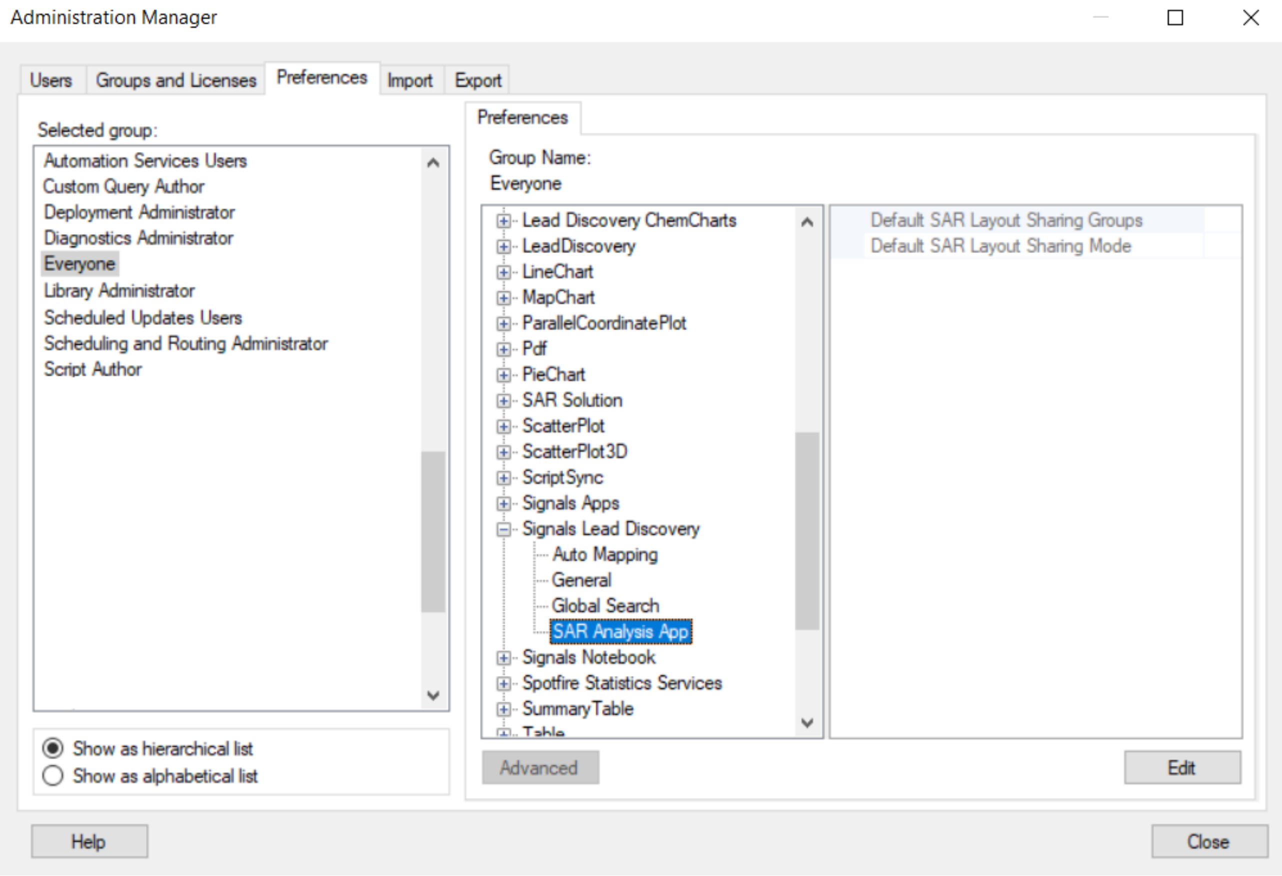
Note: If the Web Player is open, it is necessary to log out and log in again in order for the new Preference settings to take effect.

2.14 Setting the Default SAR Layout Sharing Mode in SAR Analysis App

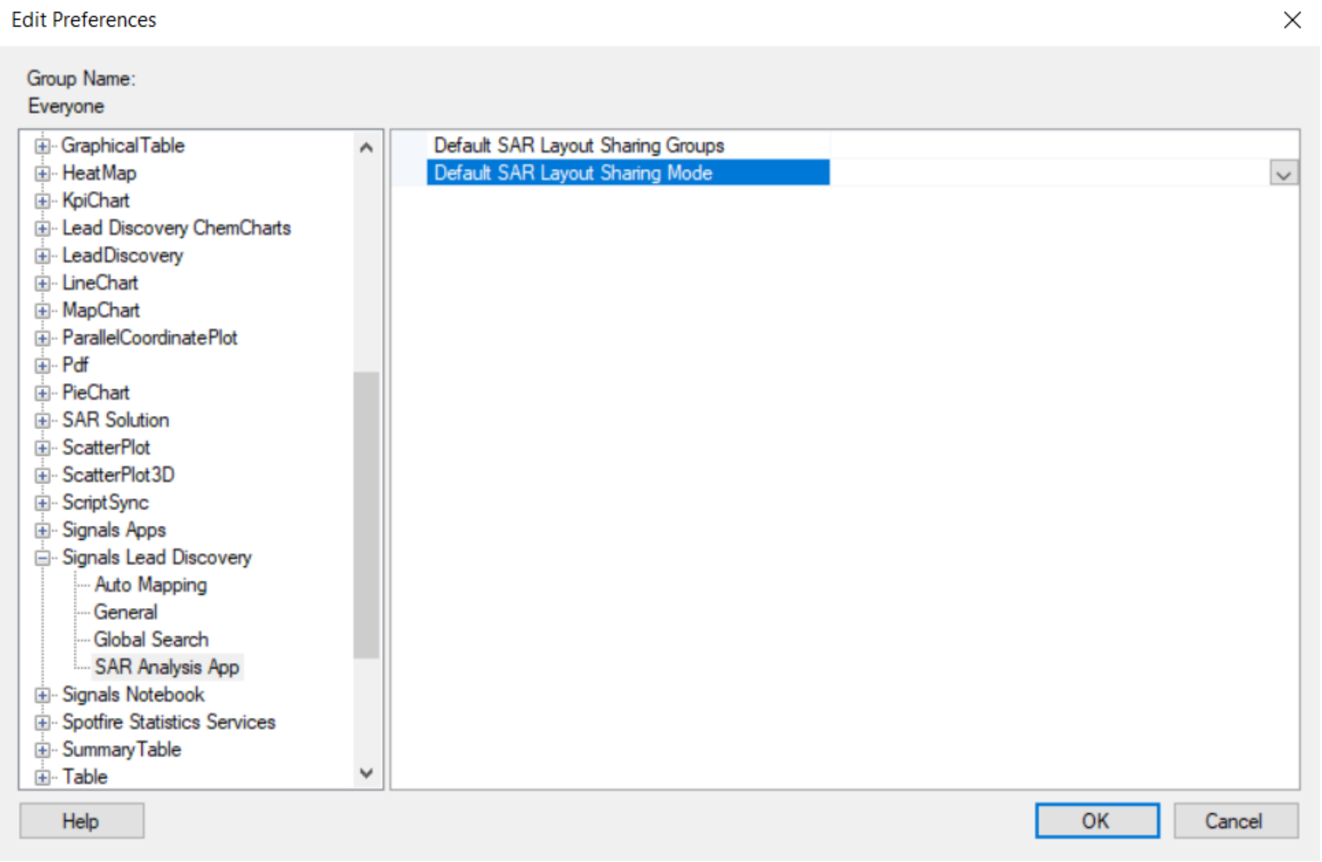
A preference can be set to define the default SAR Layout Sharing Mode in SAR Analysis App. The preference can be set to Private or Groups.

To set the Default SAR Layout Sharing Mode in SAR Analysis App:

1. Access the Signals Inventa preferences via the Administration Manager (refer to Steps 1-4 above – Accessing the Signals Inventa Preferences section).
2. Select **SAR Analysis App**.



3. Click on the **Edit** button to open the **Edit Preferences** dialog.



Note: The default value for Default SAR Layout Sharing Mode is Private. However, Spotfire does not display the default value, and therefore the field appears blank.

4. Enter Private or Groups to define the default SAR Layout Sharing Mode to be used when the SAR Analysis App is first opened.
5. Click **OK**.

Note: It is recommended that you restart the Spotfire Client in order for the new Preference settings to take effect.

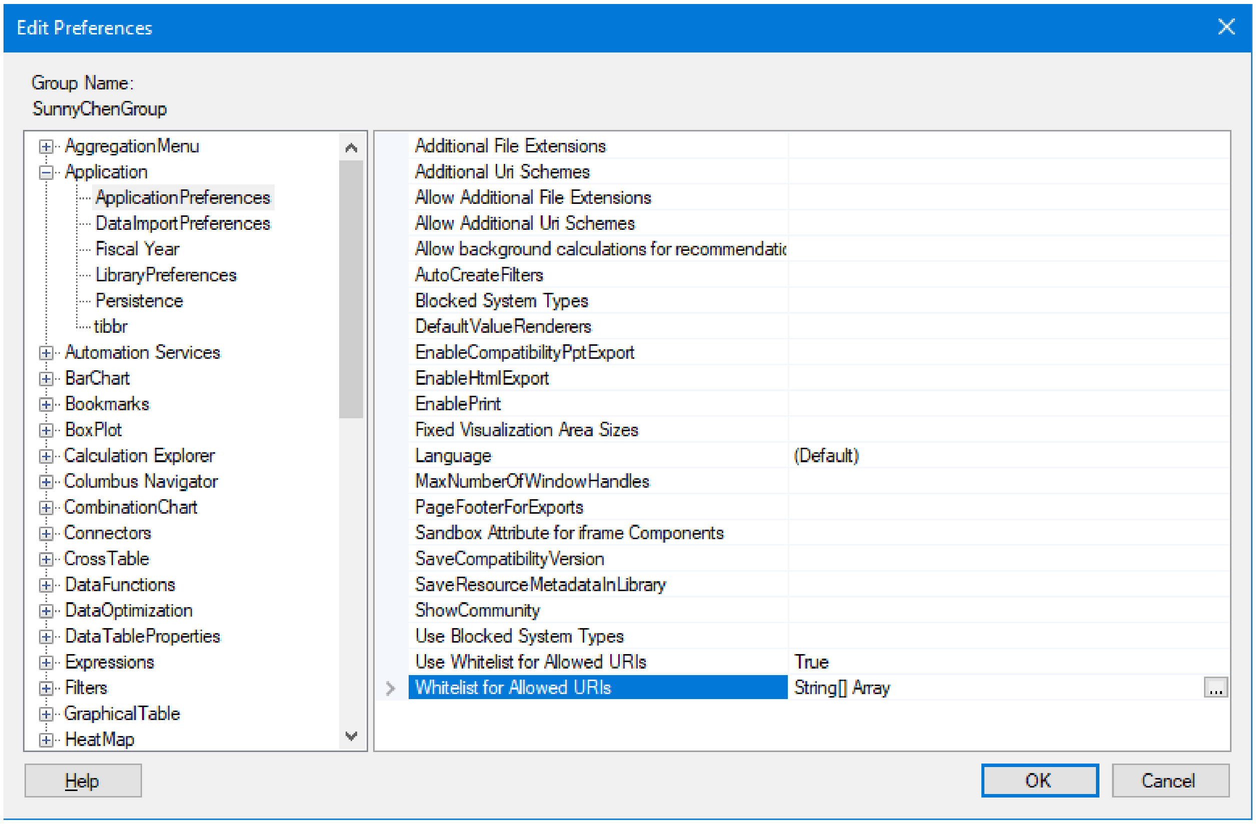
Note: If the Web Player is open, it is necessary to log out and log in again in order for the new Preference settings to take effect.

2.15 Adding the SDF Base URL to Whitelist for Allowed URIs

In order for Spotfire to open the SDF login page in a pop-up web browser window, the SDF Base URL must be added to the **Whitelist for Allowed URIs** Spotfire application preference.

To add the SDF Base URL to Whitelist for Allowed URIs:

1. Open the Spotfire client, and logon as a Spotfire Administrator. From the **Tools** menu, select the **Administration Manager** sub-menu item. The Administration Manager is only enabled if you logon connected to the Spotfire Server.
2. Click on the **Preferences** tab.
3. Select the Group Name to which the preferences should be applied.
4. Expand **Application** and select **ApplicationPreferences**.
5. Click the **Edit** button.
6. Click the ellipsis icon on the **Whitelist for Allowed URIs** item.



Group Name:
SunnyChenGroup

Additional File Extensions
Additional Uri Schemes
Allow Additional File Extensions
Allow Additional Uri Schemes
Allow background calculations for recommendatic
AutoCreateFilters
Blocked System Types
DefaultValueRenderers
EnableCompatibilityPptExport
EnableHtmlExport
EnablePrint
Fixed Visualization Area Sizes
Language (Default)
MaxNumberOfWindowHandles
PageFooterForExports
Sandbox Attribute for iframe Components
SaveCompatibilityVersion
SaveResourceMetadataInLibrary
ShowCommunity
Use Blocked System Types
Use Whitelist for Allowed URIs True
Whitelist for Allowed URIs String[] Array ...

7. In the **String Collection Editor**, add the SDF Base URL in the text box.
8. Click **OK** to close the String Collection Editor.
9. Click **OK** to close the Edit Preferences dialog.

10. Click **Close** to close the Administration Manager.

Note: It is recommended that you restart the Spotfire Client in order for the new Preference settings to take effect.

Note: If the Web Player is open, it is necessary to log out and log in again in order for the new Preference settings to take effect.

3 Manage Measurement Types Tool

The Manage Measurement Types tool allows data administrators to manage measurement types. It is implemented via a website deployed together with the metastore service. You need to configure the SDF Base URL in Spotfire Preferences before using this tool. Refer to Setting the SDF Base URL section for information on setting this preference.

3.1 Accessing the Manage Measurement Types Tool

The Manage Measurement Types tool is accessed through the main Spotfire Interface. You will be required to login to the Signals Data Factory using your SSO credentials before you can access the Manage Measurements Types tool if you have not already been authenticated or your session has expired.

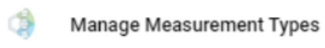
Note: If the SDF ApiKey Spotfire preference has been set, you will not be required to logon. Refer to Setting the SDF APIKey section for further information.

Note: If you are using Safari web browser, please make sure that it won’t block the pop-up dialog from Signals Data Factory domain. To enable the pop-up dialog from Signals Data Factory:

1. In Safari, select **Preferences** menu.
2. In the **Preferences** dialog, choose **Websites** tab.
3. In the Configured Websites list, make sure that the Signals Data Factory web page has been set to **Allow**.

To access the Management Measurements Type tool:

In both Spotfire Analyst Client and Web Player:

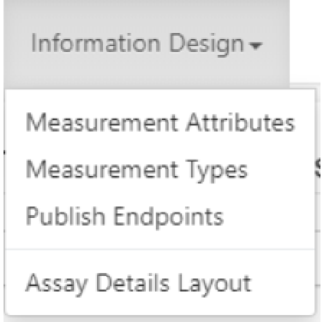
1. Open data in Spotfire.
2. Select **Tools > Signals Inventa > Manage Measurement Types** from the main menu to open the Manage Measurement Types in your system default web browser. Alternatively, you can open the Visualization types flyout and click the  item to open it.

3.2 Managing Attributes

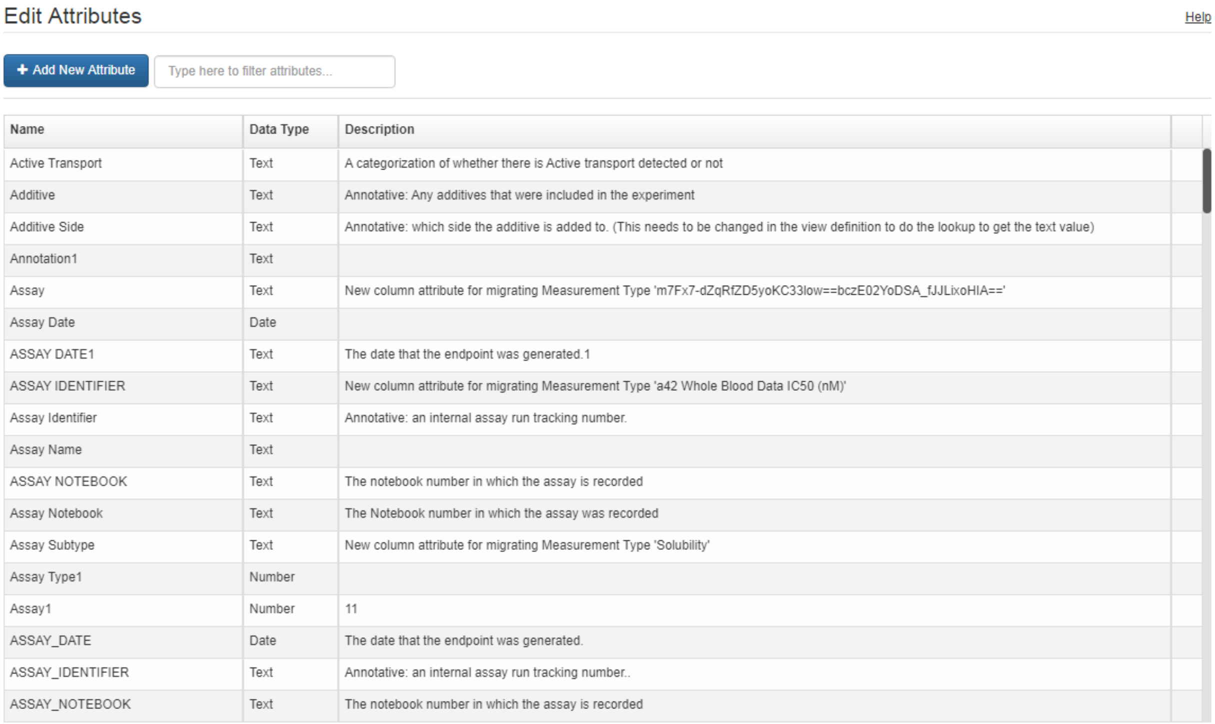
Measurement attributes are a definition of the measurement values collected. Attributes are managed in the Edit Attributes page.

To access the Edit Attributes page:

1. From the Information Design drop-down list box, select **Measurement Attributes**.



The Edit Attributes page opens, similar to the example shown below.



Name	Data Type	Description
Active Transport	Text	A categorization of whether there is Active transport detected or not
Additive	Text	Annotative: Any additives that were included in the experiment
Additive Side	Text	Annotative: which side the additive is added to. (This needs to be changed in the view definition to do the lookup to get the text value)
Annotation1	Text	
Assay	Text	New column attribute for migrating Measurement Type 'm7Fx7-dZqRfZD5yoKC33low==bczE02YoDSA_fJJLixoHIA=='
Assay Date	Date	
ASSAY DATE1	Text	The date that the endpoint was generated.1
ASSAY IDENTIFIER	Text	New column attribute for migrating Measurement Type 'a42 Whole Blood Data IC50 (nM)'
Assay Identifier	Text	Annotative: an internal assay run tracking number.
Assay Name	Text	
ASSAY NOTEBOOK	Text	The notebook number in which the assay is recorded
Assay Notebook	Text	The Notebook number in which the assay was recorded
Assay Subtype	Text	New column attribute for migrating Measurement Type 'Solubility'
Assay Type1	Number	
Assay1	Number	11
ASSAY_DATE	Date	The date that the endpoint was generated.
ASSAY_IDENTIFIER	Text	Annotative: an internal assay run tracking number..
ASSAY_NOTEBOOK	Text	The notebook number in which the assay is recorded

The Edit Attributes page is a single page application for querying, adding, editing and deleting attributes.

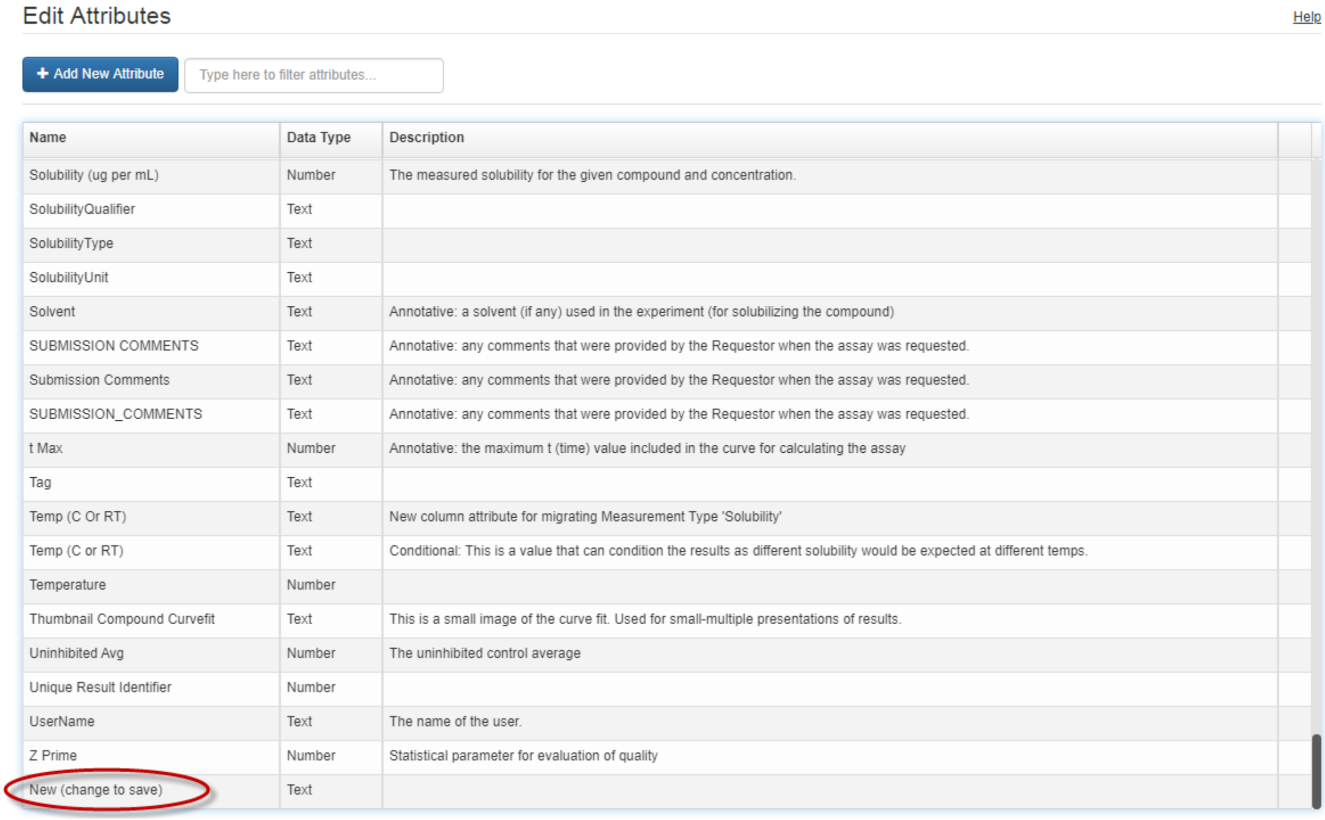
The table lists all currently defined measurements attributes. Each row represents an attribute template. From the table, attributes can be edited or deleted.

3.2.1 Defining a New Attribute

Note: You can enter a query string in the text box located to the right of the **Add New Attribute** button to filter the attributes in the table.

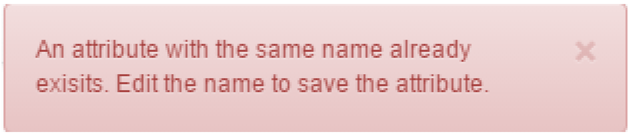
To add a new attribute:

1. Click the **+Add New Attribute** button to add a new row to the bottom of the table, similar to the example shown below.



Name	Data Type	Description
Solubility (ug per mL)	Number	The measured solubility for the given compound and concentration.
SolubilityQualifier	Text	
SolubilityType	Text	
SolubilityUnit	Text	
Solvent	Text	Annotative: a solvent (if any) used in the experiment (for solubilizing the compound)
SUBMISSION COMMENTS	Text	Annotative: any comments that were provided by the Requestor when the assay was requested.
Submission Comments	Text	Annotative: any comments that were provided by the Requestor when the assay was requested.
SUBMISSION_COMMENTS	Text	Annotative: any comments that were provided by the Requestor when the assay was requested.
t Max	Number	Annotative: the maximum t (time) value included in the curve for calculating the assay
Tag	Text	
Temp (C Or RT)	Text	New column attribute for migrating Measurement Type 'Solubility'
Temp (C or RT)	Text	Conditional: This is a value that can condition the results as different solubility would be expected at different temps.
Temperature	Number	
Thumbnail Compound Curvefit	Text	This is a small image of the curve fit. Used for small-multiple presentations of results.
Uninhibited Avg	Number	The uninhibited control average
Unique Result Identifier	Number	
UserName	Text	The name of the user.
Z Prime	Number	Statistical parameter for evaluation of quality
New (change to save)	Text	

2. Enter a unique Attribute Name in the New (change to save) text box. If the attribute name already exists, you will be notified that an attribute with the same name already exists, and that you must edit the name to save the attribute. The text in the row will change to red until this violation is resolved.



An attribute with the same name already exisits. Edit the name to save the attribute.

3. Select the Data Type (Number, Text, Date or Image) from the drop-down list. An optional description can be entered.

After navigating from this new row, the attribute is automatically saved to the metastore service.

3.2.2 Editing an Existing Attribute

To edit an attribute:

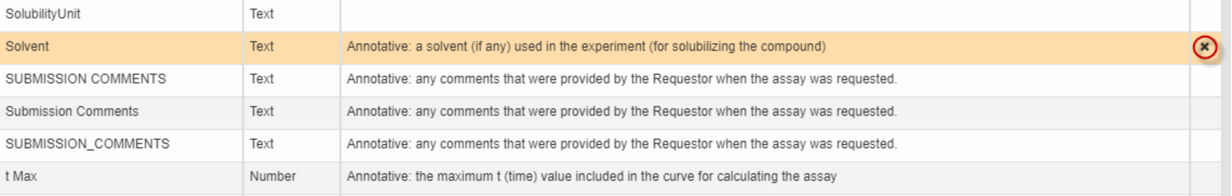
1. Click the cell to edit.
2. Make the necessary modifications.

After navigating from the cell, any edits are automatically updated in the metastore service.

3.3.3 Deleting an Attribute

To delete an attribute:

1. Hover the mouse over the attribute to delete. An 'X' icon appears in the last column for that row.



SolubilityUnit	Text	
Solvent	Text	Annotative: a solvent (if any) used in the experiment (for solubilizing the compound)
SUBMISSION COMMENTS	Text	Annotative: any comments that were provided by the Requestor when the assay was requested.
Submission Comments	Text	Annotative: any comments that were provided by the Requestor when the assay was requested.
SUBMISSION_COMMENTS	Text	Annotative: any comments that were provided by the Requestor when the assay was requested.
t Max	Number	Annotative: the maximum t (time) value included in the curve for calculating the assay

2. Click the 'X' icon. The attribute is deleted, and the following message is displayed.

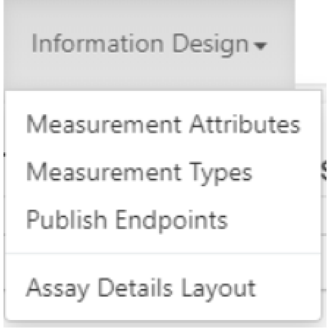
Sucessfully deleted attribute

3.3 Managing Measurement Types

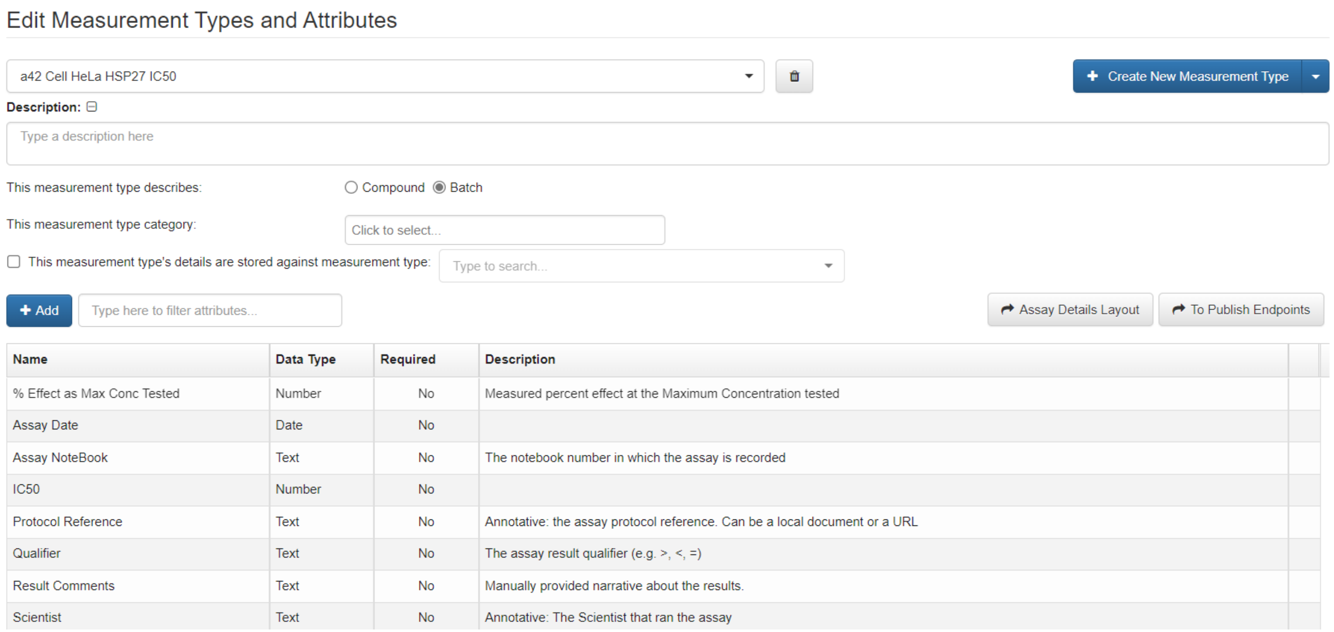
Measurement types are a category of measurements that are similar. The measurement types are managed in the **Edit Measurement Types and Attributes** page. Measurement types can be associated with a Compound or Batch.

To access the Edit Measurement Types and Attributes page:

1. From the Information Design drop-down list box, select **Measurement Types**.



The Edit Measurement Types and Attributes page opens, similar to the example shown below.



Edit Measurement Types and Attributes

a42 Cell HeLa HSP27 IC50

Description:

Type a description here

This measurement type describes: ○ Compound ● Batch

This measurement type category: Click to select...

☐ This measurement type's details are stored against measurement type: Type to search...

Name	Data Type	Required	Description
% Effect as Max Conc Tested	Number	No	Measured percent effect at the Maximum Concentration tested
Assay Date	Date	No	
Assay NoteBook	Text	No	The notebook number in which the assay is recorded
IC50	Number	No	
Protocol Reference	Text	No	Annotative: the assay protocol reference. Can be a local document or a URL
Qualifier	Text	No	The assay result qualifier (e.g. >, <, =)
Result Comments	Text	No	Manually provided narrative about the results.
Scientist	Text	No	Annotative: The Scientist that ran the assay

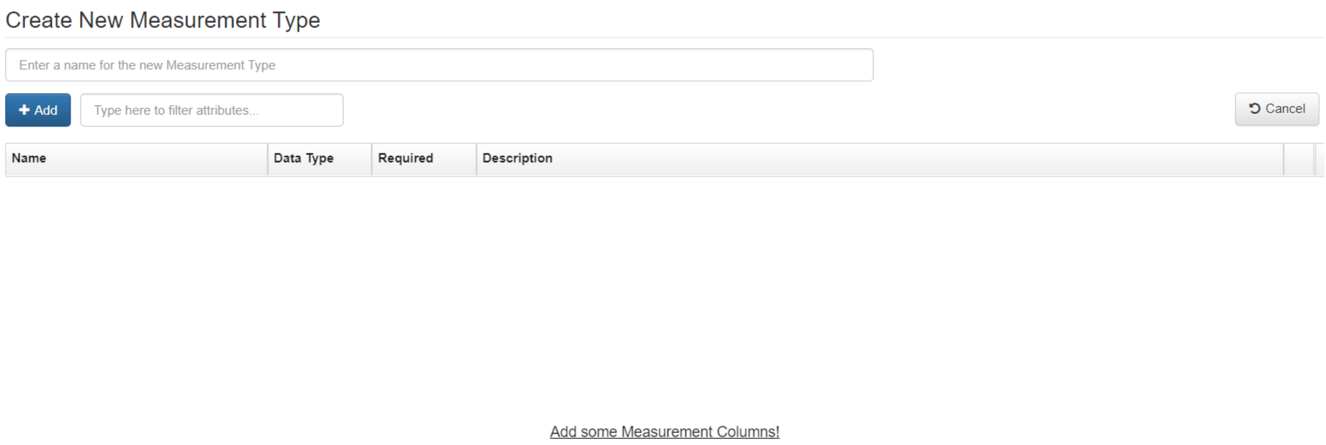
The Edit Measurement Types and Attributes page is a single page application for adding measurement attributes to a selected measurement type. In addition, you can delete attributes from the selected measurement type. From here, you can also choose a measurement type as the details of another measurement type. You can also change the ‘Required’ status from Yes to No and vice versa. From here, you can also create new Measurement Types, and proceed directly to defining the mapping for the endpoint publication map.

The table lists all currently defined measurement attributes for the selected measurement type. Each row represents an attribute template.

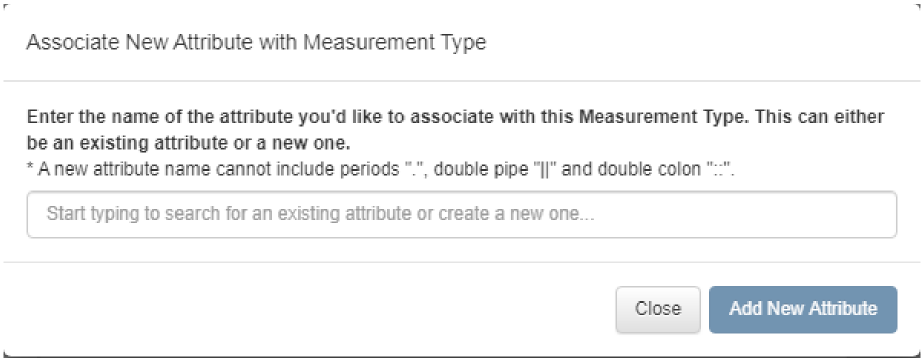
3.3.1 Defining a New Measurement Type

To create a new measurement type:

1. Click the **+ Create New Measurement Type** button to open the Create New Measurement Type page, similar to the example shown below.



2. Enter a unique name for the new Measurement Type.
3. Click the **Add** button. The Associate New Attribute with Measurement Type dialog is displayed.



Enter the name of the attribute you'd like to associate with this Measurement Type. This can either be an existing attribute or a new one.

* A new attribute name cannot include periods ".", double pipe "||" and double colon "::".

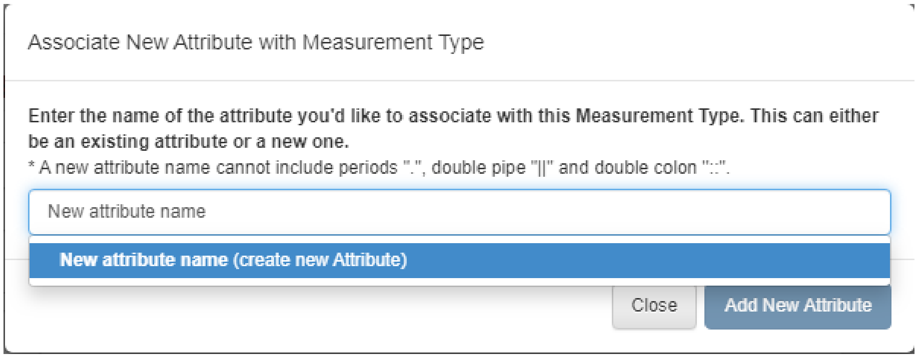
From here, you can select an existing attribute to associate with the measurement type or create a new attribute.

a) From the drop-down list box, select an existing attribute directly or type to search for an existing attribute and then click the **Add New Attribute** button to add the selected attribute to the measurement type.

b) To create a new attribute, type a new attribute name to display the Create New Attribute option, similar to the example shown below.

Note: The attributes that have already been added to the measurement type will not be shown in the drop-down list box.

Note: If you have very large number of attributes available in the system, the drop-down list box will only list 2000 items for selection. You will need to keep typing in order for it to update continuously and narrow down the available items for selection.



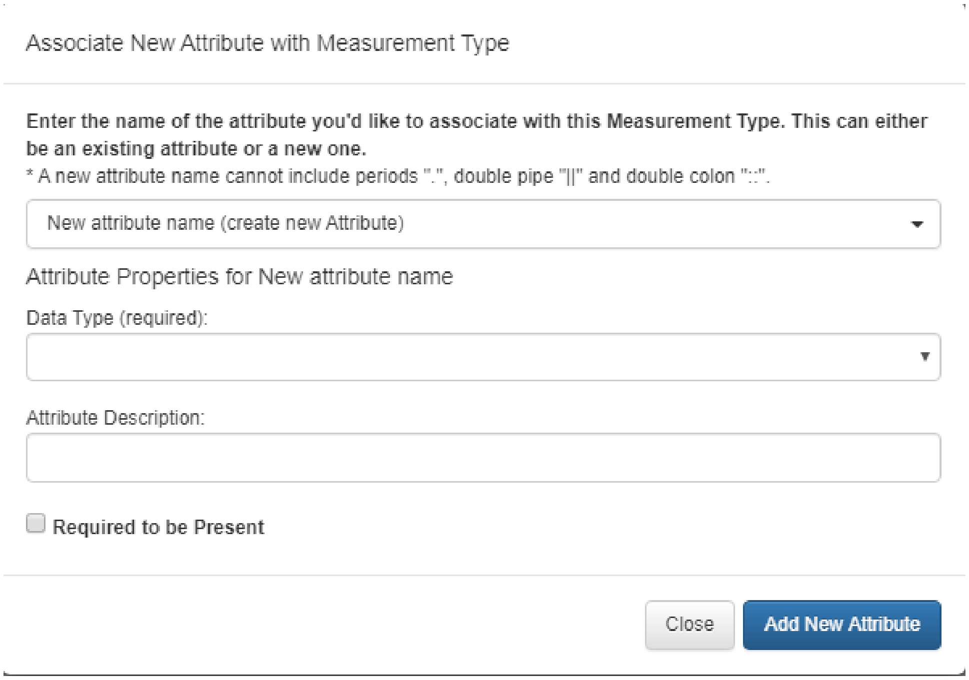
Associate New Attribute with Measurement Type

Enter the name of the attribute you'd like to associate with this Measurement Type. This can either be an existing attribute or a new one.
* A new attribute name cannot include periods ".", double pipe "||" and double colon "::".

New attribute name

New attribute name (create new Attribute)

i. Select the new attribute name (create new Attribute) to expand the dialog, similar to the example shown below.



Associate New Attribute with Measurement Type

Enter the name of the attribute you'd like to associate with this Measurement Type. This can either be an existing attribute or a new one.
* A new attribute name cannot include periods ".", double pipe "||" and double colon "::".

New attribute name (create new Attribute)

Attribute Properties for New attribute name

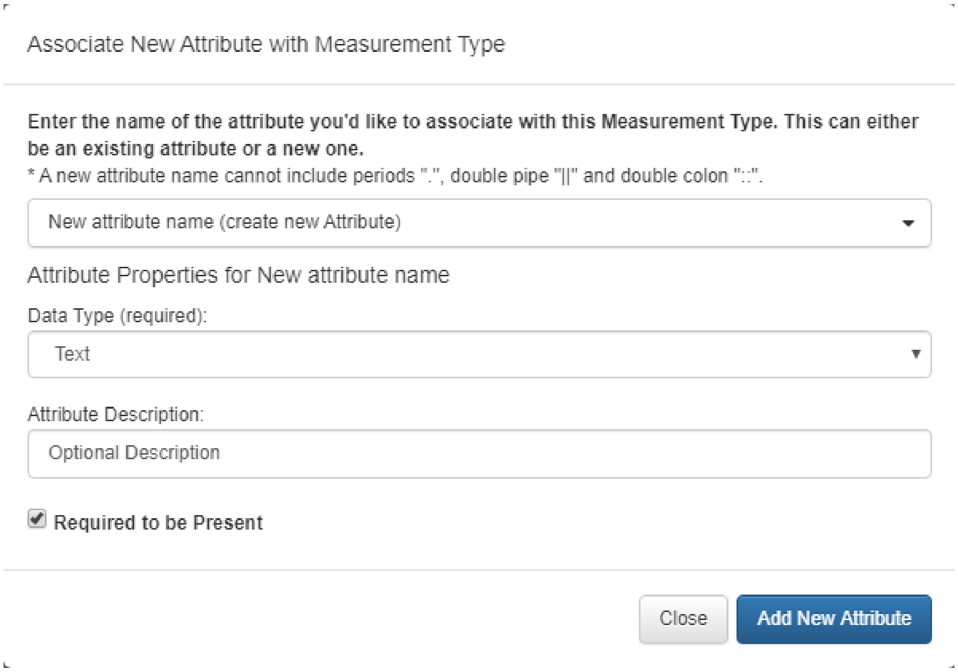
Data Type (required):

Attribute Description:

☐ Required to be Present

ii. Specify the Attribute properties for the new attribute (data type, optional description).

iii. If the attribute is required, enable the **Required to be Present** checkbox.



Associate New Attribute with Measurement Type

Enter the name of the attribute you'd like to associate with this Measurement Type. This can either be an existing attribute or a new one.

* A new attribute name cannot include periods ".", double pipe "||" and double colon "::".

New attribute name (create new Attribute)

Attribute Properties for New attribute name

Data Type (required): Text

Attribute Description: Optional Description

☑ Required to be Present

iv. Click the **Add New Attribute** button to add the new attribute to the current measurement type.

v. Repeat these steps to add additional new attributes to the measurement type. Click Close when you are finished.

vi. Enter an optional description for the measurement type.

vii. Select if the new measurement type is associated with a Compound or Batch. By default, Batch is selected.

If applicable, select the measurement type category (PKStudy, PKDetail, Ppb). These refer to measurement types from Signals VitroVivo. If a measurement type is identified with one of these categories, it will subsequently be targeted for use in the Target Engagement Profile App. For example, the PK Parameters measurement type which comes directly from Signals VitroVivo is tagged with PKStudy measurement type category, the PK Time Concentration measurement type is tagged with PKDetail measurement type category and the Plasma Protein Binding measurement type is tagged with Ppb measurement type category.

3.3.2 Configuring a Measurement Type as Details of another Measurement Type

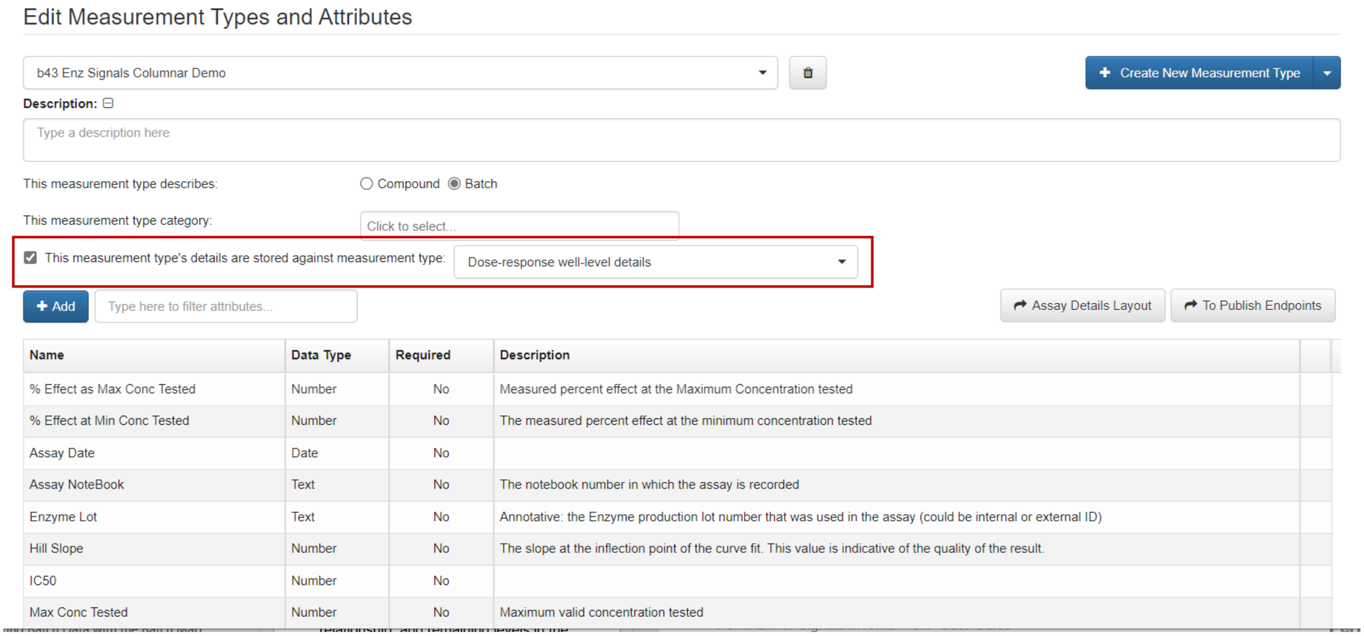
From the Edit Measurement Types and Attributes window, you can choose a measurement type as a detail of another measurement type.

Details measurements store the inputs that make up a final result (e.g. the wells of an IC50).

For example, the “Well-level % inhibition” assay could be designated as a detail of the “IC50” assay. In the Publish Measurements app, you could publish both the details result to the details Measurement Type (e.g. the well-level % inhibition assay) as well as the main assay result (e.g. the IC50 assay).

To configure a measurement type as details of another measurement type:

1. Enable the “This measurement type’s details are stored again measurement type:” checkbox.
2. From the drop-down list, select an existing measurement type to be the details of the selected measurement type. Note a measurement type cannot be the details of itself.



Edit Measurement Types and Attributes

b43 Enz Signals Columnar Demo

Description:

Type a description here

This measurement type describes: ○ Compound ● Batch

This measurement type category: Click to select...

☑ This measurement type's details are stored against measurement type: Dose-response well-level details

Name	Data Type	Required	Description
% Effect as Max Conc Tested	Number	No	Measured percent effect at the Maximum Concentration tested
% Effect at Min Conc Tested	Number	No	The measured percent effect at the minimum concentration tested
Assay Date	Date	No	
Assay NoteBook	Text	No	The notebook number in which the assay is recorded
Enzyme Lot	Text	No	Annotative: the Enzyme production lot number that was used in the assay (could be internal or external ID)
Hill Slope	Number	No	The slope at the inflection point of the curve fit. This value is indicative of the quality of the result.
IC50	Number	No	
Max Conc Tested	Number	No	Maximum valid concentration tested

Note: This drop-down box will list all the measurement types with the exception of the current one allowing you to choose any measurement type in the system to be the details of the current measurement type. In doing so, you can achieve a multi-level parent-detail hierarchy across multiple measurement types, or even a circular reference between measurement types. However, in other Signals Inventa apps, only the first two levels of the hierarchy will be used to represent the parent and detail relationship, and remaining levels in the hierarchy are ignored.

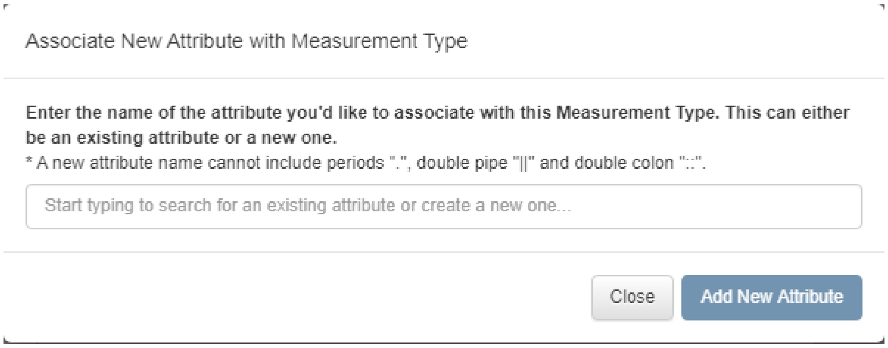
3.3.3 Editing an Existing Measurement Type

From the Edit Measurement Types and Attributes page, you can add or delete attributes to/from an existing measurement type.

Note: You can enter a query string in the text box located to the right of the **Add** button to filter the attributes in the table.

To add an attribute to an existing measurement type:

1. From the Measurement Type drop-down list, select the measurement type to which you want to add an attribute.
2. Click the **Add** button. The Associate New Attribute with Measurement Type dialog is displayed.



Associate New Attribute with Measurement Type

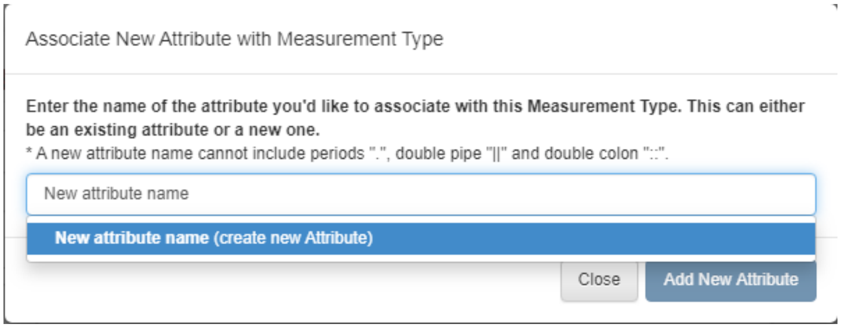
Enter the name of the attribute you'd like to associate with this Measurement Type. This can either be an existing attribute or a new one.

* A new attribute name cannot include periods ".", double pipe "||" and double colon "::".

From here, you can select an existing attribute to associate with the measurement type or create a new attribute.

a) From the drop-down list box, select an existing attribute directly or type to search for an existing attribute and then click the **Add New Attribute** button to add the selected attribute to the measurement type.

b) To create a new attribute, type a new attribute name to display the Create New Attribute option, similar to the example shown below



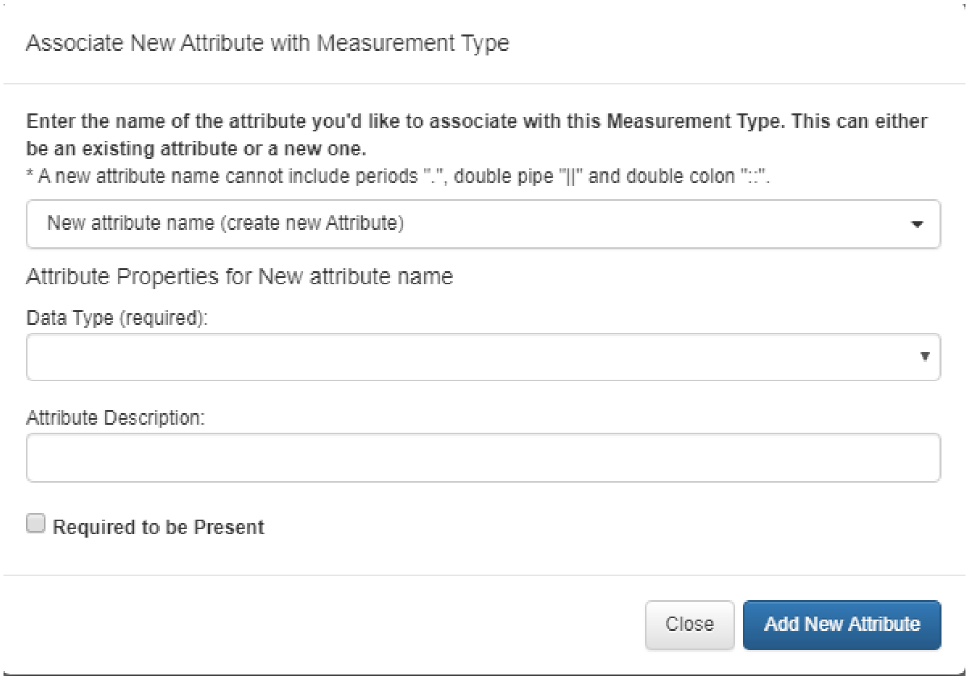
Associate New Attribute with Measurement Type

Enter the name of the attribute you'd like to associate with this Measurement Type. This can either be an existing attribute or a new one.

* A new attribute name cannot include periods ".", double pipe "||" and double colon "::".

New attribute name

i. Select the new attribute name (create new Attribute) to expand the dialog, similar to the example shown below.



Associate New Attribute with Measurement Type

Enter the name of the attribute you'd like to associate with this Measurement Type. This can either be an existing attribute or a new one.
* A new attribute name cannot include periods ".", double pipe "||" and double colon "::".

New attribute name (create new Attribute)

Attribute Properties for New attribute name

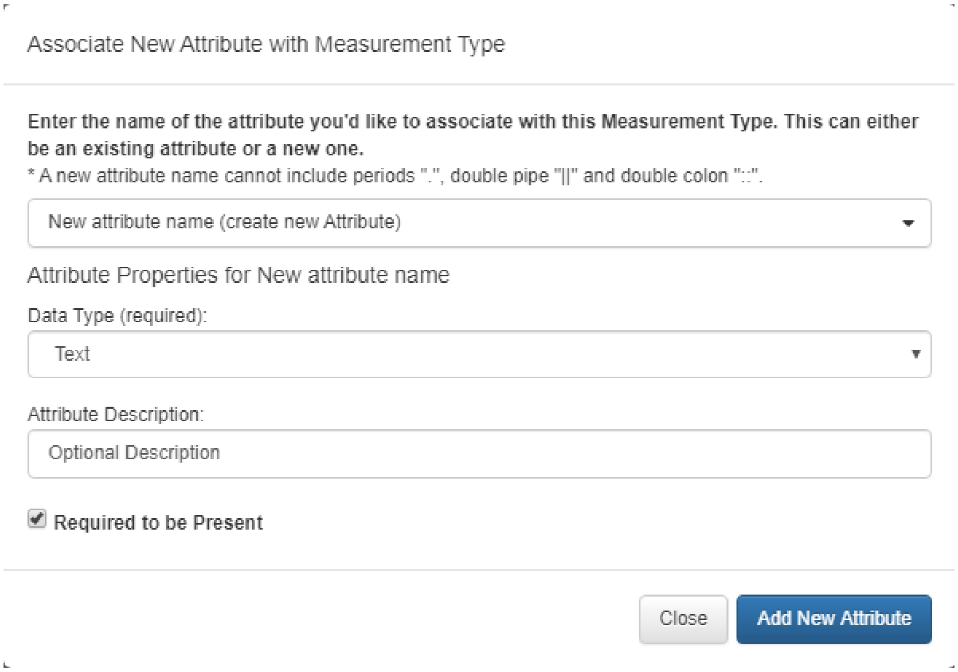
Data Type (required):

Attribute Description:

☐ **Required to be Present**

ii. Specify the Attribute properties for the new attribute (data type, optional description).

iii. If the attribute is required, enable the **Required to be Present** checkbox.



Associate New Attribute with Measurement Type

Enter the name of the attribute you'd like to associate with this Measurement Type. This can either be an existing attribute or a new one.
* A new attribute name cannot include periods ".", double pipe "||" and double colon "::".

New attribute name (create new Attribute)

Attribute Properties for New attribute name

Data Type (required): Text

Attribute Description: Optional Description

☑ **Required to be Present**

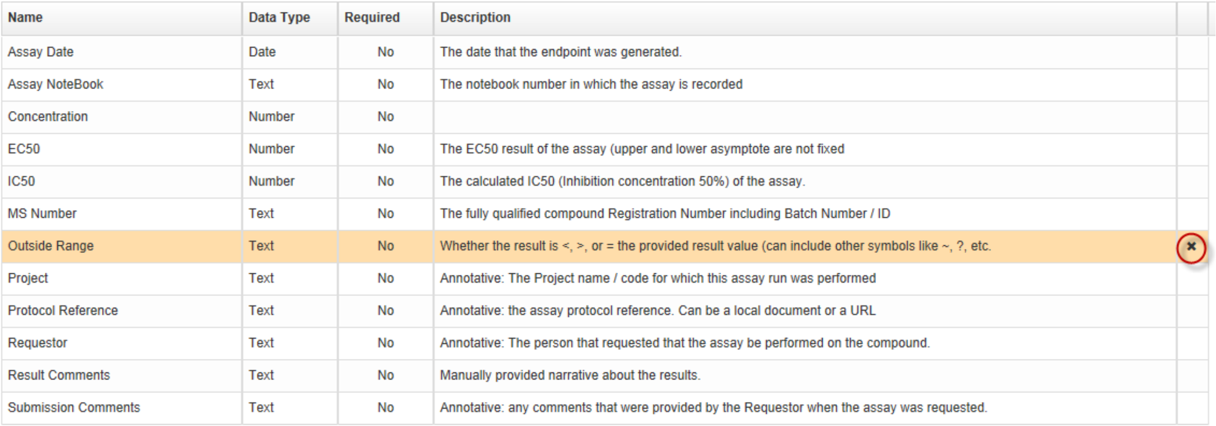
iv. Click the **Add New Attribute** button to add the new attribute to the current measurement type.

viii. Repeat these steps to add additional new attributes to the measurement type. Click **Close** when you are finished.

To delete an attribute from an existing measurement type:

1. From the **Measurement Type** drop-down list, select the measurement type from which you want to delete an attribute.

2. Hover the mouse over the attribute to delete. An ‘X’ icon appears in the last column for that row.



Name	Data Type	Required	Description	
Assay Date	Date	No	The date that the endpoint was generated.	
Assay NoteBook	Text	No	The notebook number in which the assay is recorded	
Concentration	Number	No		
EC50	Number	No	The EC50 result of the assay (upper and lower asymptote are not fixed	
IC50	Number	No	The calculated IC50 (Inhibition concentration 50%) of the assay.	
MS Number	Text	No	The fully qualified compound Registration Number including Batch Number / ID	
Outside Range	Text	No	Whether the result is <, >, or = the provided result value (can include other symbols like ~, ?, etc.	✖
Project	Text	No	Annotative: The Project name / code for which this assay run was performed	
Protocol Reference	Text	No	Annotative: the assay protocol reference. Can be a local document or a URL	
Requestor	Text	No	Annotative: The person that requested that the assay be performed on the compound.	
Result Comments	Text	No	Manually provided narrative about the results.	
Submission Comments	Text	No	Annotative: any comments that were provided by the Requestor when the assay was requested.	

3. Click the ‘X’ icon to delete the attribute from the selected measurement type.

To change the description of the measurement type:

1. From the Measurement Type drop-down list, select the measurement type for which you want to modify the description.

2. In the **Description** text box, type the description for the measurement type.

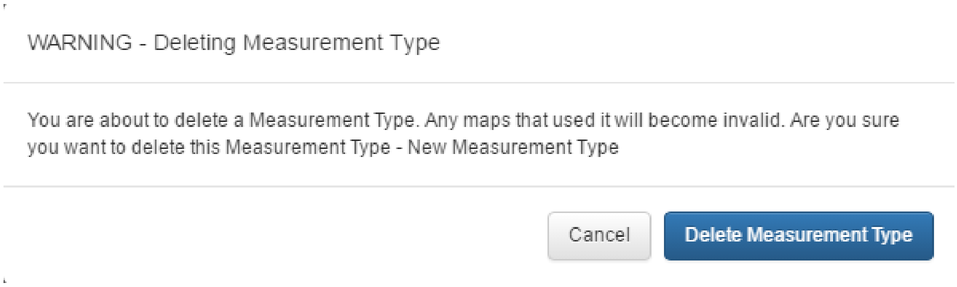
3. Move the focus out of the text box, the description will be persisted automatically.

3.3.4 Deleting a Measurement Type

To delete a measurement type:

1. From the Measurement Type drop-down list box, select the measurement type to delete.

2. Click the Delete Measurement Type 🗑 icon. You will be prompted to confirm the deletion. Any endpoint publication maps using this measurement type will also be deleted.



WARNING - Deleting Measurement Type

You are about to delete a Measurement Type. Any maps that used it will become invalid. Are you sure you want to delete this Measurement Type - New Measurement Type

3.3.5 Defining the Assay Details Layout

For each measurement type, you can define how the assay data of that measurement type will be presented. With the Assay Details Layout definition tool, you can define which attributes of a particular measurement type to display in the Assay Details page , and also you can choose the presentation layout and data format for the attributes.

The **Assay Details Layout** button on the **Edit Measurement Types and Attributes** page will redirect you to the Assay Details Layout page, which will be described in more detail in the Edit Assay Details Layout section.

3.3.6 To Publish Endpoints

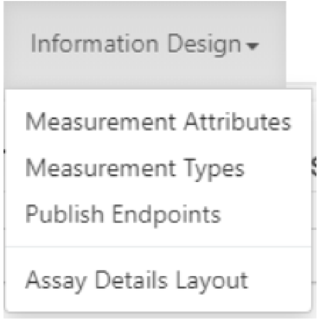
After defining a measurement type, you are encouraged to proceed with the workflow and define the mapping against the endpoint publication map. This can be accomplished by clicking on the **To Publish Endpoints** button. This will take you directly to the Prepare Measurement Types for Publication page. Refer to the section “Managing Publish Endpoints”.

3.4 Managing Publish Endpoints

Endpoint Publication maps relate a measurement type, and most importantly, the endpoints of the measurement type to the Signals Inventa data index. The Endpoint Publication Maps are managed in the Prepare Measurement Types for Publication page.

To access the Prepare Measurement Types for Publication page:

1. From the Information Design drop-down list box, select **Publish Endpoints**.



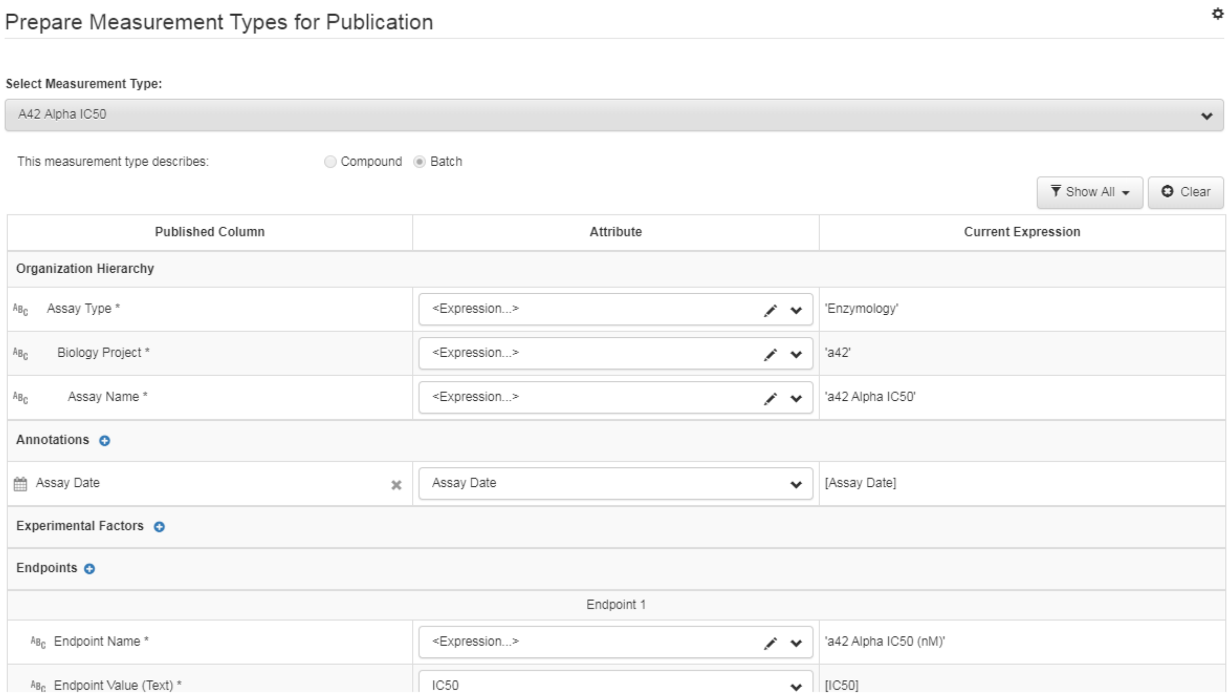
The Prepare Measurement Types for Publication page opens, similar to the example shown below.

According to the system design, each measurement type has an endpoint publication map.

To display an Endpoint Publication Map for a Measurement Type:

1. From the Select Measurement Type drop-down list, select the measurement type for which you want to display the endpoint publication map.

The endpoint publication map information is displayed for the selected measurement type, similar to the example shown below.



Prepare Measurement Types for Publication

Select Measurement Type: A42 Alpha IC50

This measurement type describes: ○ Compound ● Batch

Published Column	Attribute	Current Expression
Organization Hierarchy		
Assay Type *	<Expression...>	'Enzymology'
Biology Project *	<Expression...>	'a42'
Assay Name *	<Expression...>	'a42 Alpha IC50'
Annotations		
Assay Date	Assay Date	[Assay Date]
Experimental Factors		
Endpoints		
Endpoint 1		
Endpoint Name *	<Expression...>	'a42 Alpha IC50 (nM)'
Endpoint Value (Text) *	IC50	[IC50]

The Prepare Measurement Types for Publication page is a single page application for displaying and editing the endpoint publication maps for a measurement type. Publication refers to making the data available to an index.

The table lists the Published Columns (attributes of the index), the attributes (the definition of the published column), and the current expressions for the attributes.

The Published Columns represent different types of attributes outlined in the table below:

Type	Description
Organizational Hierarchy	Organizational hierarchy attributes are used to present the published endpoints in a hierarchy which the user can browse to locate the desired endpoints.
Annotations	Annotative attributes provide information about how the measurement was performed that may be useful to publish.
Experimental Factors	Experimental factors are conditions of the experiments that would typically affect the actual measured value. For example,

	a temperature, pH, or concentration that would affect the outcome.
Endpoints	Endpoints are the actual measured values of interest.

All the required fields (with red box) must be mapped before the measurement type can be used.

Note that adding more endpoints to a measurement does not add columns to the endpoint results table. It actually adds rows to it. On the other hand, adding Annotations or Experimental factors will add columns to results table. As each measurement type can add its own set of attributes, the endpoints results table will become wider and more sparsely populated. These types of attributes are automatically added to the published table.

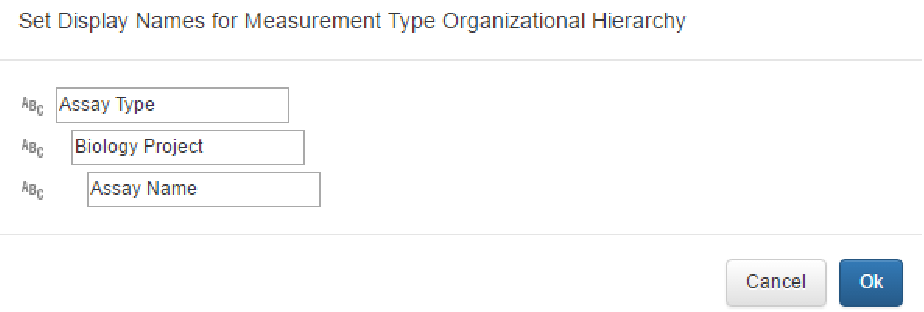
Setting the Display Names for the Measurement Type Organizational Hierarchy:

The display names for the Measurement Type Organizational Hierarchy can be customized for each endpoint publication map.

To set the Display Names for the Measurement Type Organizational Hierarchy:

1. Click on the ⚙ icon located in the top right hand corner of the page.

The Set Display Names for Measurement Type Organizational Hierarchy dialog is displayed, similar to the example shown below.



Assay Type

Biology Project

Assay Name

From here, you can define the display names for the measurement type organizational hierarchy.

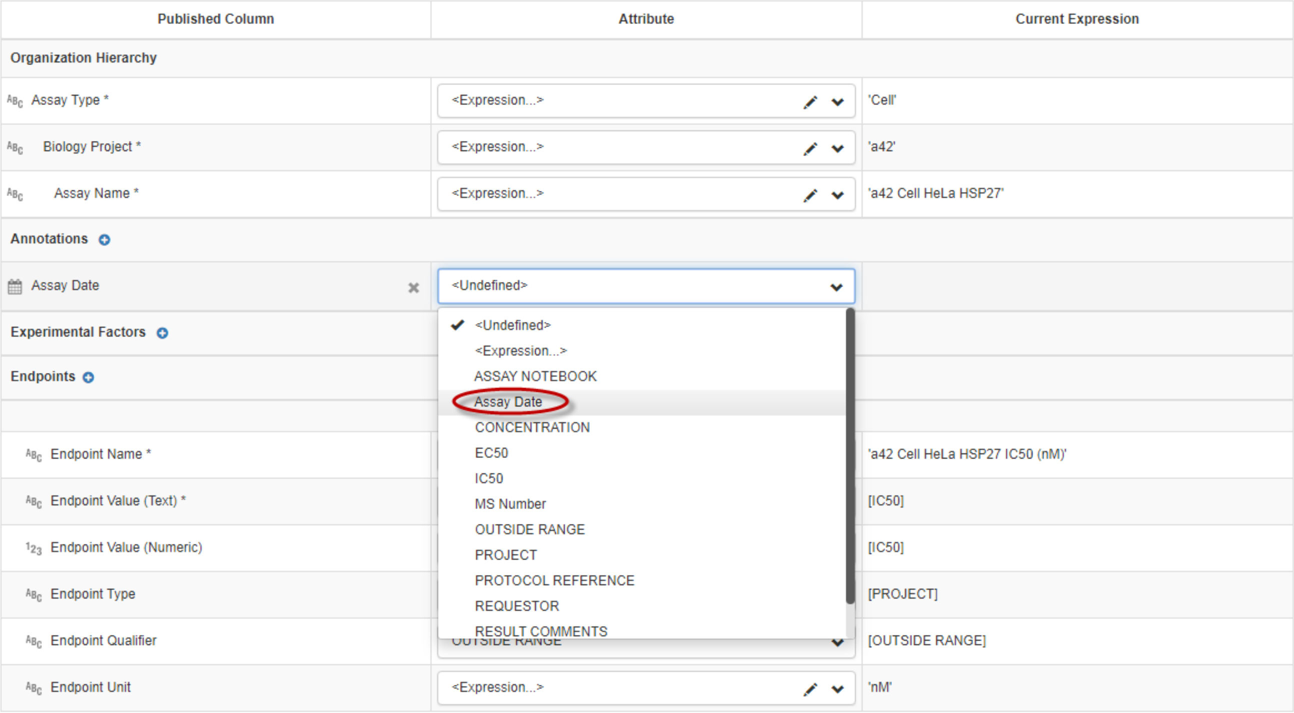
The organization hierarchy is the index (table with summary of results). In Global Search, instead of showing a long list of all endpoint names, they are organized into categories (folders). The Set Display Names for Measurement Type Organization Hierarchy screen allows the naming of those folders in the Endpoint Publication mapping screen. The actual values you will see on the tree are the values mapped in. For example, if you want the Solubility endpoint to appear under ADMET> Project Avalon > Solubility > Solubility (gr/sml) at 25C, you would map the first three values above to the top three hierarchical columns and the fourth value above to the Endpoint Name column. If you added a second endpoint to the map, it would appear in the tree under the same folder as the first endpoint. .

3.4.1 Defining the Mapping for a Published Column

For each Published column, you can define the definition of the published column (attribute). The attribute defines what values will be published. By default, the Published Columns are set to <Undefined>. You have the option to select a current attribute or create an expression.

To map to an attribute:

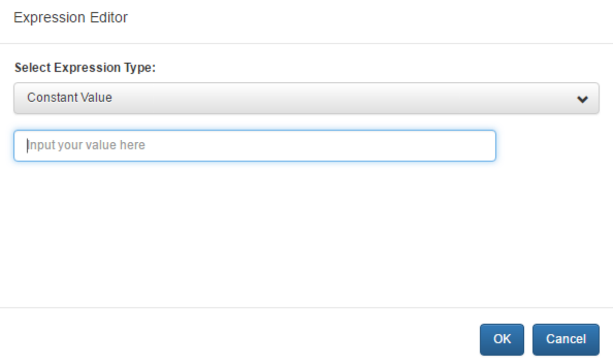
1. From the Attribute drop-down list for the selected Published Column, select the Attribute name.



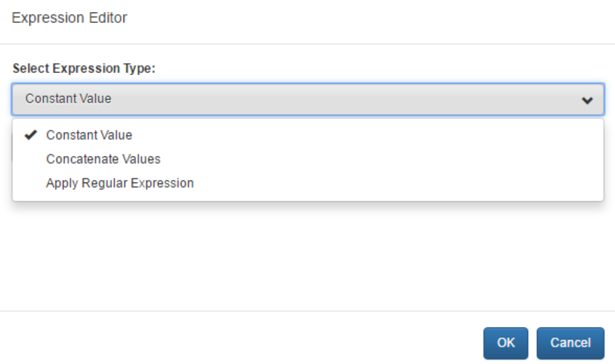
Published Column	Attribute	Current Expression
Organization Hierarchy		
Assay Type *	<Expression...>	'Cell'
Biology Project *	<Expression...>	'a42'
Assay Name *	<Expression...>	'a42 Cell HeLa HSP27'
Annotations		
Assay Date	<Undefined>	
Experimental Factors		
Endpoints		
Endpoint Name *		'a42 Cell HeLa HSP27 IC50 (nM)'
Endpoint Value (Text) *		[IC50]
Endpoint Value (Numeric)		[IC50]
Endpoint Type		[PROJECT]
Endpoint Qualifier	OUTSIDE RANGE	[OUTSIDE RANGE]
Endpoint Unit	<Expression...>	'nM'

To map to an expression:

1. From the Attribute drop-down list for the selected Published Column, select <Expression> to open the **Expression Editor** dialog.



2. From the **Select Expression Type** drop-down list box, select the expression type.

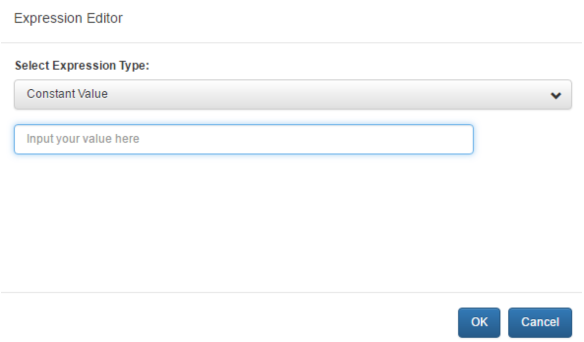


The following options are available:

Option	Description
Constant Value	The expression will return a user-defined constant value.
Concatenate Values	In this expression you can concatenate Attributes and literal strings. When the Signals Data Factory ingests CSV data, the expression will return values by concatenating the values of the Attributes and literal strings for each row.
Apply Regular Expression	In this expression, user can select an Attribute and specify a regular expression as a pattern. When the Signals Data Factory ingests CSV data, the expression will use the regular pattern to extract the result values from the Attribute for each row.

a) To create a Constant Value expression:

i. Select Constant Value from the Select Expression Type drop-down list. A dialog, similar to the example below appears.



ii. Input a value in the text box.

iii. Click **OK** to save the expression.

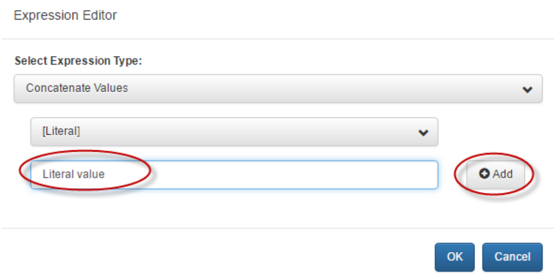
Note: When creating an expression for Organization Hierarchy published columns (e.g. Assay Type, Biology Project, Assay Name), it is important that these hierarchy names do not have the same string value with differing capitalization (e.g. cell, Cell) when they define AER mapping.

b) To create a Concatenate Values expression

i. Select Concatenate Values from the Select Expression Type drop-down list. A dialog, similar to the example below appears.

ii. Select an Attribute from the drop-down list. Click the **+Add** button to add the selected attribute to the expression.

iii. Select <Literal> from the drop-down list box. Input the literal expression in the textbox. Click **+Add** button to add the literal expression.

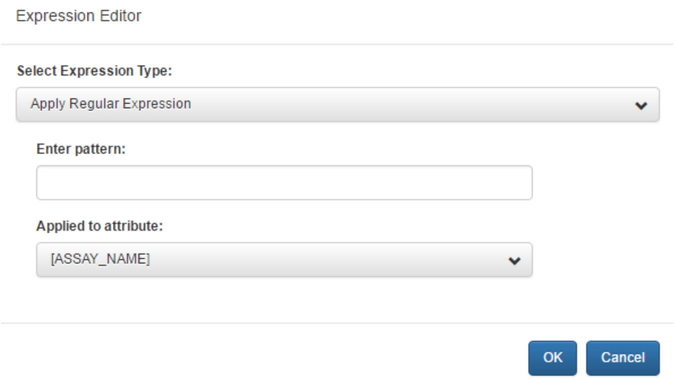


iv .Repeats steps ii and iii to add all attributes and literal values to the expression.

ix. Click **OK** to save the expression.

c) To create an Apply Regular Expression:

i. Select Apply Regular Expression from the Select Expression Type drop-down list. A dialog, similar to the example below appears.



ii. Select an attribute from the Applied to attribute drop-down list box.

iii. Enter a regular pattern in the Enter pattern text box.

iv. Click **OK** to save the expression.

To edit an expression:

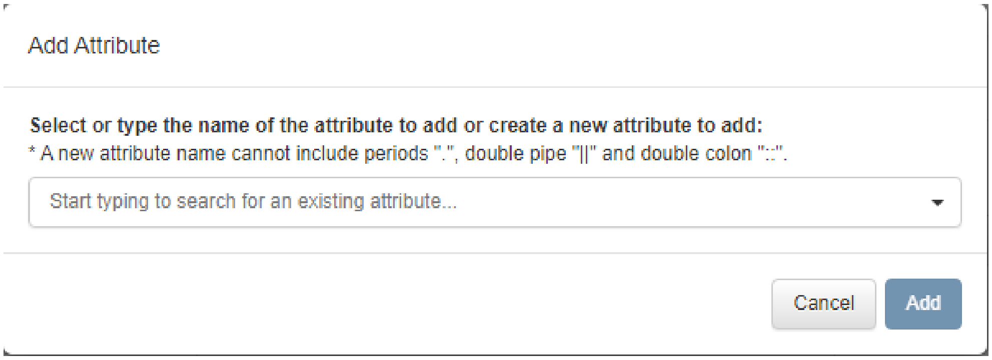
1. Select the ✎ icon to open the **Expression Editor** dialog.
2. Edit the expression
3. Click **OK** to save the expression.

3.4.2 Adding and Removing Published Columns to/from the Endpoint Publication Map

To add a published column:

1. Click on the ⊕ icon next to the heading (e.g. Annotations).

The Add Attribute dialog is displayed.



Add Attribute

Select or type the name of the attribute to add or create a new attribute to add:

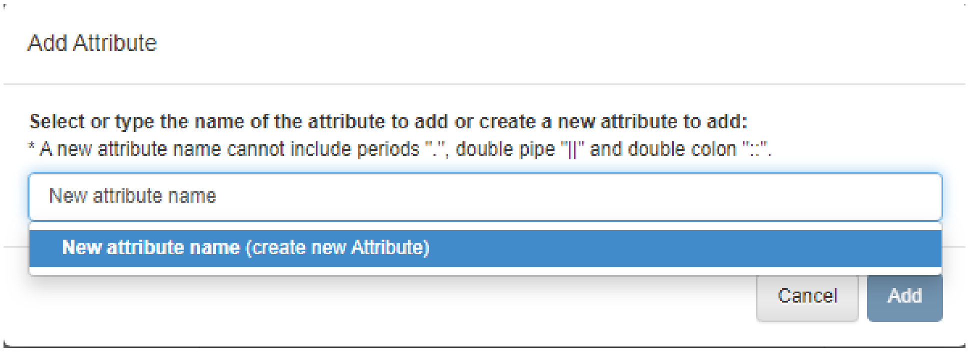
* A new attribute name cannot include periods ".", double pipe "||" and double colon "::".

2. From here, you can select an existing attribute or create a new attribute.

a) From the drop-down list box, select an existing attribute directly or type to search for an existing attribute and then click the **Add** button. The published column is added to the table.

Note: When a new attribute is created in this use case, it will also be added as a measurement attribute in the Signals Data Factory. As a result, the next time you choose an existing attribute from this dialog box, you will notice that some of the attribute names in the list are suffixed with an asterisk("*") indicating that they are already a measurement attribute in the Signals Data Factory and were created by other measurement types.

b) To create a new attribute, type a new attribute name to display the Create New Attribute option, similar to the example shown below.



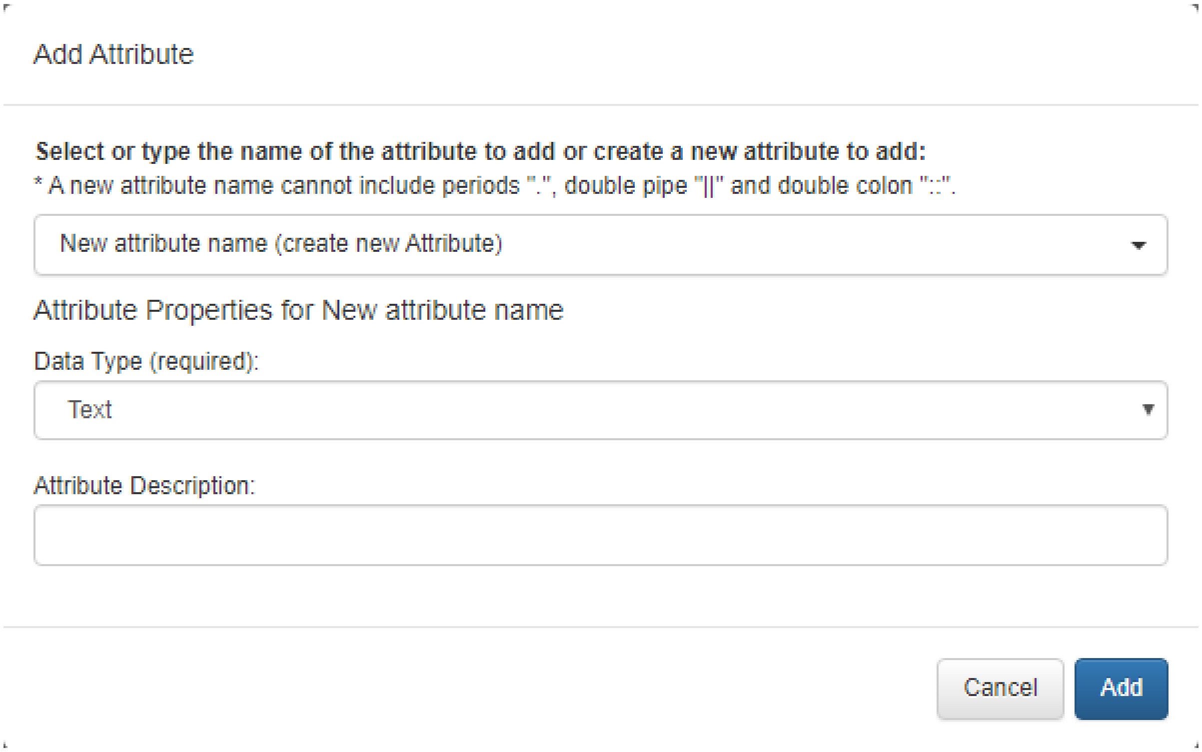
Add Attribute

Select or type the name of the attribute to add or create a new attribute to add:

* A new attribute name cannot include periods ".", double pipe "||" and double colon "::".

New attribute name

   i. Select the new attribute name (create new Attribute) to expand the dialog, similar to the example shown below.



Add Attribute

Select or type the name of the attribute to add or create a new attribute to add:
* A new attribute name cannot include periods ".", double pipe "||" and double colon "::".

New attribute name (create new Attribute)

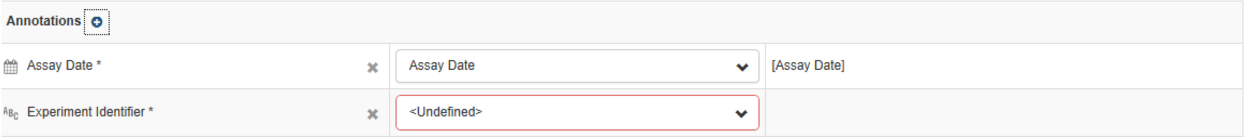
Attribute Properties for New attribute name

Data Type (required): Text

Attribute Description:

ii. Specify the Attribute properties for the new attribute (data type, optional description).

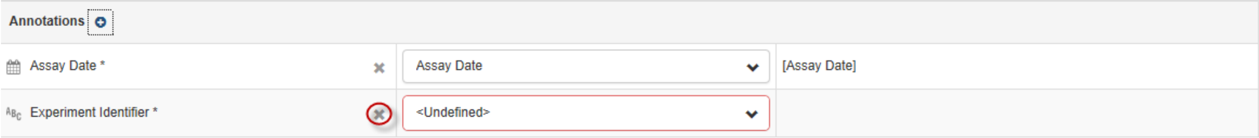
iii. Click **Add**. The published column is added to the table.



Annotations		
Assay Date *	Assay Date	[Assay Date]
Experiment Identifier *	<Undefined>	

To delete a published column:

1. Click on the ✖ icon located to the right of the published column. The published column will be deleted from the endpoint publication map.



Annotations		
Assay Date *	Assay Date	[Assay Date]
Experiment Identifier *	<Undefined>	

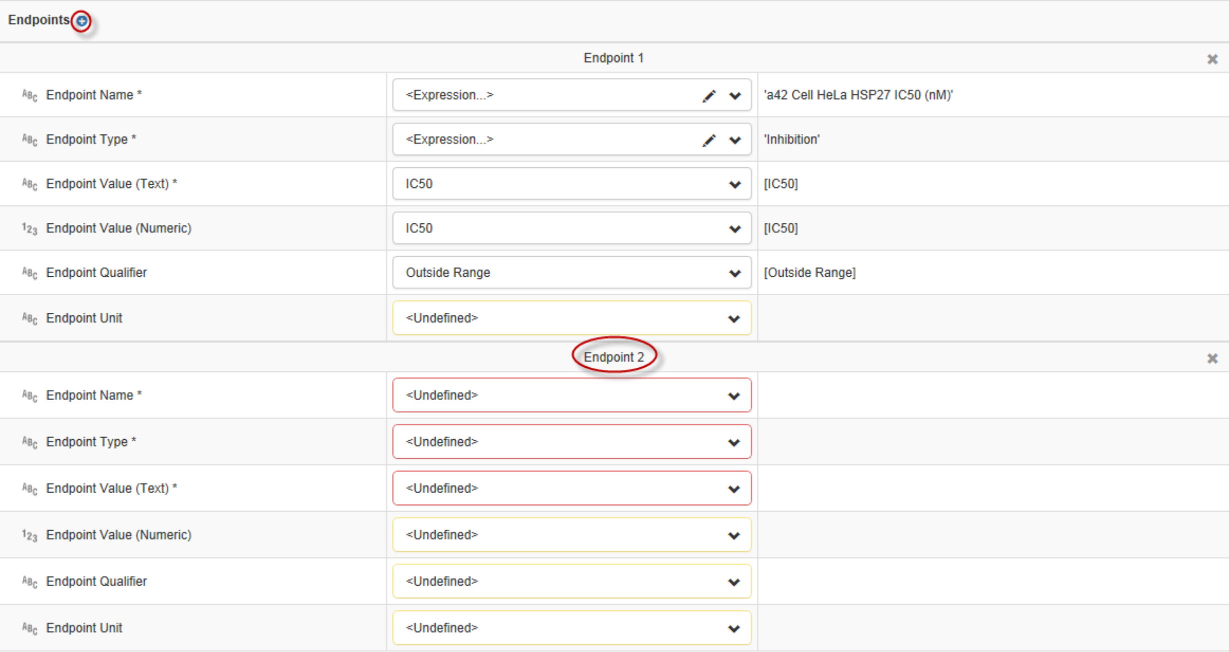
3.4.3 Adding/Removing Endpoints from the Endpoint Publication Map

Endpoints are multi-valued attributes that include the key measured value together with additional information (e.g. name, type, numerical measured value, textual measured value, qualifier, and unit).

When a new endpoint is added to the endpoint publication map, all attributes are added as Published Columns.

To add a new endpoint:

1. Click on the ⊕ icon next to the Endpoints heading.



Endpoints ⊕

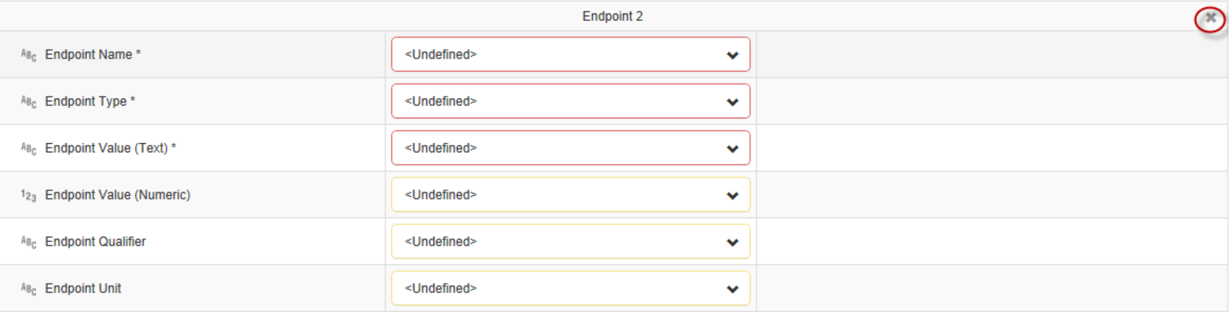
Endpoint 1		
Endpoint Name *	<Expression...>	'a42 Cell HeLa HSP27 IC50 (nM)'
Endpoint Type *	<Expression...>	'Inhibition'
Endpoint Value (Text) *	IC50	[IC50]
Endpoint Value (Numeric)	IC50	[IC50]
Endpoint Qualifier	Outside Range	[Outside Range]
Endpoint Unit	<Undefined>	

Endpoint 2		
Endpoint Name *	<Undefined>	
Endpoint Type *	<Undefined>	
Endpoint Value (Text) *	<Undefined>	
Endpoint Value (Numeric)	<Undefined>	
Endpoint Qualifier	<Undefined>	
Endpoint Unit	<Undefined>	

A new endpoint (e.g. Endpoint 2) and its attributes are appended to the table as Published Columns.

To delete an endpoint:

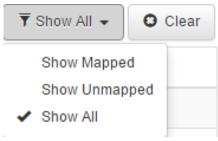
1. Click on the ✖ icon located on the right of the Endpoint row. The endpoint will be deleted from the endpoint publication map.



Endpoint 2		
Endpoint Name *	<Undefined>	
Endpoint Type *	<Undefined>	
Endpoint Value (Text) *	<Undefined>	
Endpoint Value (Numeric)	<Undefined>	
Endpoint Qualifier	<Undefined>	
Endpoint Unit	<Undefined>	

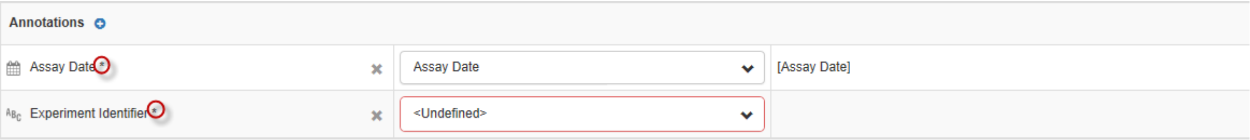
3.4.4 Viewing the Endpoint Publication Map

Clicking on the **Show All** button gives you the option to Show Mapped or Show Unmapped published columns. You can also select to Show All (mapped and unmapped).



Clicking the **Clear** button will set all mappings to <Undefined>.

Published columns with an asterisk (*) suffix indicate mandatory columns that must have a mapping defined for them, similar to the example shown below.



Annotations

Assay Date*	Assay Date	[Assay Date]
Experiment Identifier*	<Undefined>	

The Attribute field will have a red border if mapping is required for the published column but is currently <Undefined>. A yellow border indicates that mapping is optional for the published column.

Endpoint 2

Endpoint Name *	<Undefined>	
Endpoint Type *	<Undefined>	
Endpoint Value (Text) *	<Undefined>	
Endpoint Value (Numeric)	<Undefined>	
Endpoint Qualifier	<Undefined>	
Endpoint Unit	<Undefined>	

3.5 Guided Measurement Type Definition

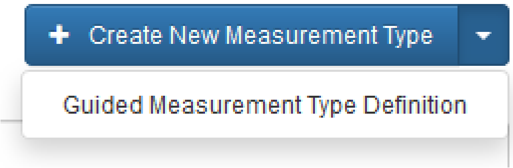
In the case where you have your assay data in CSV files , and you would like to create a measurement type and define the attributes for your assay data, typically, you would first open the Edit Attributes page to define the attributes according to the columns of your data source, then use the Edit Measurement Types and Attributes to create a new measurement type and attach the pre-created attributes to this measurement type, then define the assay endpoint mappings by using the Publish Endpoints tool, and finally use the Publish Measurements tool to define the mappings between your data and the measurement type. This workflow is often complex and be prone to error especially when your data contains a large number of columns.

The Guided Measurement Type Definition tool assists you to do all of these operations in a single screen with less typing and mouse-clicks. In this section, you will learn how to create the attributes, measurement types and generate the mappings for when you already have your data on hand.

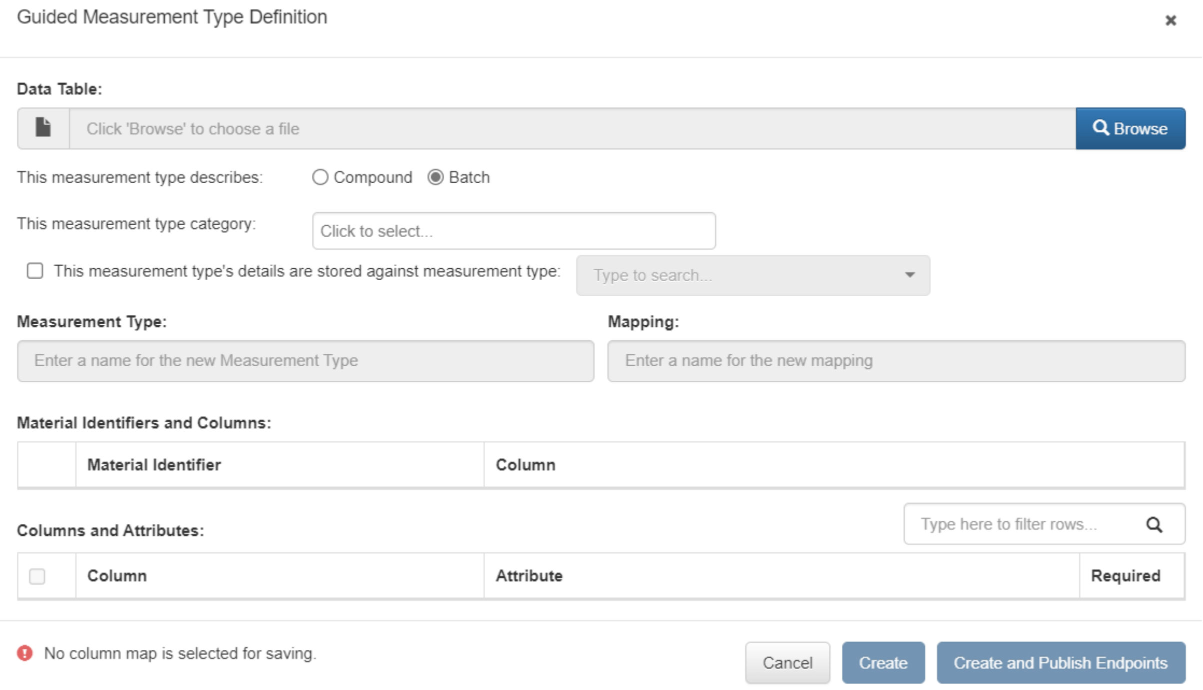
3.5.1 Creating the Measurement Type and Mappings from Flat Files

You may use the Guided Measurement Type Definition screen to create the measurement types and AER mappings from an existing flat file which contains your assay data.

1. In the **Edit Measurement Types and Attributes** page, click the down arrow icon at the right side of the **Create New Measurement Type** button. You will see the **Guided Measurement Type Definition** button.



2. Click the **Guided Measurement Type Definition** button to open the Guided Measurement Type Definition dialog.



This measurement type describes: ○ Compound ● Batch

No column map is selected for saving.

3. Click the **Browse** button to open the **File Upload** dialog, from which you can select a file with .csv, .txt, .dat extension. A file which contains the comma-separated content format but without an extension is also supported.

4. Select if the new measurement type is associated with a Compound or Batch. By default, Batch is selected.

5. If applicable, select the measurement type category (PKStudy, PKDetail, Ppb). These refer to measurement types from Signals VitroVivo. If a measurement type is identified with one of these categories, it will subsequently be targeted for use in the Target Engagement Profile App. For example, the PK Parameters measurement type which comes directly from Signals VitroVivo is tagged with PKStudy measurement type category, the PK Time Concentration measurement type is tagged with PKDetail measurement type category and the Plasma Protein Binding measurement type is tagged with Ppb measurement type category.

6. To configure a measurement type as details of another measurement type, enable the “This measurement type’s details are stored against the measurement type:” checkbox. From the drop-down list, select an existing measurement type to be the details of the newly created measurement type.

7. In the **Measurement Type** text box, input the name for the new measurement type.

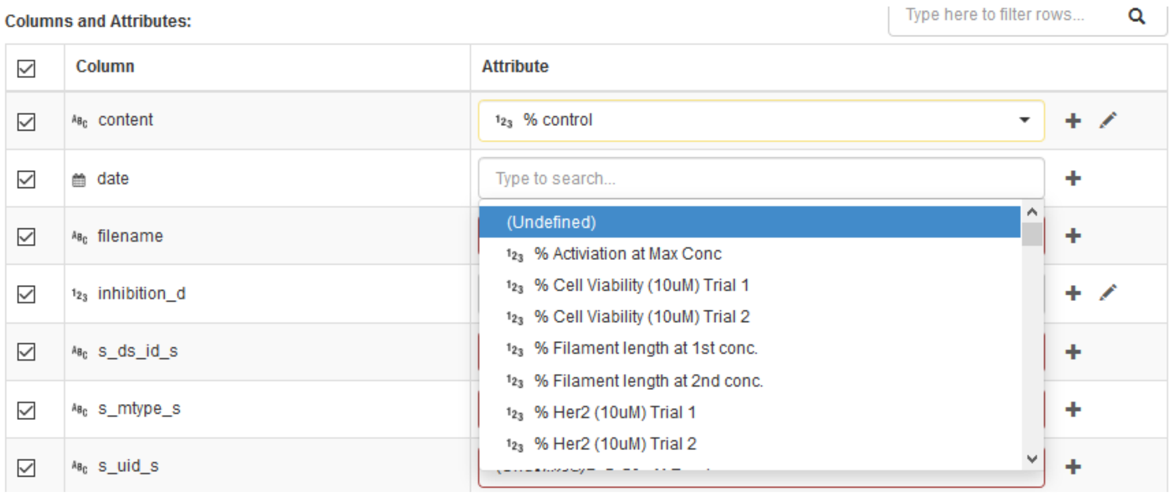
8. Select if the new measurement type is associated with a Compound or Batch.

9. In the **Mapping** text box, input the name for the mapping which maps the measurement type attributes to your data columns.

10. In the **Material Identifiers and Columns** grid, if the Measurement Type is set to Batch, choose the column which you want to map to the Compound entity and Batch entity. Specifically, choose an ID column from your measurement data to be mapped to the Compound Batch ID column, and choose an ID column from your measurement data to be mapped to the Compound ID column. Note that the Compound Batch ID is a mandatory identifier which must be mapped. Compound ID, on the other hand, is optional and if it is absent, will use the same mapping as Compound Batch ID column. If the Measurement type is set to Compound, only an ID column from your measurement data to be mapped to the Compound ID is required.

11. In the **Columns and Attributes** grid, choose the columns which you want to convert to the measurement type attributes. Once a column is selected, the corresponding drop-down box in the **Attribute** cell will be surrounded by a red rectangle if the attribute has not been defined.

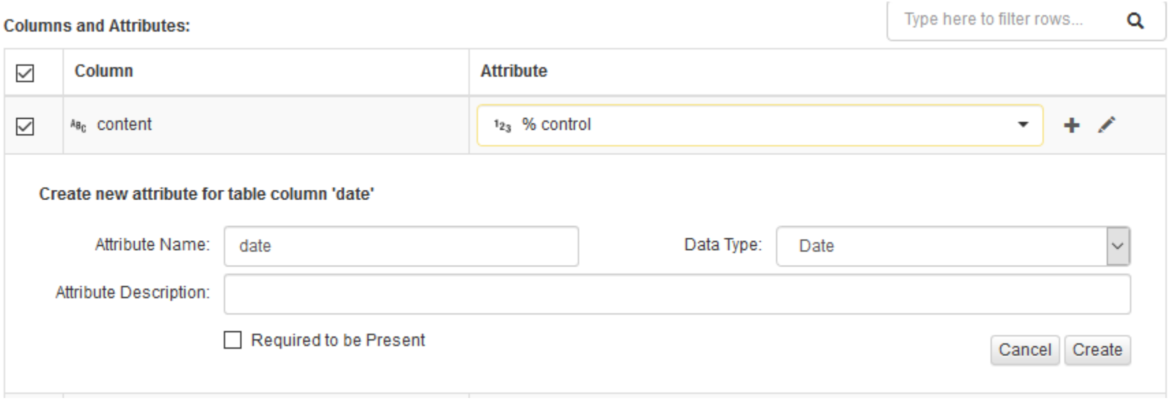
12. In the corresponding **Attribute** drop-down, select an existing attribute which you wish to map to the current data column. If the type of the selected attribute does not match with the column data type, a yellow rectangle will display.



Columns and Attributes:

☑	Column	Attribute
☑	content	% control
☑	date	Type to search...
☑	filename	
☑	inhibition_d	
☑	s_ds_id_s	
☑	s_mtype_s	
☑	s_uid_s	

13. You can also click the "**+**" button at the right side of the **Attribute** drop-down to quickly add a new attribute. By clicking this button, the grid will expand with an additional section, within which you can define the properties for the new attribute. All the properties are the same as the ones that you can see from the attribute management screen.



Columns and Attributes:

☑	Column	Attribute
☑	content	% control

Create new attribute for table column 'date'

Attribute Name: date

Data Type: Date

Attribute Description:

☐ Required to be Present

14. You can click the **Cancel** button to discard the changes or **Create** button to save the changes.

15. Similarly, once you have mapped an existing attribute to the data column, you will be able to modify the mapped attribute by clicking the "✎" icon. This will also expand the grid allowing you to modify the mapped attribute that will be attached to the newly created measurement type.

16. You will be able to filter the rows in the grid by using the type-ahead text box at the upper-right corner of the **Columns and Attributes** grid.

17. If any error occurs, the error information will be shown at the bottom of the dialog, similar to the example shown below:

A selected item must be mapped to an attribute.

In such case, you will not be able to click the **Create** button to save the measurement type

18. Once the settings have all been defined correctly, a green check icon will display at the bottom of the dialog, and you will be able to create the measurement type and corresponding mappings by clicking the **Create** button. You can also click the **Create and Publish Endpoints** button, such that the **Prepare Measurement Types for Publication** page will be shown immediately after the measurement type has created successfully.

19. After the file has been parsed and read successfully, the fields will be populated to the **Columns and Attributes** grid automatically.

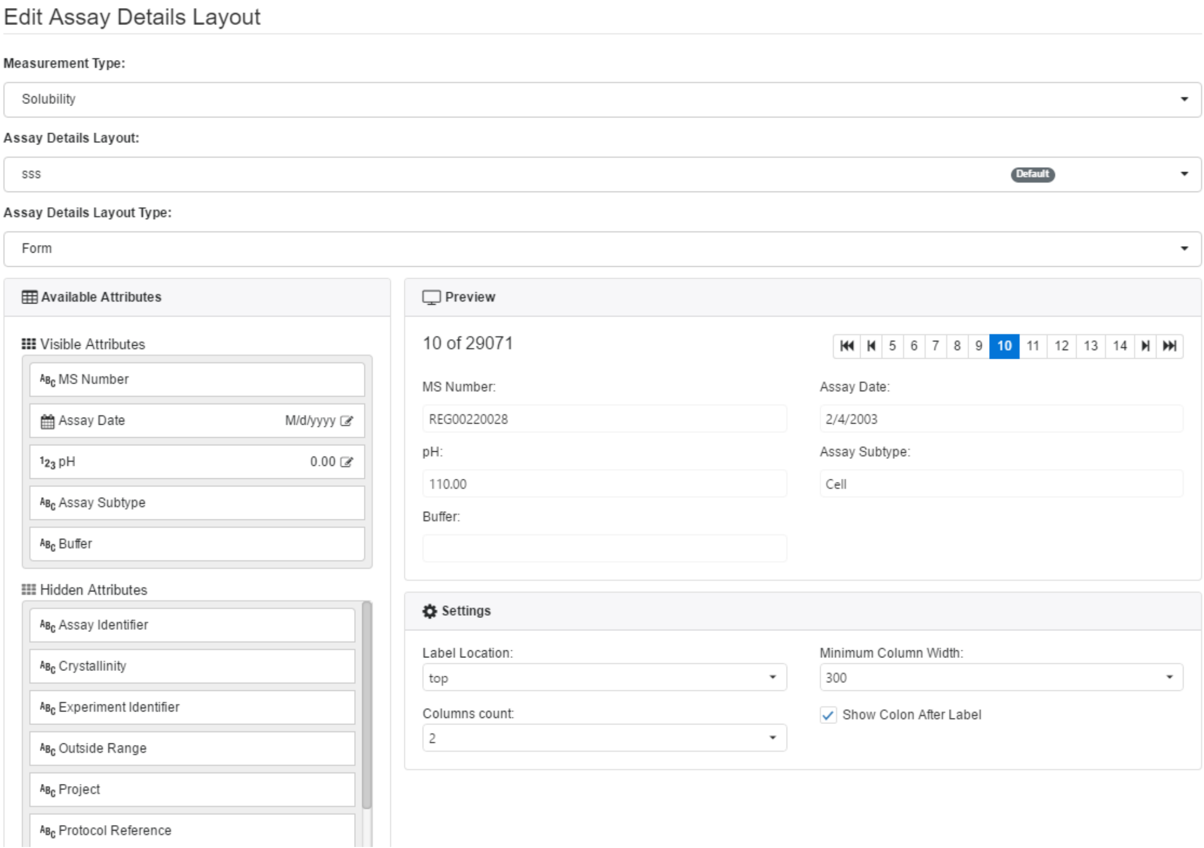
3.6 Managing Assay Details Layout

The Assay Details visualization shows the assay data from different measurement types for a particular candidate (usually chemical compound). Users can define how the assay data will be represented based on the measurement types, by using the Assay Details Layout definition page.

To open the Assay Details Layout:

In both Spotfire Analyst Client and Web Player:

1. Open data in Spotfire.
2. Select **Tools > Signals Inventa > Manage Measurement Types** from the main menu to add the Manage Measurement Types page. Alternatively, you can open the Visualization types flyout and click the  Manage Measurement Types item to add a Manage Measurement Types page.
3. From the **Information Design** navigation menu, click the **Assay Details Layout** item to open the Edit Assay Details Layout page.



Edit Assay Details Layout

Measurement Type:
Solubility

Assay Details Layout:
sss Default

Assay Details Layout Type:
Form

Available Attributes

Visible Attributes
- MS Number
- Assay Date M/d/yyyy
- pH 0.00
- Assay Subtype
- Buffer

Hidden Attributes
- Assay Identifier
- Crystallinity
- Experiment Identifier
- Outside Range
- Project
- Protocol Reference

Preview

10 of 29071

MS Number: REG00220028
Assay Date: 2/4/2003
pH: 110.00
Assay Subtype: Cell
Buffer:

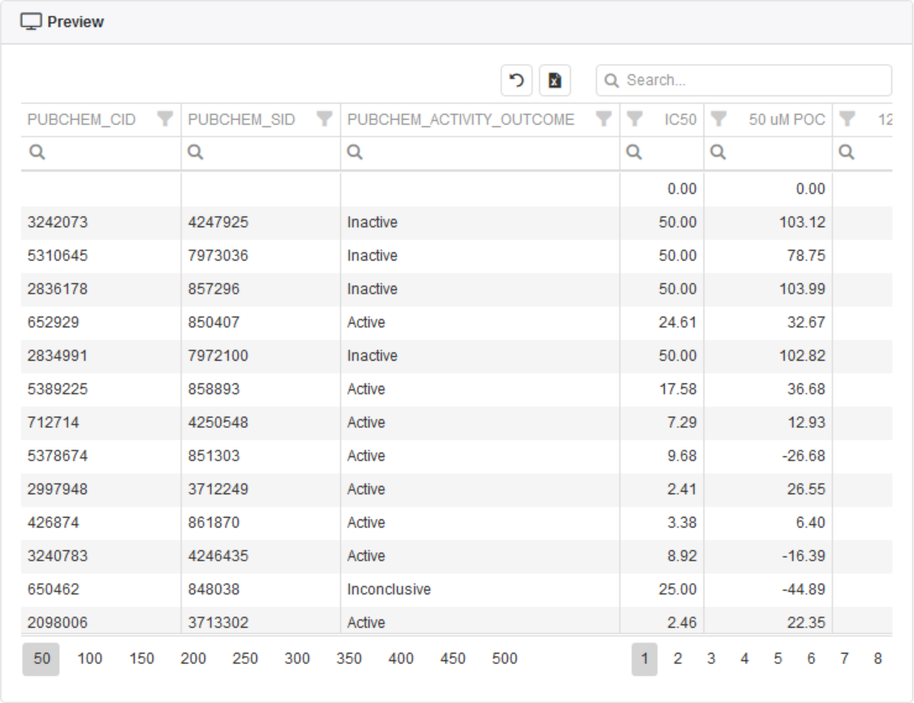
Settings

Label Location: top
Minimum Column Width: 300
Columns count: 2
☑ Show Colon After Label

In the **Edit Assay Details Layout** page:

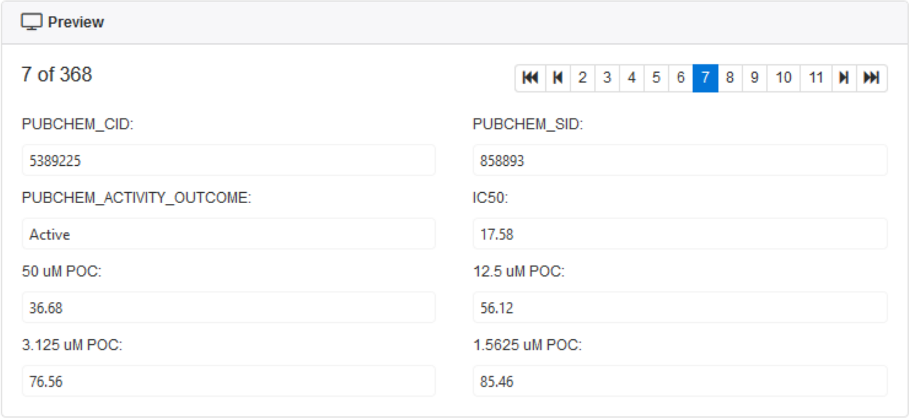
1. **Measurement Type:** The drop-down box which allows you to choose which measurement type you want to define the layout for.
2. **Assay Details Layout:** The drop-down box which shows all the available layouts for the currently selected measurement type. A measurement type may have multiple layouts; each would have different layout type and settings.
3. **Assay Details Layout Type:** The type of the layout, can be either Table or Form.

a) **Table:** This layout type will display the assay data in a table grid with multiple records per page, similar to the example shown below:



PUBCHEM_CID	PUBCHEM_SID	PUBCHEM_ACTIVITY_OUTCOME	IC50	50 uM POC	12
			0.00	0.00	
3242073	4247925	Inactive	50.00	103.12	
5310645	7973036	Inactive	50.00	78.75	
2836178	857296	Inactive	50.00	103.99	
652929	850407	Active	24.61	32.67	
2834991	7972100	Inactive	50.00	102.82	
5389225	858893	Active	17.58	36.68	
712714	4250548	Active	7.29	12.93	
5378674	851303	Active	9.68	-26.68	
2997948	3712249	Active	2.41	26.55	
426874	861870	Active	3.38	6.40	
3240783	4246435	Active	8.92	-16.39	
650462	848038	Inconclusive	25.00	-44.89	
2098006	3713302	Active	2.46	22.35	

b) Form: This layout type will display the assay data in a form with a single record for each page, similar to the example shown below:



7 of 368

PUBCHEM_CID: 5389225

PUBCHEM_SID: 858893

PUBCHEM_ACTIVITY_OUTCOME: Active

IC50: 17.58

50 uM POC: 36.68

12.5 uM POC: 56.12

3.125 uM POC: 76.56

1.5625 uM POC: 85.46

4. **Available Attributes:** This lists all the attributes from the measurement type

a) Visible Attributes: Lists the attributes that will be included in the assay details layout

b) Hidden Attributes: Lists the attributes that will not be included in the assay details layout

You can use drag-and-drop to move the attributes between Visible Attributes list and Hidden Attributes list. You can also hold the CTRL or SHIFT key to make multiple choices.

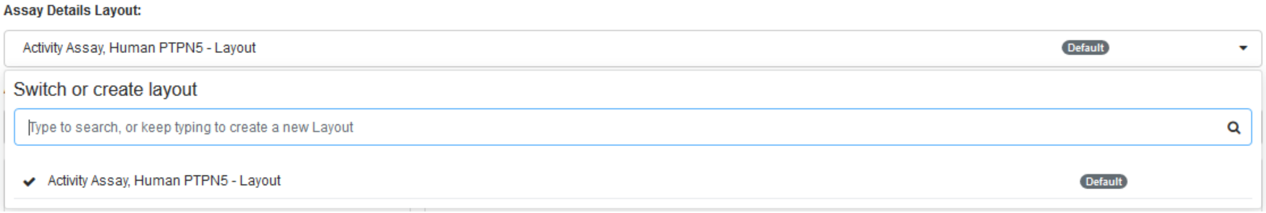
Note: Curve images are supported in Assay Details Form View and the Assay Details visualization.

5. **Preview**: Gives you a preview of how the layout will look like in the assay details page.
6. **Settings**: Layout type specific settings. For example, you will be able to choose the column width for a Form layout, or you will be able to define the line styles for a Table layout.

3.6.1 Creating a New Layout for a Measurement Type

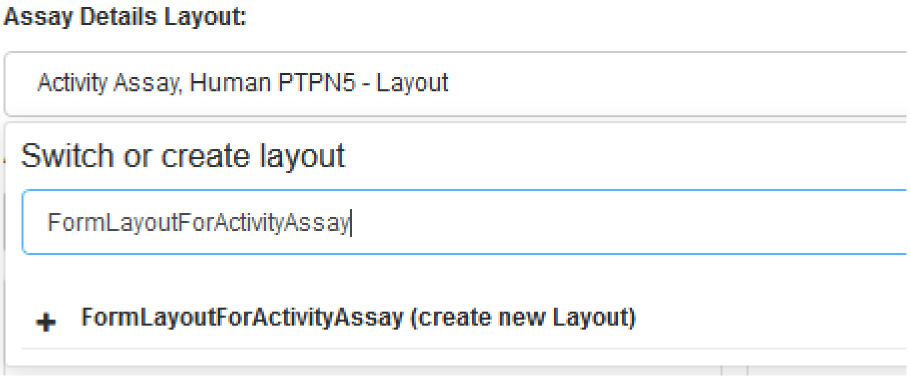
Follow the steps below to create a new layout for a measurement type.

1. From the **Information Design** navigation menu, click the **Assay Details Layout** item to open the **Edit Assay Details** Layout page.
2. Select a measurement type for which you want to define the layout from the **Measurement Type** drop-down.
3. By default, the system will create a layout automatically when you switch to a measurement type that does not have a layout defined. This auto-generated layout will have the name **<measurement_type> - Layout**, and the layout type is **Table.**
4. You can click on the **Assay Details Layout** drop-down box; this will list the layouts for the selected measurement type, with a type-ahead text box within it.



Assay Details Layout: Activity Assay, Human PTPN5 - Layout

5. Type the name of the layout you wish to create in the **Switch or create layout** text box, and then press **ENTER** or click the **Create new Layout** menu item to create a new layout for the selected measurement type.



Assay Details Layout: Activity Assay, Human PTPN5 - Layout

Switch or create layout: FormLayoutForActivityAssay

6. After the layout has been created, you can change the type of the layout by using the **Assay Details Layout Type** drop-down. You can also specify the attributes to display in the assay details by dragging them from the **Hidden Attributes** list and dropping them in the **Visible Attributes** list.

7. You can also create a layout by duplicating an existing one. To do that, simply click the ⧉ icon at the right side of the Assay Details Layout drop-down. This will create a new layout with the name of **copy of <existing_layout_name>**. You can rename and modify this new layout, according to the steps outlined in the Editing an Existing Layout section.

3.6.2 Editing an Existing Layout

Editing an existing layout is very simple. Choose the layout to edit from the **Assay Details Layout** drop-down box, and then make the necessary adjustments.

To rename the layout:

1. Click the ✎ icon located to the right of the **Assay Details Layout** drop-down box. The drop-down will change to a text box allowing you to modify the name of the layout.
2. Rename your layout by typing the new name in the text box.
3. Press **ENTER** or mouse click outside of the text box to save the changes.

To make the layout as the default layout

Each measurement type can have one default layout. This default layout will be selected automatically and will be shown in the configuration of the assay details page. For more information about the default layouts, please refer to the SAR Template User Guide.

1. Click the 📌 icon at the right side of the **Assay Details Layout** drop-down box, a Default badge will display on the drop-down, and the 📌 icon disappears. This implies that the current layout has already been set to default.
2. The changes will be saved automatically.

To change the type of the layout:

1. Choose the type of the layout from the **Assay Details Layout Type** drop-down box; you will see the Preview area is updated accordingly.
2. The changes will be saved automatically.

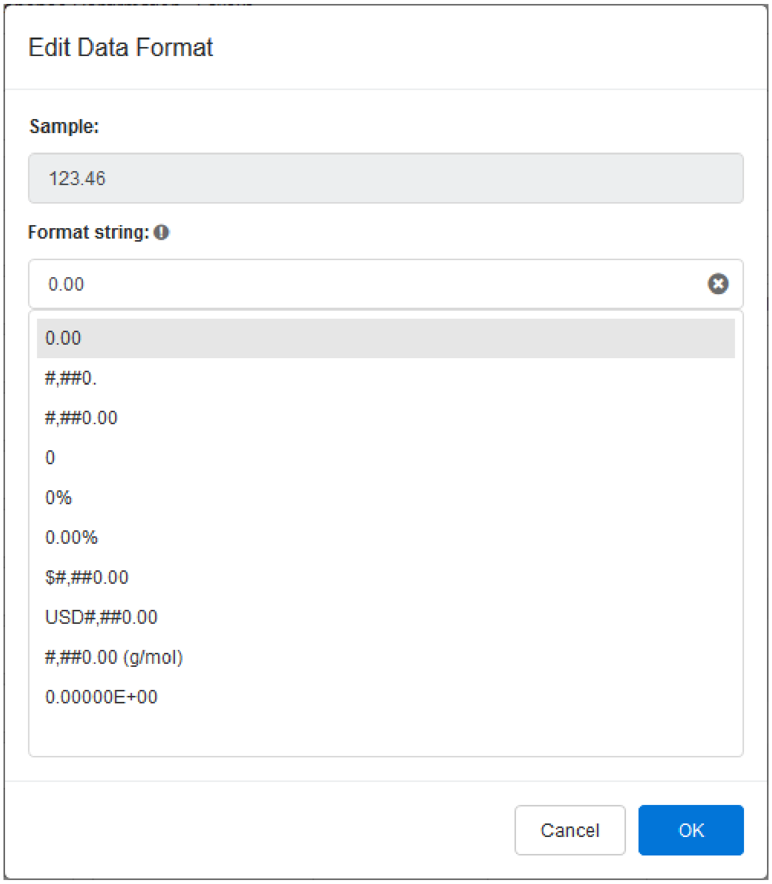
To specify the attributes to be shown in the assay details page:

1. Click the name of the attributes in the **Hidden Attributes** list that you want to show. Holding the **CTRL** or **SHIFT** keys will make the multiple selections.
2. Drag the selected attributes and drop them into the **Visible Attributes** list.
3. The changes will be saved automatically.
4. Similarly, you can remove the attributes from the assay details page by moving them from **Visible Attributes** into **Hidden Attributes**.

To change the data format for numeric or date/time attributes:

Users are able to change how the numeric or date/time attribute values will be represented in the assay details layout, by specifying the data format for those attributes. Follow the steps below to change the data format for either numeric or date/time attributes.

1. In the **Available Attributes** area, select a numeric or date/time attribute for which you want to change the data format.
2. Click the ✎ icon at the right side of the attribute to open the **Edit Data Format** dialog.



Edit Data Format

Sample: 123.46

Format string: 0.00

- 0.00
- #,##0.
- #,##0.00
- 0
- 0%
- 0.00%
- $#,##0.00
- USD#,##0.00
- #,##0.00 (g/mol)
- 0.00000E+00

3. In the **Edit Data Format** dialog, choose the preferred format; an example will be displayed at the top of the dialog.
4. You can also input your own format string in the **Format string** text box. The specification of the format string is explained in a later section.
5. Click **OK** button to save and close the dialog. Clicking **Cancel** button will discard your selection.
6. The selected data format will be used in the assay details layout; you can see the results in the **Preview** area.

Specification of the Format Strings for Numeric Values

The following table shows the detailed information about the elements that can be used to compose a valid numeric value format string.

Format Specifier	Name	Description
“0”	Zero placeholder	Replaces the zero with the corresponding digit if one is present; otherwise, zero appears in the result string.
“#”	Digit placeholder	Replaces the "#" symbol with the corresponding digit if one is present; otherwise, no digit appears in the result string.
“.”	Decimal point	Determines the location of the decimal separator in the result string.
“,”	Group separator and number scaling	Serves as both a group separator and a number scaling specifier. As a group separator, it inserts a localized group separator character between each group. As a number scaling specifier, it divides a number by 1000 for each comma specified.
“%”	Percentage placeholder	Multiplies a number by 100 and inserts a localized percentage symbol in the result string.
“E”	Scientific E-notation sign	For example, mEn indicates a value of $m \times 10^n$
Other	All other characters	The character is copied to the result string unchanged.

The following table shows some examples of the formatted numeric values based on the given format string:

#	Description	Input	Format	Output
Most common world wide				
1	Simple	123456.789	#,##0.00	123,456.79
2	Random	20110628.15	#,##0.###0	20,110,628.15

3	Random	0	#,###.##0	0
4	Long number	1234567890	#,###.##0	1,234,567,890.12
5	Negative value	-0.1	#	
6	Negative value	-0.1	0	0
7	Negative value	-0.13	0.#	-0.1
8	Negative value	-5000.123457	#,##0.######	-5,000.12
Localization format				
9	US, UK and many more	1234567.89	#,##0.00	1,234,567.89
10	Estonia, France	-128983833.5	### ###,##	-128 983 833,46
11	Germany, Italy	-1234560.1	##.000,00	-1.234.560,10
12	Japan	963852741	###,####.00	963,852,741.00
13	Switzerland	33445566.78	#'###'#00.00	33'445'566.78
Any format				
14		-1234.5678	##.000,00	-1.234,57
15		4651321.841	##^000*00	4^651^321*84
16		3411.498	-##¿000$00	-3¿411$50
17		465456456.9	00!00@00	4!65!45!64!56@88
18	Force comma as separator	1112341.435	###,###.	1,112,341
19	Force space as separator	2344441.435	### ###.	2 344 441
20	Force dot as separator	2345341.435	###.###	2345341.435
Prefix & Suffix				
21	No spaces	123456790	$#,##0.00USD	$123,456,789.99USD
22	Extra spaces (set white-space: pre; in cells)	123456790	$ #,##0.00 USD	$ 123,456,789.99 USD
23		123456790	##.000,00 €	123.456.789,99 €
24		123456790	###,####.00 ¥	1,2345,6789.99 ¥
25		123456790	### ###,### ¢ and stuff	123 456 789,988 ¢ and stuff
26		123456790	#,##0.00 a b c	123,456,789.99 a b c

27	Spaces & parenthesis (indicates a negative value, but the input is positive)	123456790	$ (#,###.00) Money	$ (123,456,789.99) Money
28	Spaces & parenthesis (negative)	-123456790	$ (#,###.00) Money	$ (-123,456,789.99) Money
29	Prefix with comma	123456790	a, b c? #.00 yep!	a, b c? 123456789.99 yep!
30	Prefix with a period	123456790	cost... #,##0.00 yep!	cost... 123,456,789.99 yep!
31	Suffix with comma & period	123456790	$# ###,00 USD, or euros.	$123 456 789,99 USD, or euros.
32	Suffix with period	123456790	It costs $# ###,00 euros.	It costs $123 456 789,99 euros.
33	Hanging decimal	123456790	test:### ###. ing	test:123 456 790 ing
Scientific Notation				
34	Scientific Notation	123.456	0.00000E+00	1.23456E+2

Specification of the Format Strings for date/time Values

The following table shows the detailed information about the elements that can be used to compose a valid date/time value format string.

Format Specifier	Description
fff	milliseconds, 3-digits
s	seconds
ss	seconds, 2-digits
m	minutes
mm	minutes, 2-digits
h	hours, 12-hour clock
hh	hours, 12-hour clock, 2-digits
H	hours, 24-hour clock
HH	hours, 24-hour clock, 2-digits
d	date number
dd	date number, 2-digits
ddd	day name, 3-characters (like "Sun")

dddd	day name, full (like "Sunday")
M	month number (Jan=1, Feb=2, etc)
MM	month number, 2-digits
MMM	month name, 3-characters (like "Jan")
MMMM	month name, full (like "January")
yy	year, 2-digits
yyyy	year, 4-digits
t	a/p
tt	am/pm
T	A/P
TT	AM/PM
z	timezone offset hour (like "-7") or "Z"
zz	timezone offset hour, 2-digits (like "-07") or "Z"
zzz	timezone offset hour, 2-digits, and minutes (like "-07:00") or "Z"
w	ISO week number
ww	ISO week number, 2 digits
S	day-of-week ordinal (like "st", "nd", "rd")
i	ISO8601 format, without a timezone indicator
u	ISO8601 format, with a timezone indicator

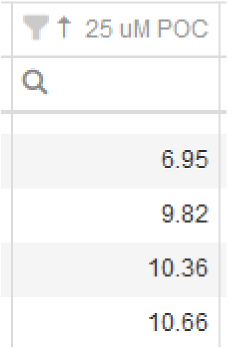
The following table shows some examples of the formatted date/time values based on the given format string:

#	**Input**	**Format**	**Output**
1	11/9/2017 11:02:13	M/d/yyyy	11/9/2017
2	11/9/2017 11:02:13	d-MMM-yy	9-Nov-17
3	11/9/2017 11:02:13	d-MMM	9-Nov
4	11/9/2017 11:02:13	MMM-yy	Nov-17
5	11/9/2017 11:02:13	h:mm AM/PM	11:02 AM
6	11/9/2017 11:02:13	h:mm:ss AM/PM	11:02:13 AM
7	11/9/2017 11:02:13	H:mm	11:02
8	11/9/2017 11:02:13	H:mm:ss	11:02:13
9	11/9/2017 11:02:13	M/d/yyyy H:mm	11/9/2017 11:02:13

10	11/9/2017 11:02:13	HH:ss	11:13
11	11/9/2017 11:02:13	HH:ss.0	11:13.0
12	11/9/2017 11:02:13	dddd, MMMM dd, yyyy	Thursday, November 09, 2017
13	11/9/2017 11:02:13	dddd, MMMM dd, yyyy hh:mm tt	Thursday, November 09, 2017 11:02 am
14	11/9/2017 11:02:13	dddd, MMMM dd, yyyy hh:mm:ss TT	Thursday, November 09, 2017 11:02:13 AM

To change the sorting of the columns in the Table layout:

For the layouts in the Table layout type, you can change the sorting of the columns by clicking the column header. A small arrow will appear when there is a sorting applied to the current column, for example:



↑ 25 uM POC
6.95
9.82
10.36
10.66

The column above has the ascending sorting applied. Clicking the column header with sorting will toggle the sorting order. This sorting will be persisted to the assay details layout definition. Note that in the assay details page, you will also be able to change the sorting of the columns, however, the changes will not be persisted.

To change the width of the columns in the Table layout:

For the layouts in the Table layout type, you can change the width of the columns by dragging the column splitters. When you hover the mouse over the splitters, it will turn into a splitter cursor. Drag the column splitter to a proper position and release the mouse. The width of the column will be adjusted and persisted to the assay details layout definition. Note that in the assay details page, you can also change the width of the columns, however, the changes will not be persisted.

You can also restore the width settings by clicking the ↺ button in the Table layout.

3.6.3 Changing the Layout Settings

Both Table and Form layout type have their own specific settings. For example, for the Table layout type, you can show or hide the header filters. For the Form layout type, you can choose the number of field columns. This section describes each setting option for the two layout types.

Layout Settings for Table Layout Type

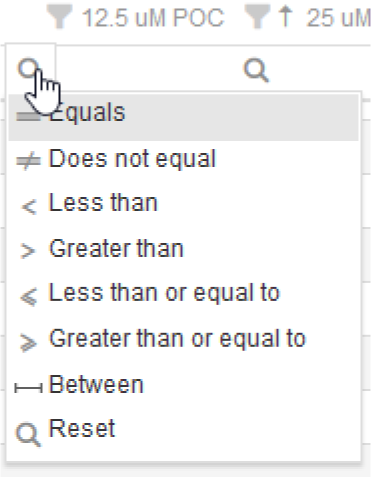
- **Show Column Lines:** If checked, will display the column splitter lines between two columns, unchecking this option will hide the splitter lines.

- **Show Row Lines:** If checked, will display the row splitter lines between two rows, unchecking this option will hide the splitter lines.

- **Show Borders:** If checked, the border line will display outside of the Table grid, unchecking this option will hide the table border.

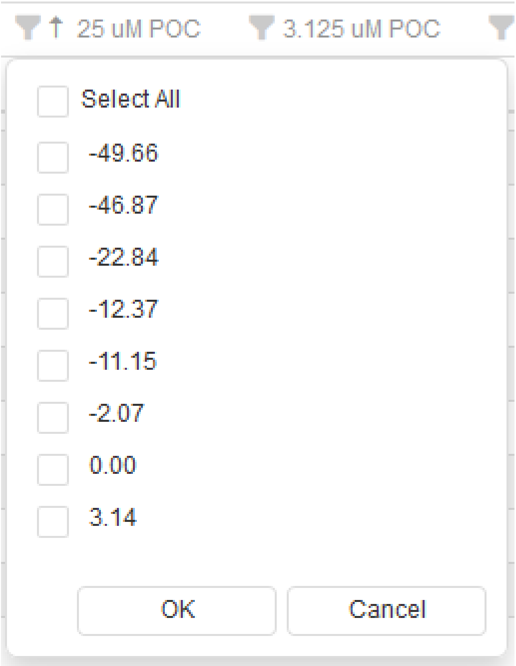
- **Alternating Row Color:** If checked, will show the alternating row color in the Table grid, unchecking this option will only use the single color to render the data rows.

- **Show Filter Row:** Check this option to show the filter row below the column header. In the filter row, there will be a magnifier icon in each cell. Clicking the magnifier icon allows you to specify the filter criteria:



You can choose a criteria and input the value in the text box to perform the filtering. Unchecking this option will hide this filter row.

- **Show Header Filter:** Checking this option will display a filter icon at the left side of each column name. Clicking the filter icon will give you the filter options based on the row values.

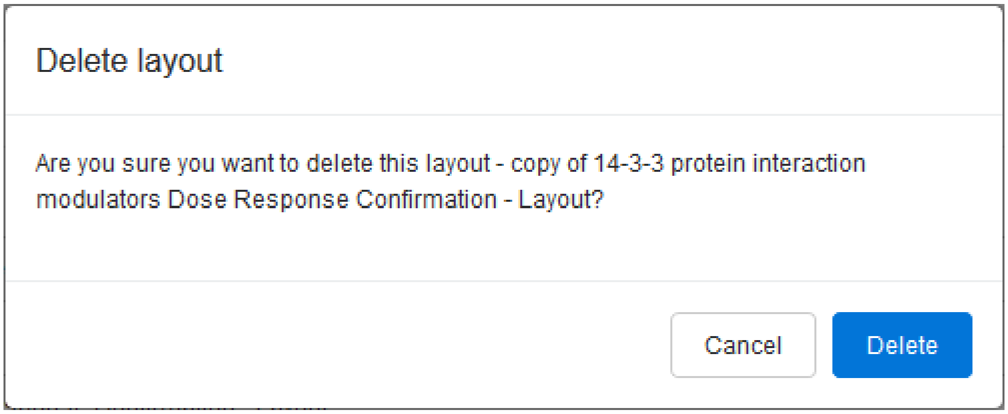


- **Show Search Panel:** Checking this option will display a search text box at the upper-right corner of the table grid. You can input a value in the search box to search for a value in the current page of the grid. Unchecking this option will hide the search panel.
- **Show Export Button:** Checking this option will display the export button on the top of the table grid. Clicking the export button allows you to export the data of the current page in the table grid. Unchecking this option will hide the export button.
- **Layout Settings for Form Layout Type**
- **Label Location:** Specifies the location of a field label. There are two choices: left and top.
- **Minimum Column Width:** Specifies the minimum width of the form columns. When the Columns count option has been specified to auto, the number of form columns will be determined by this minimum column width setting.
- **Columns count:** Specifies the number of columns to display in the form layout.
- **Show Colon After Label:** When checked, will display the colon right after the field label. Unchecking this option will hide the colon.

3.6.4 Deleting a Layout

To delete an existing layout:

1. Select the layout that you want to delete from the **Assay Details Layout** drop-down box.
2. Click the 🗑 icon at the right side of the drop-down box, a confirmation dialog will appear.



Delete layout

Are you sure you want to delete this layout - copy of 14-3-3 protein interaction modulators Dose Response Confirmation - Layout?

3. Click the **Delete** button to delete the selected layout.

4 Configuring Signals Data Factory

Signals Data Factory (SDF) is an infrastructural component of Signals Inventa which provides data transforming, indexing and query capabilities. After the measurement metadata has been correctly defined and measurement data is in Spotfire, you are able to publish the measurements into the Signals Data Factory such that the measurement data can be transformed and indexed and then searched using complex queries in Signal Inventa's Global Search.

4.1 Configuring Security Features

Signals Data Factory (SDF) provides the security features with which administrator users can determine what kind of resources could be seen or be used by which user groups. For example, the System Administrator can set up the security on the projects, so that some of the projects can only be seen by users belonging to a specific group.

To configure users, roles and groups, please refer to Manage Users section in this documentation.

Signals Data Factory allows administrators to configure the permissions based on the following resources:

- Projects
- Measurement Types
- Entity Rows

To configure project permissions, please refer to Appendix B - Projects section in this documentation.

To configure measurement type permissions, please refer to Measurement Type - Security Settings section in this documentation.

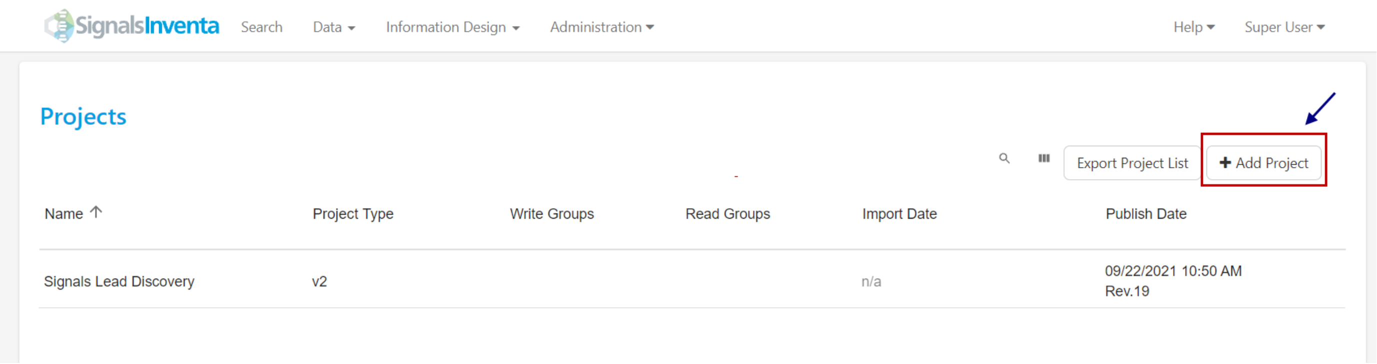
To configure the permission on entity rows, please refer to Advanced Security section in this documentation.

4.2 Creating a Project

In the Signals Data Factory, data is organized by project. Before you can publish measurement data into the Signals Data Factory, a project needs to be created.

To create a project:

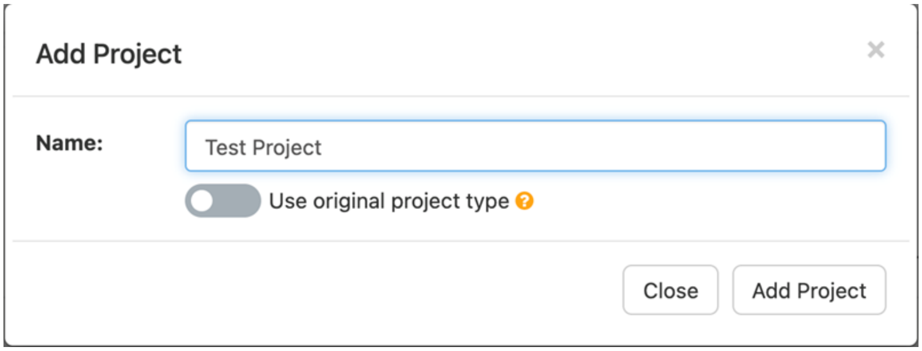
1. Log in to Signals Data Factory with username and password.
2. From **Data** menu, click **Projects.**
3. New projects can be created from the Projects page.
4. In the **Projects** page, in the upper-right corner of the project list, click **Add Project** button.



Projects

Name	Project Type	Write Groups	Read Groups	Import Date	Publish Date
Signals Lead Discovery	v2			n/a	09/22/2021 10:50 AM Rev.19

5. In the **Add Project** dialog, choose a name for your project.



Name: Test Project

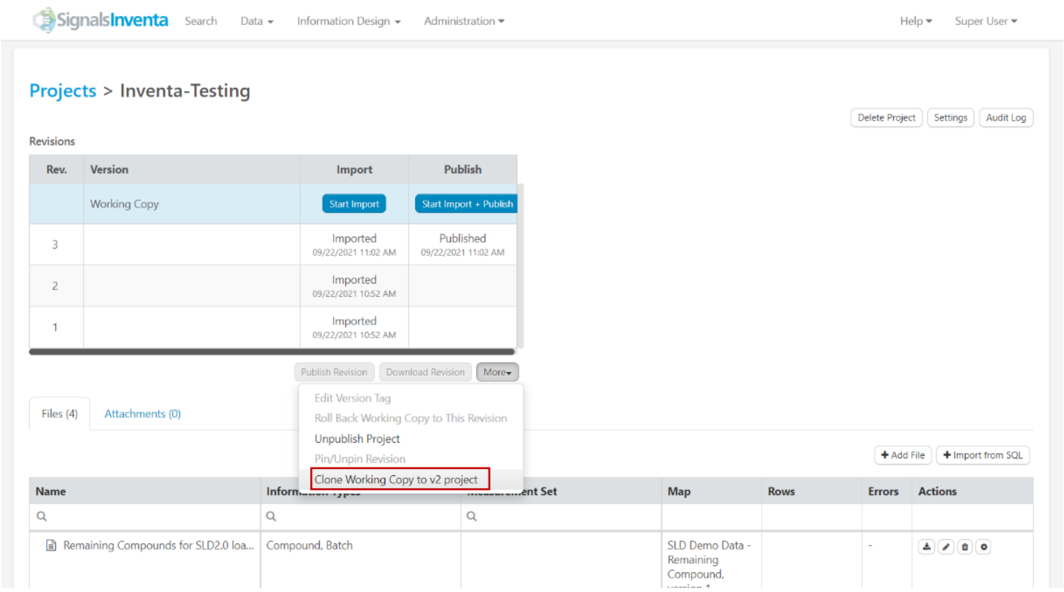
6. A ‘Use original project type’ toggle is available for you to choose the project type. By default, this toggle is disabled and will create a V2 project type (incremental project) which includes load-new and datasets functionality. You can create an original project type (V1) by clicking the slider bar which excludes load-new and dataset funtionalities. Use this toggle to define the project type.

7. Click on the **Add Project** button to append the Project to the Projects list. The Project Type will be listed as v1 (original) or v2 on the Projects page.

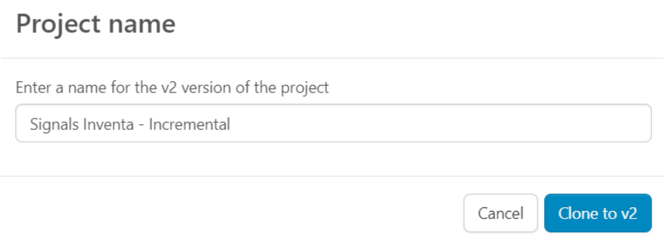
To convert a v1 (original) project to v2 (incremental project):

If you have an original project (v1) that you want to convert to an incremental project (v2), you have the option to do this from the original project.

1. From the Projects details page, select the ‘Clone Working Copy to v2 project’ sub-menu item from the More drop-down menu.



2. Enter a name for the v2 version of the project.


Project name

Enter a name for the v2 version of the project: Signals Inventa - Incremental

3. Click the **Clone to v2** button.

The v2 version of the product be appended to the Projects list page.

Note: When installing Signals Inventa, there is an environment variable which determines the name of the SIA project. The name of the environment variable is ‘sdfProject’ in the Helm chart. It is strongly recommended to remain consistent with the project name you choose when deploying Signals Inventa and the project name you save here. Otherwise, you will not be able to see the preview data when you are creating layouts for your measurement types in Signals Inventa.

4.3 Loading Batch Data

You need to prepare the batch data via Signals Data Factory rather than the publishing features in Signals Inventa, before the measurements data published to the project is transformed and indexed. Batch data must be provided and mapped correctly.

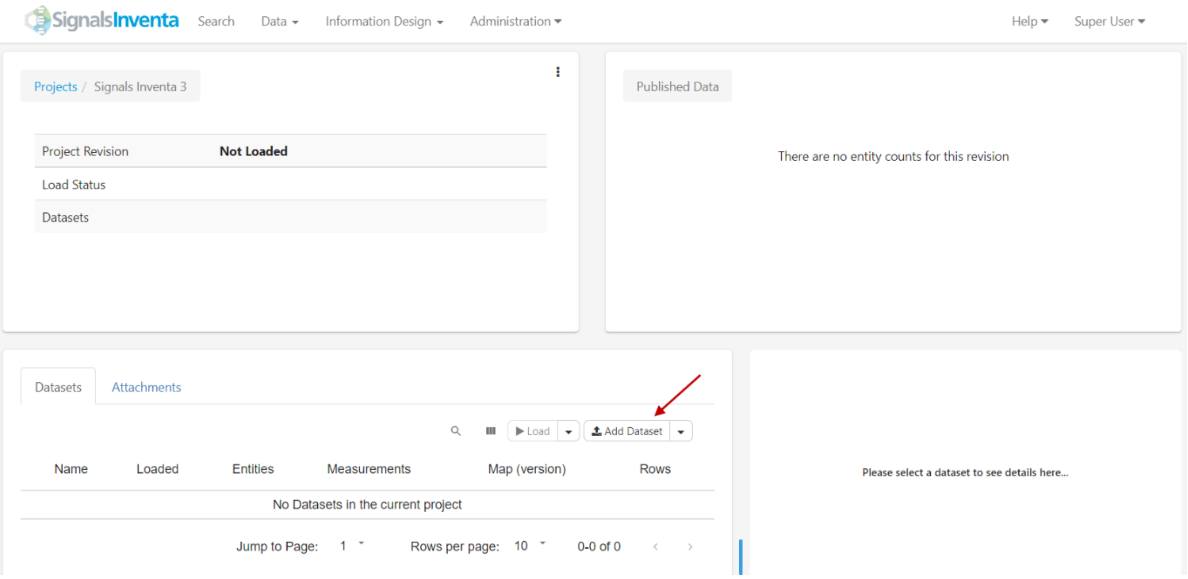
Signals Data Factory provides two methods for loading batch data:

- using a tabular text file
- importing from SQL relational databases

4.3.1 Loading Batch Data from Tabular Text File

To load the batch data from a text file:

1. Log in to Signals Data Factory with the username and password.
2. From **Data** menu, click **Projects.**
3. In the **Projects** page, click the name of the project to which you want to load batch data.
4. On the project details page, click the **Add Dataset** button to add a new dataset:



Project Revision: Not Loaded
Load Status
Datasets

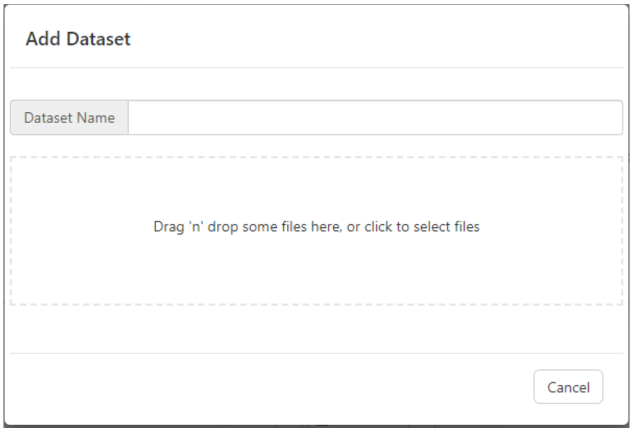
There are no entity counts for this revision

No Datasets in the current project

Jump to Page: 1 Rows per page: 10 0-0 of 0

Please select a dataset to see details here...

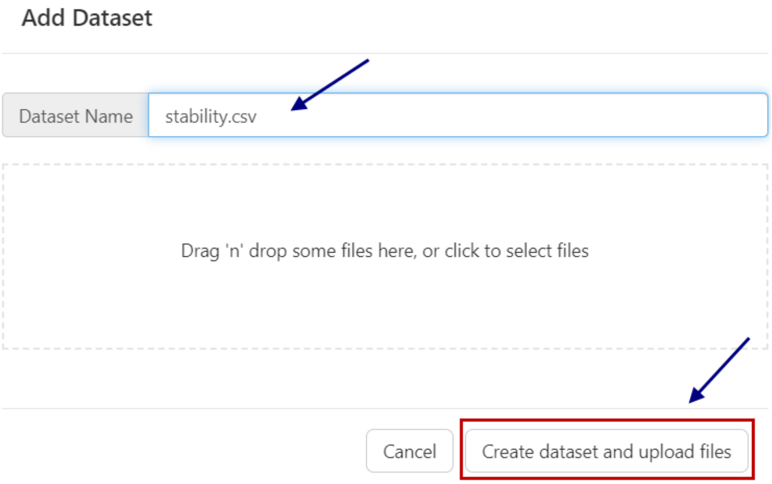
5. Drag ‘n’ drop files or click to select files.



Drag 'n' drop some files here, or click to select files

6. Once the file is ready to be added, the **Dataset Name** is populated with the name of the chosen file by default. You can also modify the **Dataset Name** before the dataset is created.

7. Click the **Create dataset and upload files** button to upload the file and create the dataset.



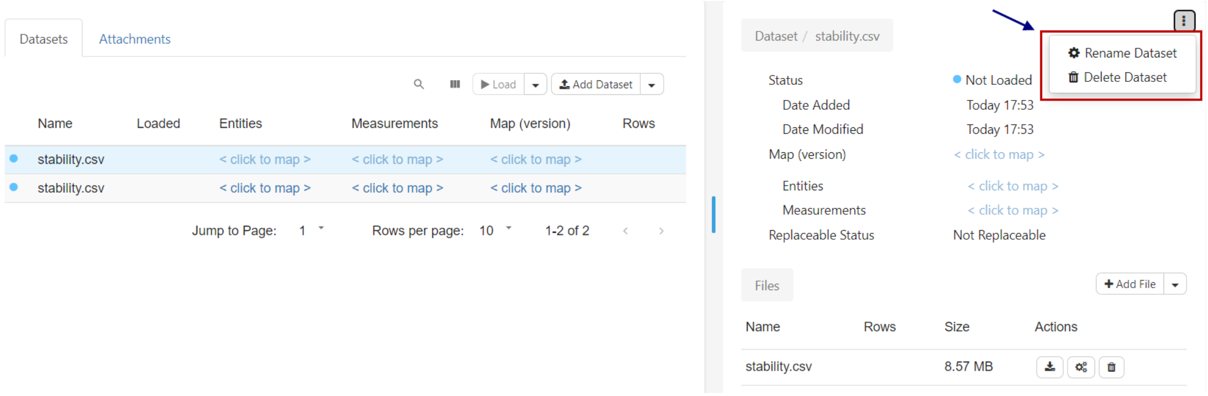
Dataset Name: stability.csv

Note: Ideally, a dataset is a group of files that can share the same mapping. In practice, files under the same dataset will have the same number of columns and column names. In Signals Inventa, usually a dataset will have only one file in it.

Note: Only text files in tabular format, such as comma-separated values (CSV), tab-separated values (TSV) are supported

Note: SDFiles are not directly supported by Signals Data Factory, however, the Signals Inventa Utilities command line tool included in the Signals Inventa release package can convert an SDFile into a CSV file, such that the compound information defined in the SDFile can also be loaded into Signals Data Factory. For more information, please refer to the "Converting SD file into CSV file" section below.

After the file has been added to the project, it will be displayed under the **Datasets** tab. At the right side of the Datasets list, there is an area showing the status of the selected dataset and the files under it. You can click the ellipse icon at the upper-right corner to either rename or delete the dataset.

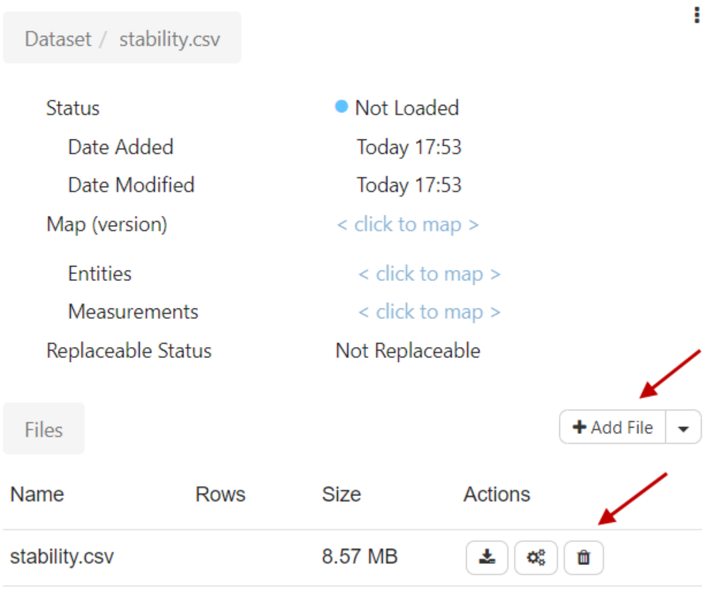


Name	Loaded	Entities	Measurements	Map (version)	Rows
stability.csv		< click to map >	< click to map >	< click to map >	
stability.csv		< click to map >	< click to map >	< click to map >	

Status: Not Loaded
Date Added: Today 17:53
Date Modified: Today 17:53
Map (version): < click to map >
Entities: < click to map >
Measurements: < click to map >
Replaceable Status: Not Replaceable

Name	Rows	Size	Actions
stability.csv		8.57 MB	

You can also add additional files to the selected dataset by clicking the **Add File** button, or delete an existing file by clicking the trash icon.



Status: Not Loaded
Date Added: Today 17:53
Date Modified: Today 17:53
Map (version): < click to map >
Entities: < click to map >
Measurements: < click to map >
Replaceable Status: Not Replaceable

Name	Rows	Size	Actions
stability.csv		8.57 MB	

4.3.2 Importing Batch Data from SQL

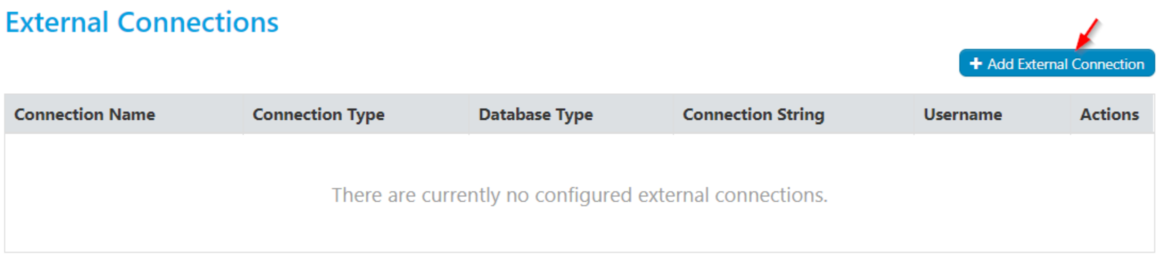
Signals Data Factory supports connections to external data sources – currently SQL data sources are supported which can be used to connect to other databases.

To load from an external connection, an administrator first configures the external connection.

Connections are managed on the ‘External Connections’ page within the ‘Information Design’ main menu.

To define the database connection:

1. Log in to Signals Data Factory with username and password.
2. From **Administration** menu, click **External Connections.**
3. On the **External Connections** page, click **Add External Connection** button in the upper-right corner of the External Connections list.



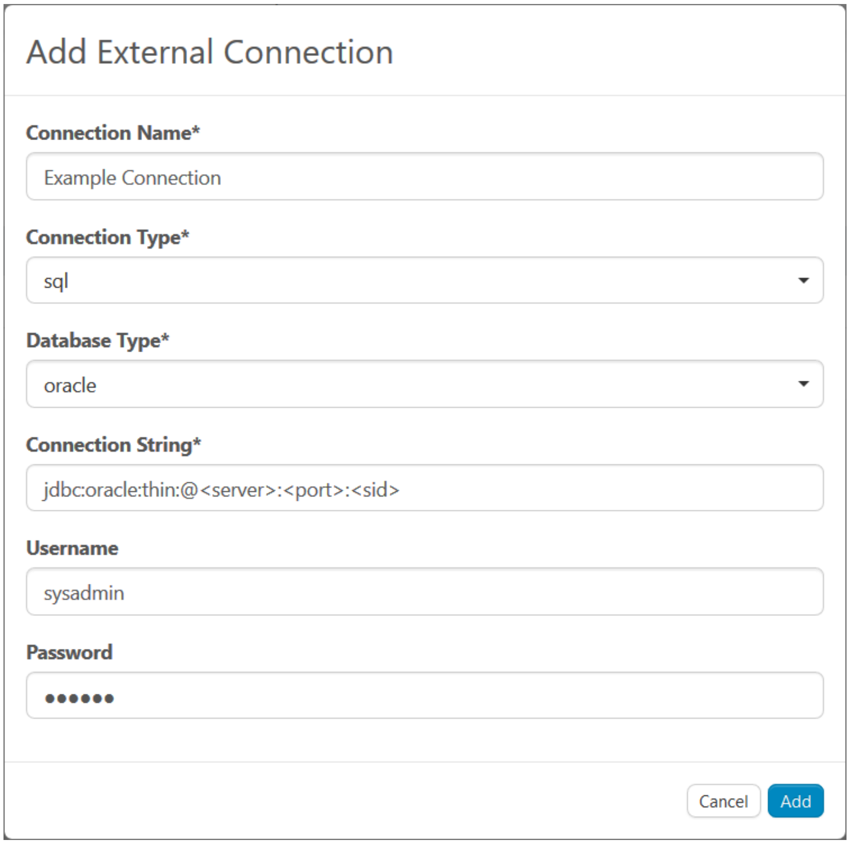
Connection Name	Connection Type	Database Type	Connection String	Username	Actions

There are currently no configured external connections.

4. When adding a connection, the following information is required in the **Add External Connection** dialog:

- Assign a name to the connection

- the connection type (currently only SQL is available)
- the database type
    - Oracle
    - MySQL
    - MSSQL
    - Redshift (also supports Redshift Spectrum)
    - Impala
    - Postgres
    - Snowflake
- the connection string
- username and password credentials



Add External Connection

Connection Name*: Example Connection

Connection Type*: sql

Database Type*: oracle

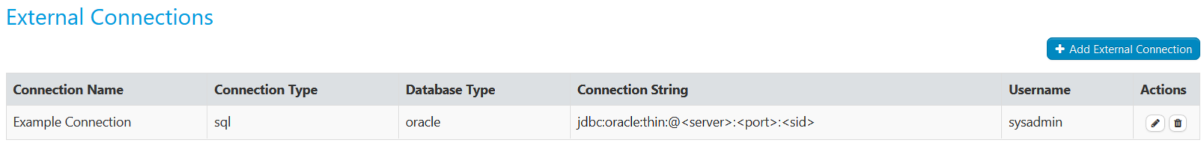
Connection String*: jdbc:oracle:thin:@<server>:<port>:<sid>

Username: sysadmin

Password: ••••••

5. Click on the **Add** button.

6. After the connection has been added successfully, you should be able to find it in the **External Connections** list:



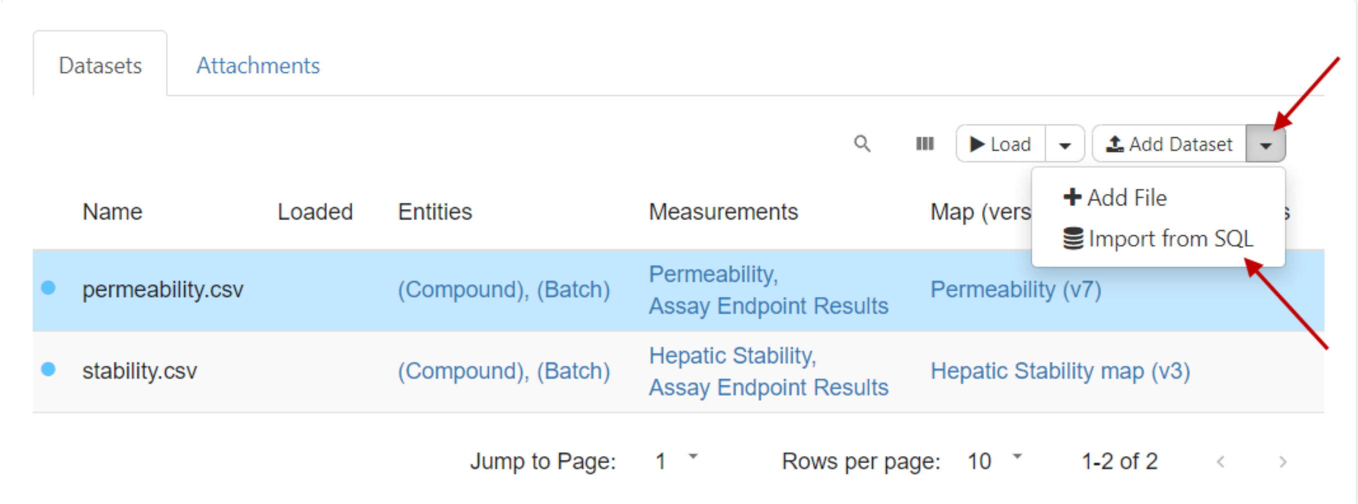
External Connections

Connection Name	Connection Type	Database Type	Connection String	Username	Actions
Example Connection	sql	oracle	jdbc:oracle:thin:@<server>:<port>:<sid>	sysadmin	✎ 🗑

Once configured, project administrators will be able to import using this connection on the project details page.

To import data from SQL by using an existing database connection:

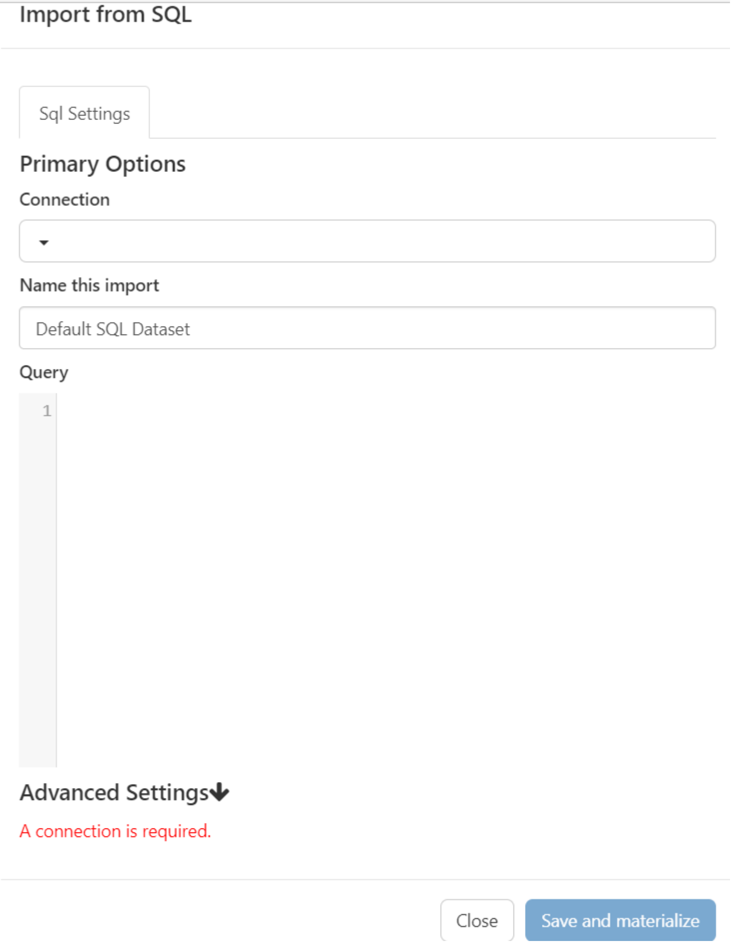
1. Log in to Signals Data Factory with username and password
2. From **Data** menu, click **Projects.**
3. Click the name of the project to which you want to import data from SQL.
4. On the project detail page, click on the **Import from SQL** menu from the Add Dataset drop-down button.



Name	Loaded	Entities	Measurements	Map (vers
permeability.csv		(Compound), (Batch)	Permeability, Assay Endpoint Results	Permeability (v7)
stability.csv		(Compound), (Batch)	Hepatic Stability, Assay Endpoint Results	Hepatic Stability map (v3)

Jump to Page: 1 Rows per page: 10 1-2 of 2

The Import from SQL window is displayed.



Import from SQL

Sql Settings

Primary Options

Connection

Name this import

Default SQL Dataset

Query

Advanced Settings

A connection is required.

5. Select the pre-configured connection, assign a name to the data being added, and enter the SQL to run:
    - **Connection**: Choose the database connection you wish to use
    - **Name this import**: Input the name of the import, this will be the name of the data set listed in the Files list.
    - **Query**: Input the SQL query for pulling in the data
6. Click **Save and materialize** button to import the data.

When the details for an SQL retrieval are saved, a new process is started to materialize the results of the query.

Any modifications to the settings to the SQL retrieval will also begin a new materialization process.

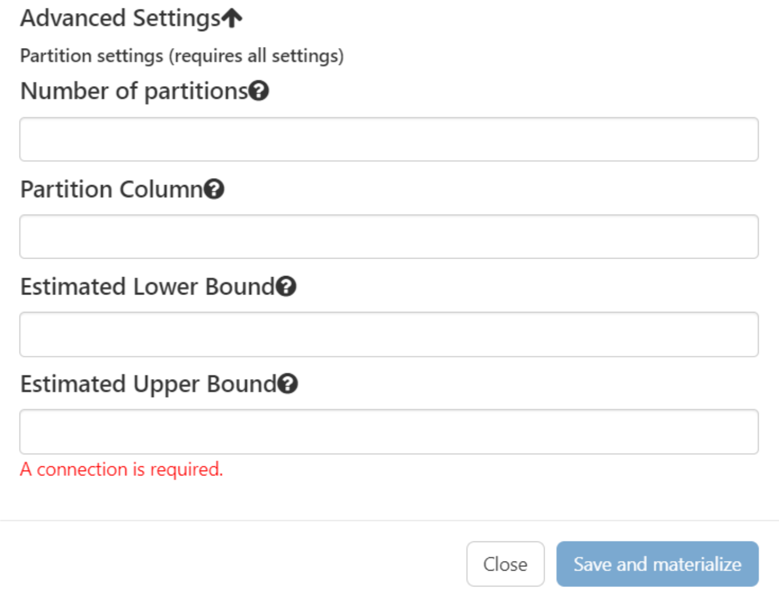
An active materialization will be indicated with a spinner alongside the file.

Should there be any issues/errors in this process, the spinner will be replaced with a ! icon, which can be clicked to view the output log and diagnose the problem (there is also a shortcut to the log in the Actions column).

If an import job is started before a materialization is complete, then a failed materialization will result in a failed import (and any dependent publish jobs).

Advanced Settings

For larger datasets it is possible to tune the retrieval mechanism via the ‘Advanced Settings’ option.



Advanced Settings

Partition settings (requires all settings)

Number of partitions

Partition Column

Estimated Lower Bound

Estimated Upper Bound

A connection is required.

Here you can specify

- **Partition Settings** (if used, all of the settings are required) When provided with a partition column along with an estimated lower and upper value, Signals Data Factory will split the data according to the number partitions requested and run these queries in parallel. This can result in significant performance improvements when materializing the data for large datasets.
  - **Number of Partitions**: The number of queries to run in parallel
  - **Partition Column**: A numeric or date column to use to split the query into multiple parts.
  - **Estimated Lower Bound**: An estimate of the lower bound of the partition column’s values
  - **Estimated Upper Bound**: An estimate of the upper bound of the partition column’s values

4.4 Converting SDFile into CSV file

SDFiles are not by default supported by Signals Data Factory. However, the Signals Inventa Command Line Utilities tool (siautils.exe) included in Signals Inventa distribution package can convert an SDFile into CSV file, which can then be supported in Signals Data Factory.

Note: The Signals Inventa Command Line Utilities tool can only work under Microsoft Windows with .NET Framework version 6.0 installed. For more information about the tool, please refer to **Revvity Signals Command Line Utilities User Guide.**

To convert an SDFile into CSV file with siautils.exe, please ensure that your machine is running Microsoft Windows and has the .NET Framework 6.0 installed, then follow the steps below:

1. Extract the **siautils.exe** from the distribution package.
2. Under the path where the **siautils.exe** exists, execute the following command from a Windows shell:

```
C:\> siautils.exe sdf2csv -i InputFile.sdf
```

Where `InputFile.sdf` is the file name of the SDFile that you wish to convert.

The generated CSV file will be named after the input file name by default, with the ".csv" as its extension. You may also specify the name of the generating CSV file explicitly by supplying `-o` (or `--output`) parameter. For other available parameters of the sdf2csv command, please refer to **Revvity Signals SIA Utilities Command Line User Guide**

Once complete, follow the steps described in "**Loading Batch Data from Tabular Text File**" section above to load the generated CSV file into Signals Data Factory.

4.5 Uploading Batch Maps

In Signals Data Factory, batch data will be transformed into two kinds of entities: Compound and Batch. Compound entity contains the compound ID, chemical structure data as well as its indexing fingerprint for searching purposes, whereas the Batch entity contains the compound ID and additional batch/chemical properties. The batch map is a type of metadata which maps the batch data into these two entities. Before the batch data can be processed by Signals Data Factory, the batch map should be correctly defined.

There are two ways of defining the batch map for a batch data file, either by using the Signals Data Factory mapping user interface, or by providing a JSON mapping file which can be uploaded into Signals Data Factory.

For more information about how to use the mapping user interface to define the maps, please refer to Appendix B - Signals Data Factory.

If uploading a JSON mapping file, first, you need to compose a mapping file. A mapping file is usually a JSON file which has the schema similar to the following example:

```
{

  "name": "BatchesMap",

  "entities": [

    {

      "entityType": "Compound",

      "ID": "CompoundID",

      "attributes": [

        {
```

```
          "attributeName": "Chemical Structure",

          "valueLocator": {

            "inputs": [

              "Structure"

            ],

            "function": {

              "type": "chemicalStructureNormalization",

              "chemicalStructureType": "chemical/x-cdx"

            }

          }

        }

      ],

      "validated": true

    },

    {

      "entityType": "Batch",

      "ID": "BatchID",

      "validated": true,

      "attributes": [

        {

          "attributeName": "Batch Project ID",

          "valueLocator": "batch_project_id"

        },

        {

          "attributeName": "BatchPropDate",

          "valueLocator": {

            "inputs": [

              "BatchPropDate_t"

            ],

            "function": {
```

```
              "type": "dateNormalization",
              "dateStyle": "year"
            }
          }
        },
        {
          "attributeName": "BatchPropNumeric",
          "valueLocator": "BatchPropNumeric_d"
        },
        {
          "attributeName": "BatchPropText",
          "valueLocator": "BatchPropText_s"
        },
        {
          "attributeName": "Chemical Structure Format",
          "valueLocator": {
            "function": {
              "type": "constant",
              "value": "chemical/x-cdx"
            }
          }
        }
      ]
    }
  ]
}
```

In this example batch map, “name” is the name of the map, and there are two entity types defined in the “entities” array: Compound and Batch.

For the Compound entity:

- `entityType` must be "Compound"
- `ID` should be the name of the column in the uploaded batch data, which represents the identifier of the compound conceptually
- `attributes` hold a list of compound attributes that will be added to the Compound entity. Specifically, the `Chemical Structure` attribute must be in place and mapped with a `chemicalStructureNormalization` custom function, with the name of the structure column as its input, and the `chemicalStructureType` as its parameter. The `chemicalStructureType` represents the MIME type of the chemical structure data which could have three options: `chemical/x-cdx`, `chemical/smiles` and `chemical/x-mdl-molfile`
  Note: The name of the Chemical Structure attribute must match the name of the Compound entity attribute defined in the Signals Data Factory whose Data Type is Chemical Structure:

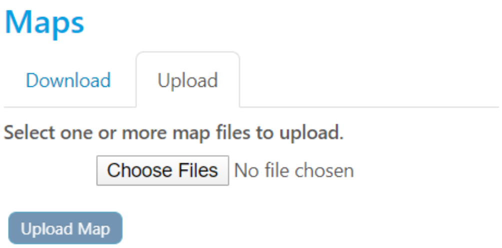
Name ↓	Data Type	Searchable	Description
Chemical Structure	Chemical Structure	Yes	
Chemical Structure Format	Keyword	No	

For the Batch entity:

- `entityType` must be "Batch"
- `ID` should be the name of the column in the uploaded batch data, which represents the identifier of the batch conceptually
- `attributes` hold a list of batch attributes that will be added to the Batch entity. For most of the batch attribute mappings, they are a simple name-to-name mapping between the column in the batch data and the attribute in the batch entity. For a date type attribute, it uses the dateNormalization function to convert the format of the value.

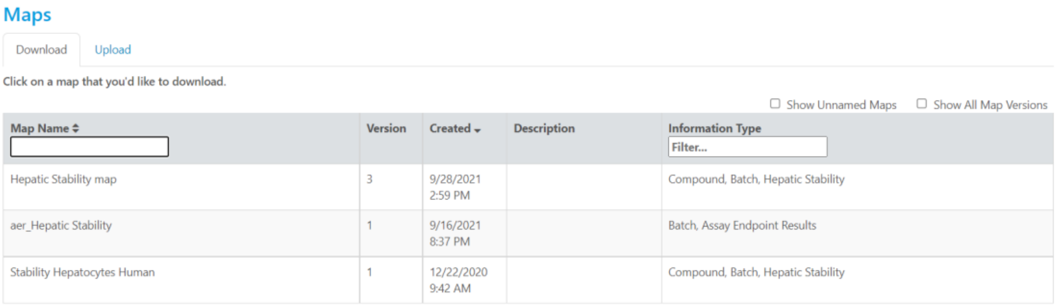
Once the mapping file is ready, you can upload it to the Signals Data Factory by following the steps below:

1. Log in to the Signals Data Factory with username and password.
2. From **Data**, click **Maps.**
3. On the **Maps** page, click **Upload** tab.
4. Click **Choose Files** button, which will open a file selection dialog.



Select one or more map files to upload.

5. In the popup dialog, choose the mapping file.
6. Click the Upload **Map** button. A message will appear indicating that the map loaded successfully.
7. Click the **Download** tab on the **Maps** page, make sure that you can see the map that you have just uploaded:



Click on a map that you'd like to download.

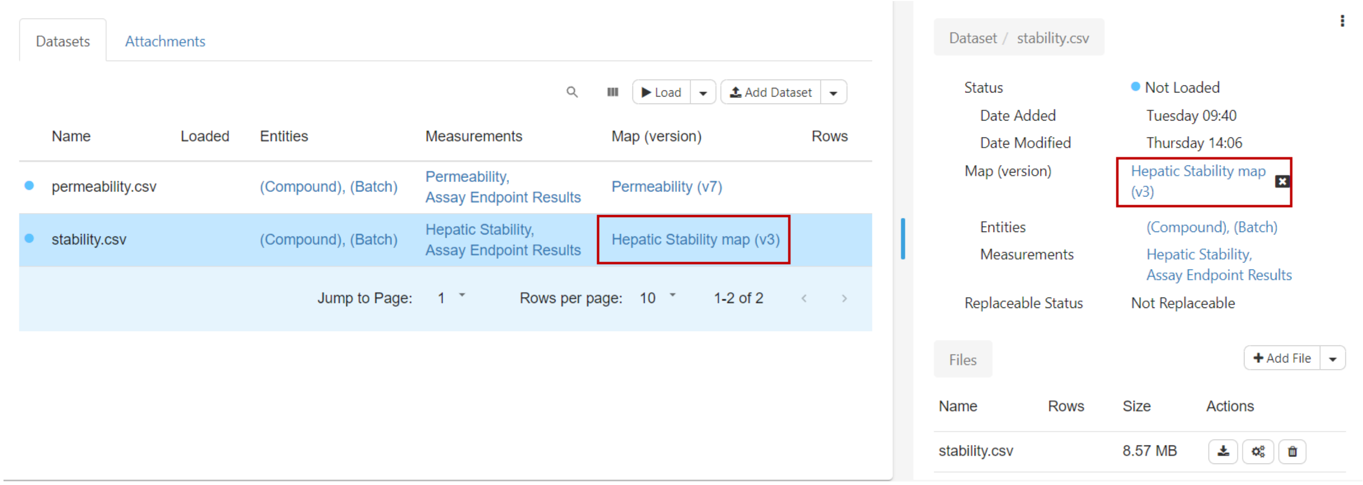
Map Name	Version	Created	Description	Information Type
				Filter...
Hepatic Stability map	3	9/28/2021 2:59 PM		Compound, Batch, Hepatic Stability
aer_Hepatic Stability	1	9/16/2021 8:37 PM		Batch, Assay Endpoint Results
Stability Hepatocytes Human	1	12/22/2020 9:42 AM		Compound, Batch, Hepatic Stability

4.6 Associating Batch Data with the Batch Map

By associating the batch data with the batch map, Signals Data Factory can transform and index the batch data.

To associate the batch data with the batch map:

1. Log to Signals Data Factory with username and password.
2. From **Data** menu, click **Projects.**
3. Click on the project of interest.
4. From the **Datasets** list, locate the uploaded batch data file. Click on the map hyperlink to edit.



Name	Loaded	Entities	Measurements	Map (version)	Rows
permeability.csv		(Compound), (Batch)	Permeability, Assay Endpoint Results	Permeability (v7)	
stability.csv		(Compound), (Batch)	Hepatic Stability, Assay Endpoint Results	Hepatic Stability map (v3)	

Jump to Page: 1 Rows per page: 10 1-2 of 2

Dataset / stability.csv

Status	Not Loaded
Date Added	Tuesday 09:40
Date Modified	Thursday 14:06
Map (version)	Hepatic Stability map (v3)
Entities	(Compound), (Batch)
Measurements	Hepatic Stability, Assay Endpoint Results
Replaceable Status	Not Replaceable

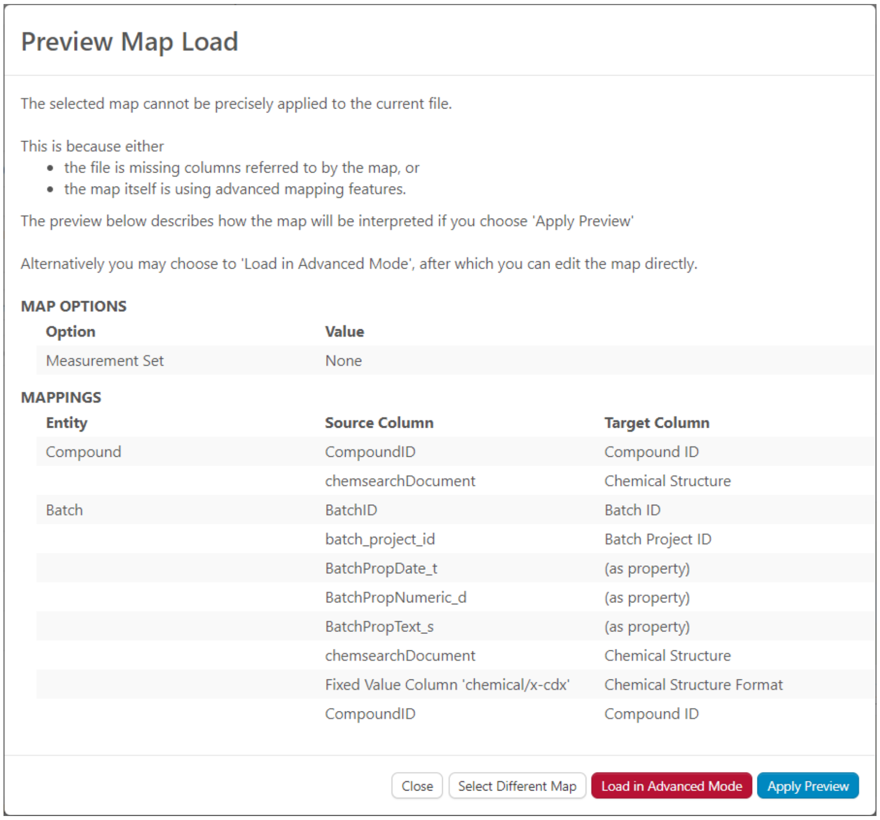
Files

Name	Rows	Size	Actions
stability.csv		8.57 MB	

5. On the **Map Details** page, you can either create a new map by using the interface or you can upload an existing mapping file. To upload an existing mapping file, click **Load Map** button.

The Load Previously Used Map dialog box is displayed. By default, only maps that are compatible with the current file and its available source columns will be displayed. To view all available maps, de-select the ‘Only Compatible Maps’.

6. On the **Load Previously Used Map** dialog box, click on the name of the map you want to use, then in the **Preview Map Load** dialog, review the map option and the mappings. You can either click the **Load in Advanced Mode** to review the mapping in JSON format or click the **Apply Preview** button directly.



Preview Map Load

The selected map cannot be precisely applied to the current file.

This is because either

- the file is missing columns referred to by the map, or
- the map itself is using advanced mapping features.

The preview below describes how the map will be interpreted if you choose 'Apply Preview'

Alternatively you may choose to 'Load in Advanced Mode', after which you can edit the map directly.

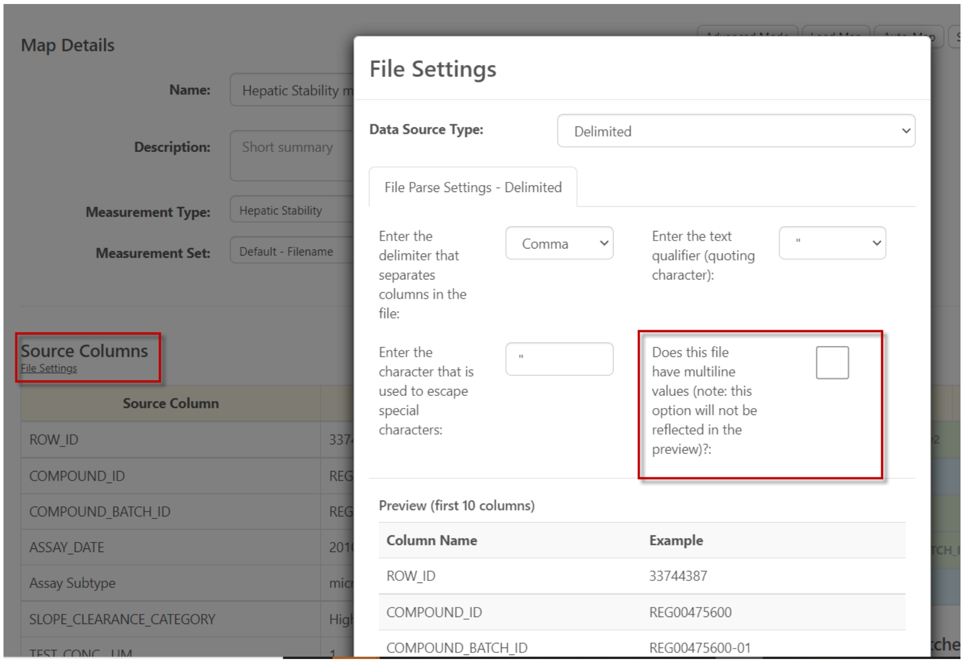
MAP OPTIONS

Option	Value
Measurement Set	None

MAPPINGS

Entity	Source Column	Target Column
Compound	CompoundID	Compound ID
	chemsearchDocument	Chemical Structure
Batch	BatchID	Batch ID
	batch_project_id	Batch Project ID
	BatchPropDate_t	(as property)
	BatchPropNumeric_d	(as property)
	BatchPropText_s	(as property)
	chemsearchDocument	Chemical Structure
	Fixed Value Column 'chemical/x-cdx'	Chemical Structure Format
	CompoundID	Compound ID

Note: If your batch data file contains columns that have multi-line values (e.g., in a CSV file converted from an SDFile, the chemical structure column will be in MolFile format which is represented by a multi-line text), please remember to check the **Does this file have multiline values** checkbox on the **File Settings** dialog, similar to the example shown below.



Map Details

Name: Hepatic Stability m

Description: Short summary

Measurement Type: Hepatic Stability

Measurement Set: Default - Filename

Source Columns

File Settings

Source Column	
ROW_ID	337
COMPOUND_ID	REG
COMPOUND_BATCH_ID	REG
ASSAY_DATE	201
Assay Subtype	mic
SLOPE_CLEARANCE_CATEGORY	Hig
TEST_CONC_UM	1

File Settings

Data Source Type: Delimited

File Parse Settings - Delimited

Enter the delimiter that separates columns in the file: Comma

Enter the text qualifier (quoting character): "

Enter the character that is used to escape special characters: "

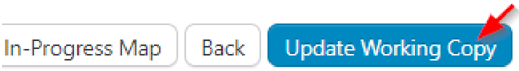
Does this file have multiline values (note: this option will not be reflected in the preview)?: ☐

Preview (first 10 columns)

Column Name	Example
ROW_ID	33744387
COMPOUND_ID	REG00475600
COMPOUND_BATCH_ID	REG00475600-01

Note: You may also need to specify the delimiter used in your batch data file, by choosing the setting in the **Enter the delimiter that separates columns in the file** drop down box on the **Import Settings** dialog shown above.

7. On the **Map Details** page, click **Update Working Copy** button to apply the map.



Once the batch data is uploaded and mapped, you can continue with the measurement data publishing workflow from within Signals Inventa.

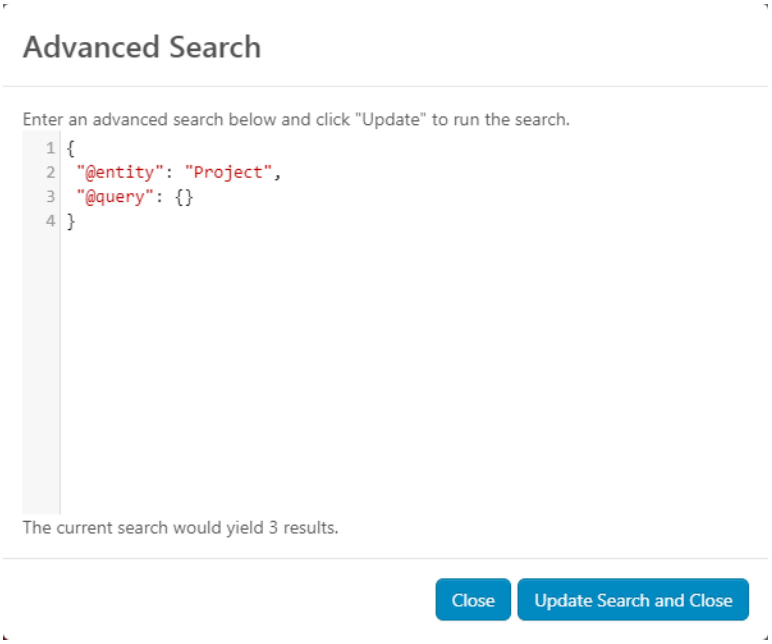
4.7 Creating a Query Template for use in Assay Results Review (ARR) App

The Assay Results Review app is designed to compare the historical Data of a measurement type with the current data for the same measurement type.

Using the Advanced Search feature in Signals Data Factory, you can create a query template to search the historical data of a measurement type by inputting parameters in an advanced search definition.

To create a query template:

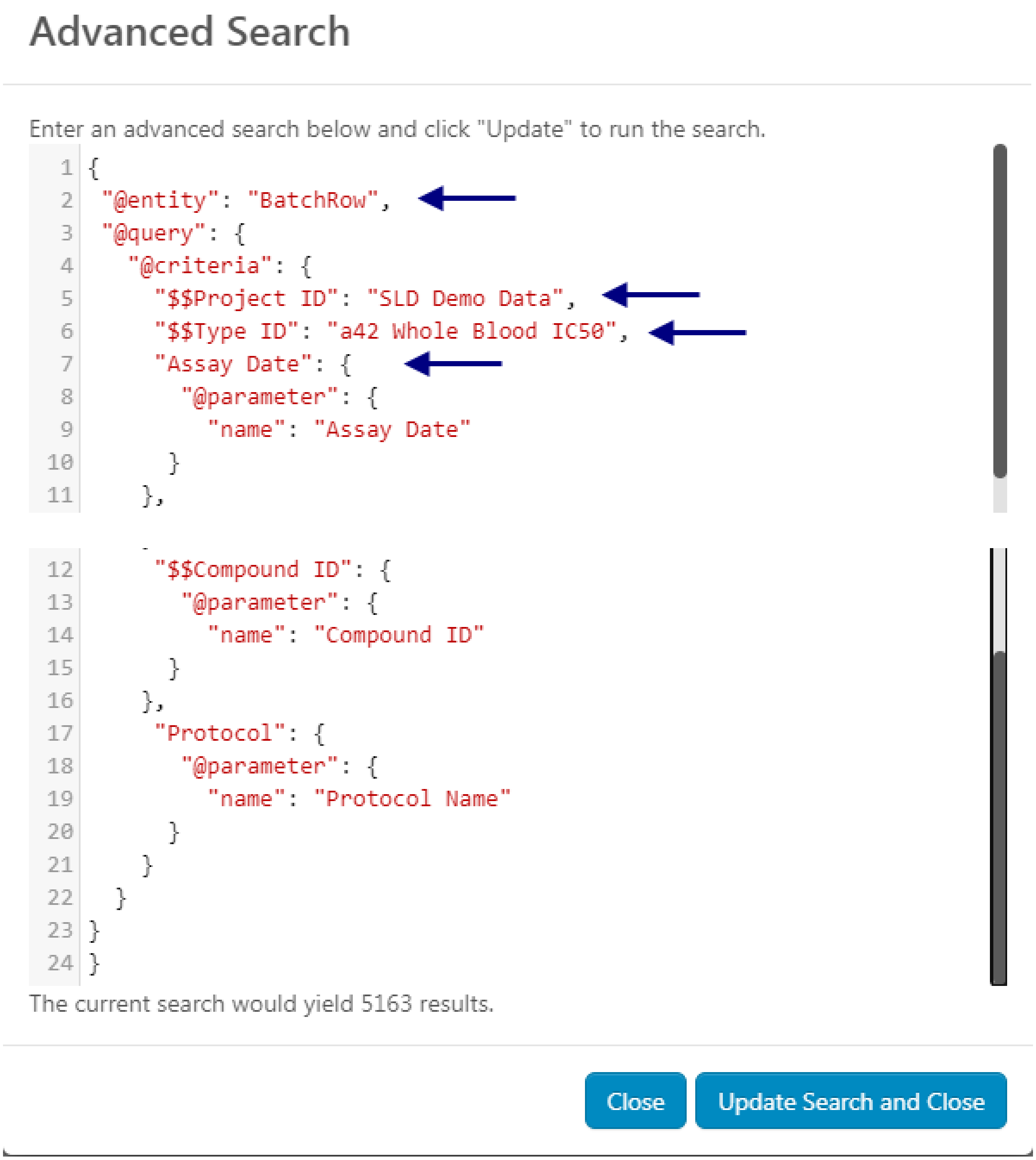
1. From the main Search page, click on the **Advanced Search** button located beneath the search facets in the left pane.



Enter an advanced search below and click "Update" to run the search.

```
{
 "@entity": "Project",
 "@query": {}
}
```

The current search would yield 3 results.



Advanced Search

Enter an advanced search below and click "Update" to run the search.

```
{
 "@entity": "BatchRow",
 "@query": {
   "@criteria": {
     "$$Project ID": "SLD Demo Data",
     "$$Type ID": "a42 Whole Blood IC50",
     "Assay Date": {
       "@parameter": {
         "name": "Assay Date"
      }
    },
     "$$Compound ID": {
       "@parameter": {
         "name": "Compound ID"
      }
    },
     "Protocol": {
       "@parameter": {
         "name": "Protocol Name"
      }
    }
  }
}
}
```

The current search would yield 5163 results.

2. Input the following locators:

- The type of entity is “BatchRow” or “CompoundRow” depending on if the Measurement Type is associated with Batch or Compound.
- The name of the SDF Project
- The name of the Measurement Type
- Pre-defined parameters based on any attribute of the measurement type. For example, you can define the Assay Date attribute (from the a42 Whole Blood IC50 measurement type) as a parameter, such that when

Assay Results Review app generates the UI, it will create a date/time picker UI component from which the user can specify the criteria of the Assay Date to query for the historical assays.

The advanced search criteria are entered by means of a JSON document defining all of the search criteria.

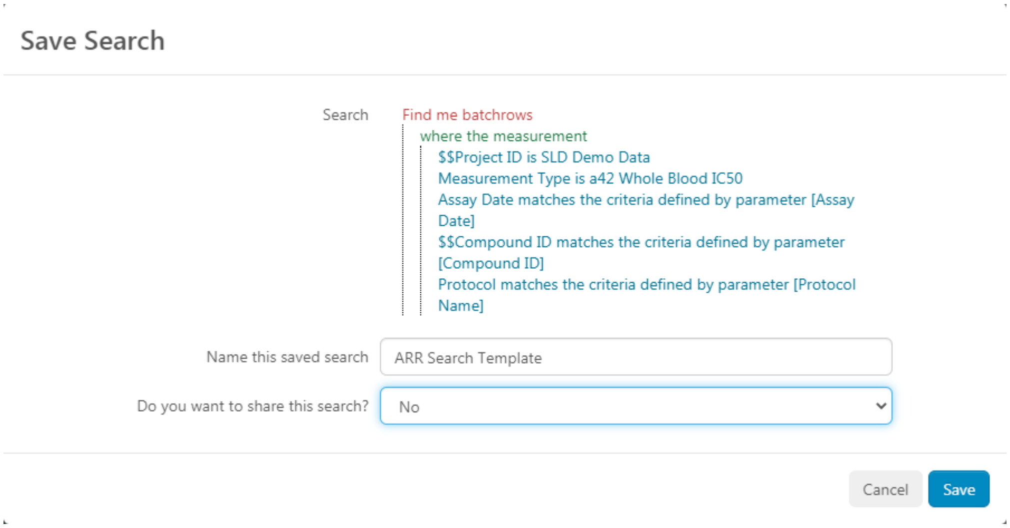
The advanced search is periodically validated as it is modified. Invalid JSON, or an invalid search structure will display an error beneath the criteria preventing the search from being saved. A valid search will result in the hit count for that search.

For the Assay Results Review app to work correctly, it is imperative that the query template follows a similar structure to that shown above. The execution of the query MUST return the data for a particular measurement type.

Note: The parameters in the SDF query must be named identically to the column name in the Current Data workflow in Spotfire. For example, you must name your **Assay Date** parameter as **MeasurementDate** if the column that contains the current assay data in the Spotfire table is named “**MeasurementDate**”.

3. After entering the search criteria, click **Update Search and Close**.

4. Click **Save Search** button.



Search
Find me batchrows
where the measurement
$$Project ID is SLD Demo Data
Measurement Type is a42 Whole Blood IC50
Assay Date matches the criteria defined by parameter [Assay Date]
$$Compound ID matches the criteria defined by parameter [Compound ID]
Protocol matches the criteria defined by parameter [Protocol Name]

Name this saved search: ARR Search Template

Do you want to share this search?: No

The current Search narrative is displayed.

5. Enter a name for the saved search.

6. You can choose to share the search. If you want to share this search, select ‘Yes, with everyone’. ‘No’ is selected by default.

7. Click **Save** button.

The Assay Results Review app will retrieve all visible saved queries from the Signals Data Factory and only make available the query templates (saved searches with ‘@parameter’ contained in the definition) in the app.

Refer to [Assay Results Review App](#) section for more detailed information on this app.

4.8 Signals Inventa Configuration

Signals Data Factory also provides the features and user interface components for managing measurement types, attributes and maps. However, these are general features that support common scientific data transformation use cases. With the exception of Compound/Batch attribute management, it is strongly recommended you use the measurement type, attributes and maps management features in Signals Inventa to accomplish information design, as the features in Signals Inventa may provide you advanced capabilities such as assay endpoint mapping definition, guided measurement type creation, etc. Refer to Appendix B – Signals Data Factory for more information.

To access the Signals Inventa configuration for measurement types, attributes and maps, select the **Inventa Configuration** sub-menu from **Information Design** in Signals Data Factory. Once you have been redirected to the Signals Inventa configuration page, you can navigate back to Signals Data Factory by selecting the **SDF Configuration** sub-menu from **Information Design** in Signals Inventa.

5 Publish Measurements Tool

The Publish Measurements tool allows data producers to define table mapping, validate, and publish the data set to the Results index.

5.1 Accessing the Publish Measurements tool

The Publish Measurements tool is accessed through the main Spotfire Interface. You will be required to login to the Signals Data Factory using your SSO credentials before you can access the Publish Measurements tool if you have not already been authenticated or if your session has expired.

Note: If the SDF ApiKey Spotfire preference has been set, you will not be required to logon. Refer to Setting the SDF APIKey section for further information.

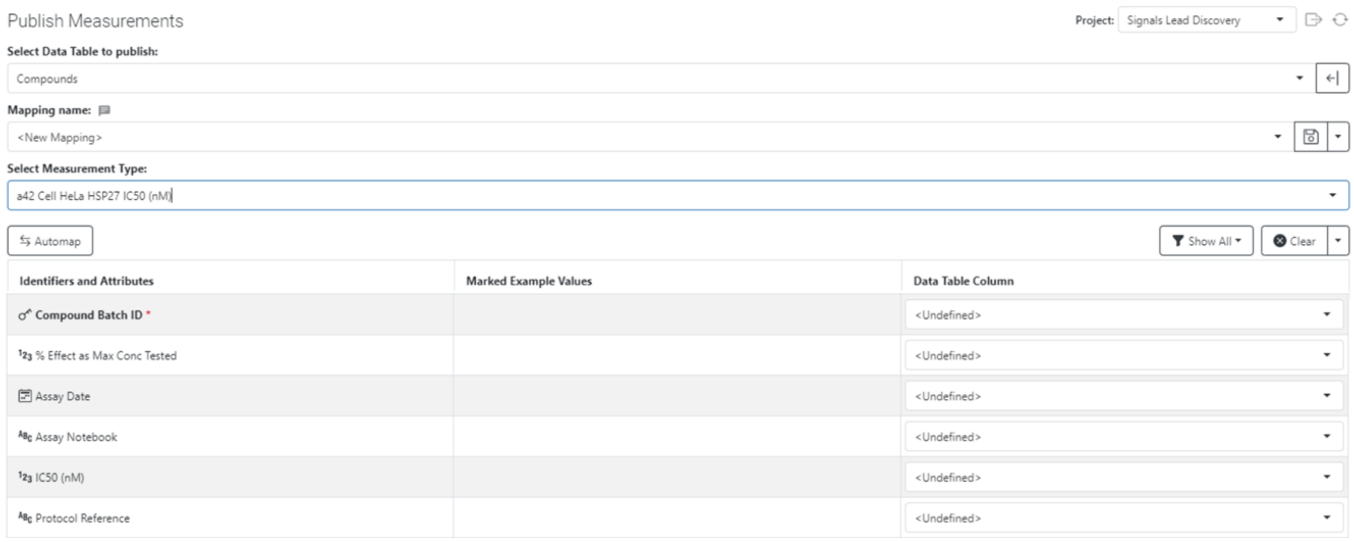
Note: If you are using Safari web browser, please make sure that it won't block the pop-up dialog from Signals Data Factory domain. To enable the pop-up dialog from Signals Data Factory:

1. In Safari, select **Preferences** menu.
2. In the **Preferences** dialog, choose **Websites** tab.
3. In the **Configured Websites** list, make sure that Signals Data Factory web page has been set to **Allow.**

To access the Publish Measurements tool:

In both Spotfire Analyst Client and Web Player:

1. Open data in Spotfire.
2. Select **Tools > Signals Inventa > Publish Measurements** from the main menu to add the Publish Measurements page. Alternatively, you can open the Visualization types flyout and click the **Publish Measurements** item to add a Publish Measurements page.



Project: Signals Lead Discovery

Select Data Table to publish: Compounds

Mapping name: <New Mapping>

Select Measurement Type: a42 Cell HeLa HSP27 IC50 (nM)

Identifiers and Attributes	Marked Example Values	Data Table Column
Compound Batch ID *		<Undefined>
% Effect as Max Conc Tested		<Undefined>
Assay Date		<Undefined>
Assay Notebook		<Undefined>
IC50 (nM)		<Undefined>
Protocol Reference		<Undefined>

5.2 Understanding the Publish Measurements Page

The Publish Measurements page allows you to define the mappings between a measurement type and a Spotfire data table and then publish the measurements. The following table describes the Publish Measurements page and the options available to you.

Option	Description
"Publish Measurements" visualization	The Publish Measurements visualization provides a user interface for you to define measurement type mappings and publish measurements.
Project Selector	A Project Selector drop down allows you to select the project to use for the Publish Meaurements tool. By default, the Publish Measurements tool opens with the project defined in the Spotfire preference. Refer to the Setting the Signals Data Factory Project Name preference for more information. You have the option to hide the Project Selector through a Spotfire preference. Refer to the Show SDF Project Selector preference section for information on setting this preference.
"Measurements (TableName)" Table plot visualization	The Table plot visualization allows you to preview the data of selected data table for publication.
➜	The logout button logs out the current user from the Publish Measurements Tool.
⟳	The Refresh button reads measurement types and mappings from the Metastore service. Click this button to refresh the **Select Measurement Type** and **Mapping name** drop-down list box.
Select Data Table to publish:	A drop-down list box for selecting a data table from the current Spotfire document.
|→ ←|	The Show/Hide table details buttons are used to show/hide table detail for the "Measurements (TableName)" Table plot visualization.
Mapping name:	A drop-down list box for selecting an existing measurement type mapping. The Mapping name list is retrieved from the Metastore service. <New Mapping> is selected if the current mapping definition is not saved in the Metastore service. **Note:** Only maps generated via Signals Inventa through the Publish Measurements Tool or through the Guided Measurement type creation workflow are available for selection here. Maps generated via Signals Data Factory are not available for selection.
💾 ▾	A drop-down button to create, overwrite or save the current mapping. Refer to the Saving Mapping section.
Select Measurement Type:	A drop-down list for selecting the measurement type for defining table mapping. The measurement type list is retrieved from the Metastore service. **Note:** Only the measurement types which have a defined Endpoint Publication Map are displayed in the drop-down list box. Refer to the section Managing Publish Endpoints.
⇆ Automap	Click the **Automap** button to automatically map the Measurement Type Attribute to the Spotfire Data Table Column. Refer to the Automapping section.

	Clicking on the **Show All** button gives you the option to Show Mapped or Show Unmapped measurement type attributes. You can also select to Show All (mapped and unmapped).
	A drop-down button to clear or reset a measurement type map.
<Mapping> table control	The table control allows you to define the mapping for each measurement type identifiers (Compound entity and Batch entity) and attributes. This table is comprised of 3 columns: **Identifiers and Attributes**, **Marked Example Values** and **Data Table. Identifiers and Attributes** column contains the attribute names for the selected measurement type, **Data Table Column** provides a list box for each line allowing the user to choose an expression or a column from the selected Spotfire data table to be mapped to the current measurement type attribute. The **Example Values** column displays the exemplary mapping result depicting how the data will look when it is transformed by Signals Data Factory. If the Measurement Type is associated with a Compound Batch, only an ID column from your measurement data to be mapped to Compound Batch ID is required. In this case, the Compound ID is not displayed as an identifier column. If the Measurement type is associated with a Compound, only an ID column from your measurement data to be mapped to the Compound ID is required. In this case, the Compound Batch ID is not displayed as identifier column.
Publish data from Data Table "Table Name"	A radio group control for choosing the rows for publication from the selected data table.
Map saving status bar	A status bar to indicate if the current measurement type map has been saved to the metastore service.
	Click the **Validate** to validate the mapping for the selected published data. Refer to the Validating Data section.
	Click the **Publish** button to begin the publish process. Refer to the Publishing Data section.

5.3 Defining Table Mapping

From the Publish Measurements page, you can define the mappings between a measurement type and a Spotfire data table.

5.3.1 Selecting Measurement Type

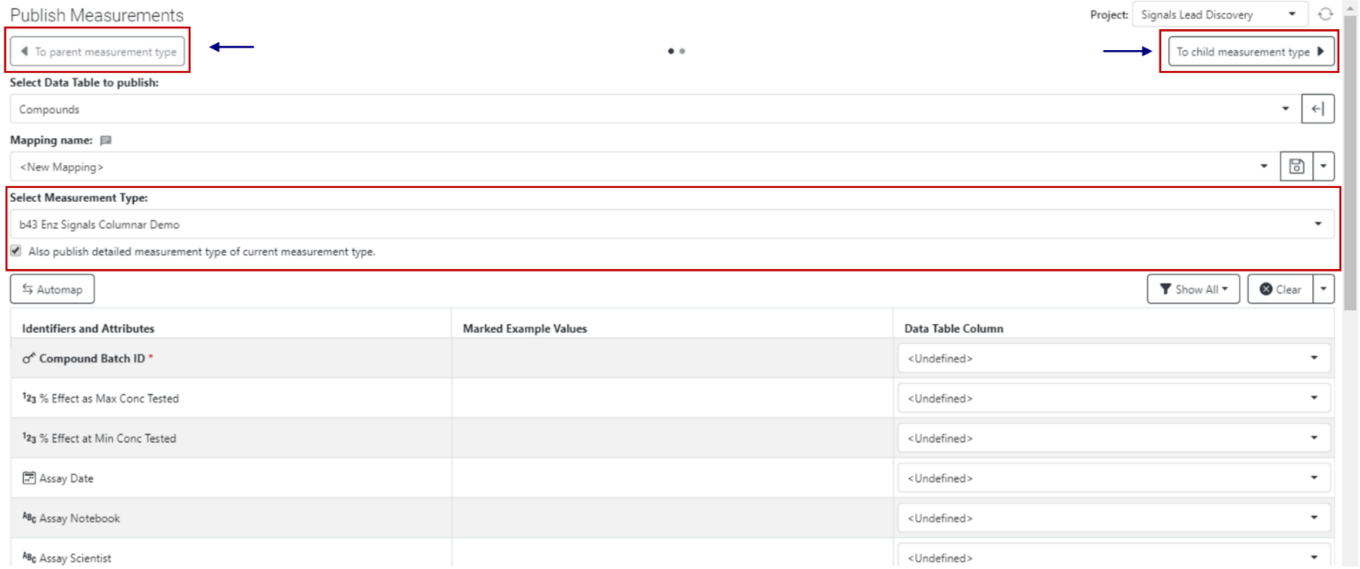
During the initialization of the Publish Measurements visualization, all existing measurement types will be retrieved from the metastore service and displayed in the Select Measurement Type drop-down list box. By default, the first measurement type is selected. You can change the measurement type at any time.

To select a measurement type:

1. From the **Select Measurement Type** drop-down list box, select the measurement type.

Note: Selecting a different measurement type will cause the current mapping data to be overwritten without prompting you for confirmation. You can click the **Undo** button to revert your changes.

Note: If the selected measurement type has a details measurement type, and you have two or more data tables in your current analysis with table relationships being defined in Data Table Properties dialog, an option to publish the detailed measurement type of the current measurement type becomes available.



Project: Signals Lead Discovery

Select Data Table to publish: Compounds

Mapping name: <New Mapping>

Select Measurement Type: b43 Enz Signals Columnar Demo

☑ Also publish detailed measurement type of current measurement type.

Identifiers and Attributes	Marked Example Values	Data Table Column
Compound Batch ID *		<Undefined>
% Effect as Max Conc Tested		<Undefined>
% Effect at Min Conc Tested		<Undefined>
Assay Date		<Undefined>
Assay Notebook		<Undefined>
Assay Scientist		<Undefined>

Using the ‘To parent measurement type’ and ‘To child measurement type’ toggles, you can toggle between the parent measurement type and child measurement type to define mapping for both. You are able to validate the mappings for each of the measurement types. You can publish both the details results to the details Measurement Type (e.g. Well-level % inhibition assay) as well as the main result assay (e.g. IC50 assay). Refer to the sections below for more information.

Note: When selecting data table for both parent and detail measurement types, you should choose the data tables that have data table relations defined. In most cases, such data table relations represent which table is the parent and which table is the child. During the data publishing, the publish tool will generate unique identifiers for the rows in both parent and child table according to the table relations. These unique identifiers act as the primary keys in the parent table and foreign keys in the child table so that when importing, the data transformer can understand the relations between the two. After Global Search has downloaded both parent and detail measurement data, the data table relation are rebuilt based on this unique identifier column.

5.3.2 Setting Data Table to Publish

The first (default) data table in the current Spotfire document is selected in the **Select Data Table to publish** drop-down list box by default. You can change the value at any time. Changing the data table will clear the map definition.

To select a data table to publish:

1. From the **Select Data Table to publish** drop-down list box, select the data table.

Note: Changing the data table will clear the current map definition without prompting you for confirmation. You can click the **Undo** button in toolbar to revert your changes.

5.3.3 Loading an Existing Measurement Type Map

Existing measurement type maps are retrieved from the metastore service and displayed in the **Mapping name** drop-down list box. By default, <New Mapping> is selected. You can select an existing map in the drop-down list at any time. After selecting a different map, Signals Inventa will apply the map definition in the current page.

To select a measurement type map:

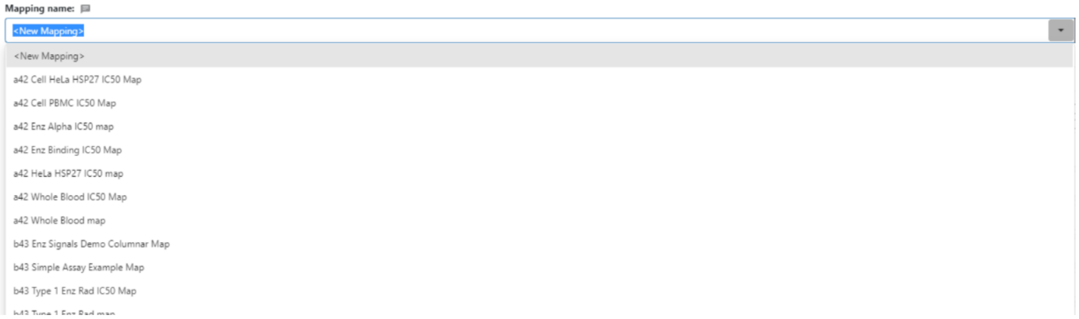
1. From the Mapping Name drop-down list box, select the mapping name.

Note: Selecting a different map will cause the current mapping data to be overwritten without prompting you for confirmation. You can click the **Undo** button in toolbar to revert your changes. The measurement type will be updated to reflect the selected measurement type map.

To filter the mappings:

The **Mapping name** drop-down list box also provides a text box where you can input a filter string. Using this feature, you can quickly navigate to the map of interest.

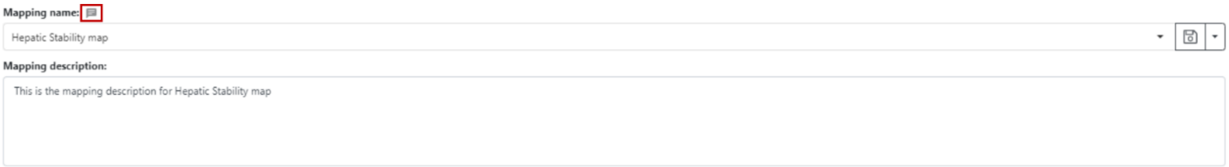
1. Select the ⌄ drop-down icon in the Mapping Name drop-down list box.
2. In the search text box, type to search for a mapping name.



Mapping name: <New Mapping>

To view the map description:

1. Click the 💬 icon to the right of the **Mapping name** label to show/hide the Mapping description text box.



Mapping name:

Hepatic Stability map

Mapping description:

This is the mapping description for Hepatic Stability map

5.3.4 Automapping

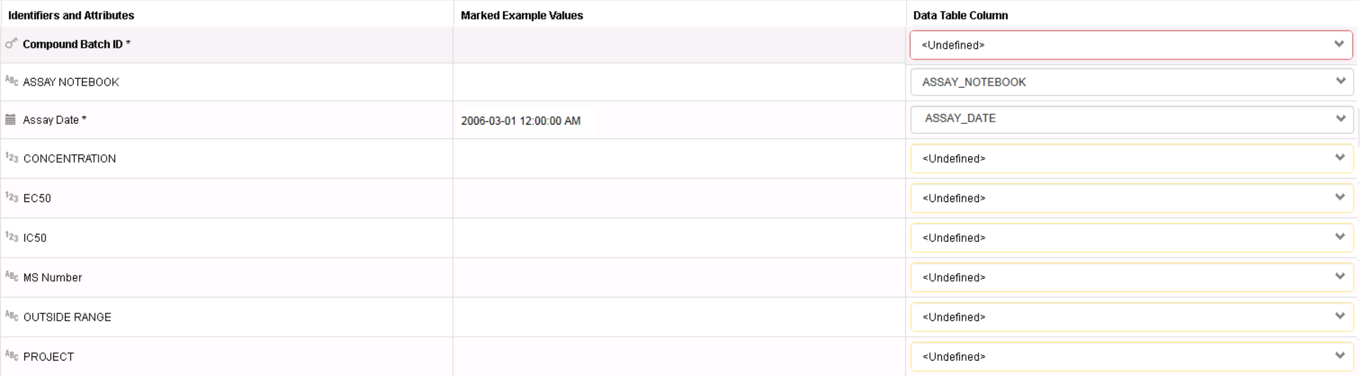
You can click the **Automap** button at any time to reset the mapping between the measurement type attributes and the Spotfire data table columns automatically. This feature will automatically find the best matching Spotfire data table column for each measurement type attribute by using a string comparison algorithm.

The algorithm used in **Auto Mapping** feature of the Publish Measurements tool is dependent on a threshold value to adjust the accuracy of the mapping result. The default value for Auto Mapping is 0.4. If you find that the automapping behavior is too fuzzy or not fuzzy enough, you can modify the threshold for the comparison algorithm in the Spotfire preferences.

Refer to the section [**Setting the Auto Mapping Threshold**]() for more information.

5.3.5 Defining the Mapping Manually

The table in the **Publish Measurements** visualization allows you to manually define the mapping for the identifiers and measurement type attributes. You have the option to select a Spotfire data table column or create an expression.



Identifiers and Attributes	Marked Example Values	Data Table Column
Compound Batch ID *		<Undefined>
ASSAY NOTEBOOK		ASSAY_NOTEBOOK
Assay Date *	2006-03-01 12:00:00 AM	ASSAY_DATE
CONCENTRATION		<Undefined>
EC50		<Undefined>
IC50		<Undefined>
MS Number		<Undefined>
OUTSIDE RANGE		<Undefined>
PROJECT		<Undefined>

The table consists of three columns. Each is described below.

Identifiers and Attributes

The identifiers and attributes for the selected measurement type are listed. The icon displayed to the left of the attribute represents the data type. There are four data types:

Icon	Data Type
🔑	Unique Value
ABC	Text

123	Number
📅	Date
🖼	Image

Identifier and attribute names with an asterisk (*) suffix indicate that the identifier/attribute is mandatory and must have a mapping defined for it.

Note: In measurement types that are ONLY mapped to a Batch, the “Compound ID” key is not available in the ‘Identifiers and Attributes’ column during mapping.

Marked Example Values

This column displays the marked example values for a mapping definition.

- For <Undefined> mapping, it is blank
- For <Expression…> mapping, it displays the result of the expression.
- For Spotfire data table column mapping, it displays the mapped column value in the first selected row.

Data Table Column

From here, you can specify the mapping for each measurement type identifier and attribute.

The drop-down list box contains three mapping options:

- <Undefined>: is the default value which indicates that nothing will be mapped to the measurement type attribute. The publication will ignore any <Undefined> columns in the CSV output. Setting a measurement type identifier/attribute to <Undefined> for a mandatory measurement type identifier/attribute will result in a violation. Refer to the section “Validating Data”.
- <Expression…>: indicates that the publication will use the result of an expression in the output column for the measurement type identifier/attribute. Refer to the section “Creating an Expression”.
- Spotfire data table column: indicates that the publication will use the data of the selected Spotfire table column in the output column for the measurement type identifier/attribute.

Mapping Status

The drop-down list box controls in the Data Table Column use color to indicate the status of the mapping. Border color is used to represent violation information.

- A red border indicates that the measurement type identifier/attribute is mandatory, and you must define a valid mapping for it before publishing.
- A yellow border indicates that the measurement type identifier/attribute is optional, and you can publish without defining a mapping for it.
- A black border indicates that mapping has been defined for the measurement type identifier/attribute.

5.3.6 Creating an Expression

In the case where there is not a proper data table column to map to the measurement type identifier/attribute, you can add a Spotfire calculated column. The data in the calculated column is the result of a Spotfire expression which you defined in the Spotfire Expression Editor. The Spotfire expression is stored in the current Spotfire document. For other documents which use the same measurement type map, you will be required to add the calculated column again.

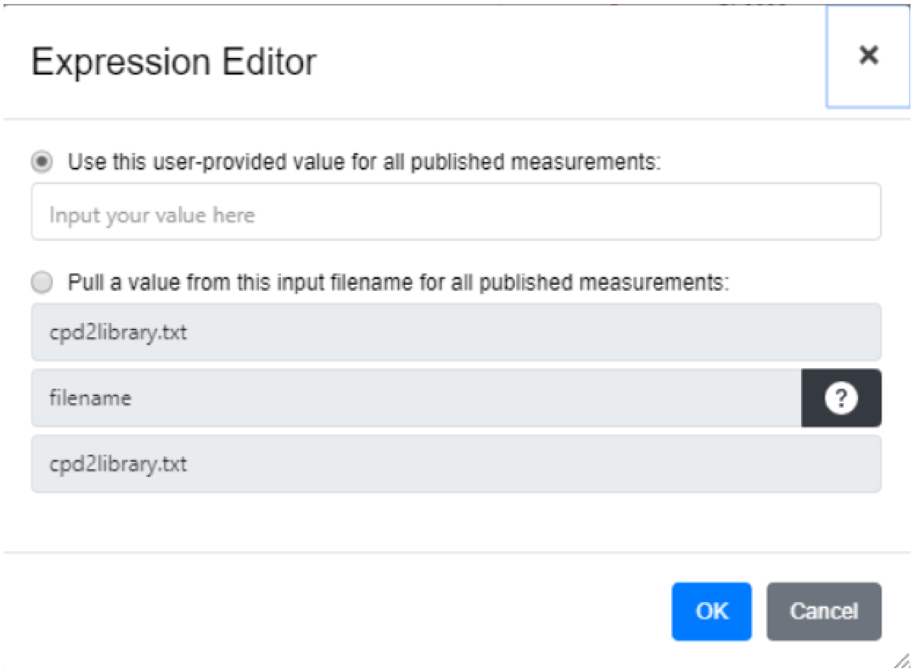
The <Expression…> option in the Data Table Column drop-down allows you to create an expression and store the definition with the mapping.

The Publish Measurements visualization supports two types of expression:

- Use this user-provided value for all published results
- Pull a value from this input filename for all published measurements

5.3.6.1 About the Expression Editor dialog

Selecting the <Expression…> option from the Data Table Column drop-down list box will open the Expression Editor dialog, similar to the example shown below.



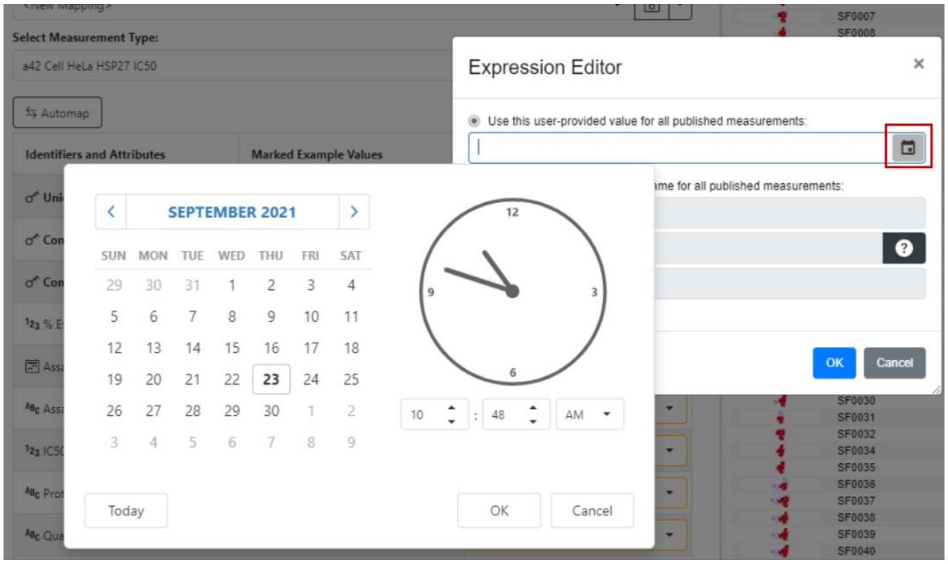
Option	Description
Use this user-provided value for all published measurements	Selecting this option will result in the publication using a user-provided value in the output column for the measurement type attribute.
<Input your value here>	To input the user-provided value.

Pull a value from this input filename for all published measurements	Using this option, you can select a file name from all the source files in the current Spotfire document and specify a JavaScript expression to extract a string value from the file name.
<File Name> drop-down	The drop-down list which contains all the source files in the current Spotfire document. You can select a file name as the value of the filename variable in the JavaScript expression.
<Expression> text box	Text box to input the JavaScript expression.
?	Clicking this icon will launch the **Help of Expression** dialog.
<Result> text box	A read-only text box to show the result of the expression.

5.3.6.2 Using the User-provided value

By selecting “Use this user-provided value for all published measurements” option in **Expression Editor** and entering a constant string in the text box, you can define a constant expression.

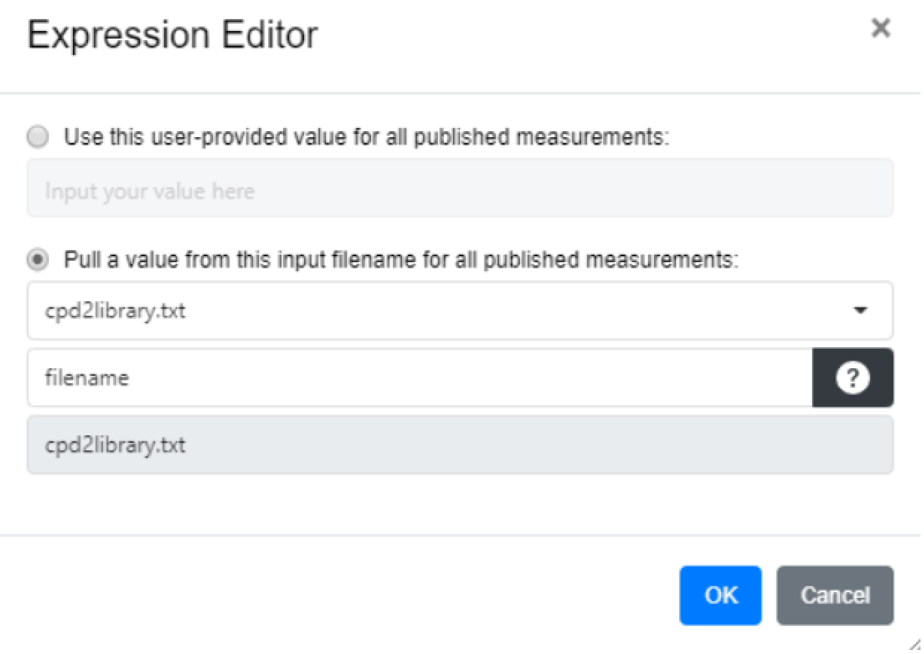
The expression editor respects the data type of the attribute. For example, if the attribute (e.g. Assay Date) is a Date data type, the expression editor provides a date/time picker for you to select the .



This expression will be stored as part of the map definition when you save the mapping. The publication will use the user-provided value in the output column for the measurement type attribute. **Note**: The user-provided value is validated during the validation process. If a violation is found, you will have to modify the expression or select another mapping option. You are not permitted to set replace value for an expression column mapping.

5.3.6.3 Pull a value from input filename

The “Pull a value from this input filename for all published measurements” option is designed to generate the expression value based on a Spotfire source file name and a JavaScript expression.



Expression Editor

○ Use this user-provided value for all published measurements:

Input your value here

● Pull a value from this input filename for all published measurements:

cpd2library.txt

filename

cpd2library.txt

<File Name> Drop-down

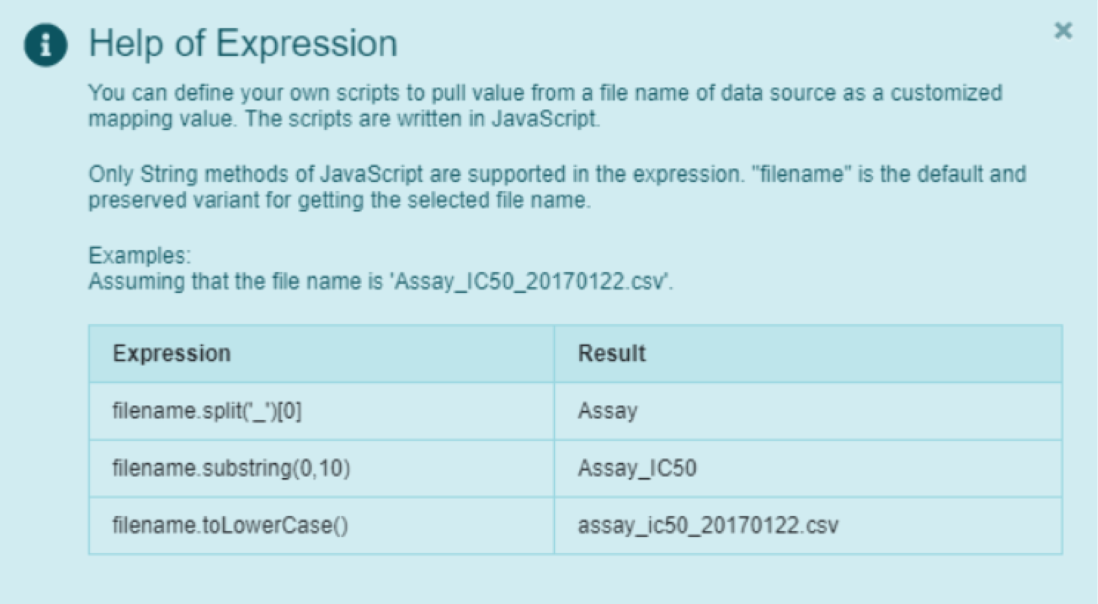
The Publish Measurements tool displays all source file names in the current Spotfire document in this drop-down list box. You can select a file name as the value of filename variable in the JavaScript expression.

Note: When you open an **Expression Editor** for a filename expression map, if the source file name does not exist in the current document, the first file name in the drop-down list box is automatically selected.

<Expression> Text Box

The file name selected in <File Name> drop-down is assigned to a string variable “filename”. Here you can write a JavaScript expression and use the variable in the expression.

The usage of the expression is described in a help page. You can open the Help dialog it by clicking the ? icon.



Help of Expression

You can define your own scripts to pull value from a file name of data source as a customized mapping value. The scripts are written in JavaScript.

Only String methods of JavaScript are supported in the expression. "filename" is the default and preserved variant for getting the selected file name.

Examples:
Assuming that the file name is 'Assay_IC50_20170122.csv'.

Expression	Result
filename.split('_')[0]	Assay
filename.substring(0,10)	Assay_IC50
filename.toLowerCase()	assay_ic50_20170122.csv

<Result> text box

The result of your expression will be displayed in the last text box. You cannot directly edit in this text box. It will be updated automatically each time you modify the expression and file name.

Note: When you open the **Expression Editor** for a filename expression map, if the source file name does not exist in the current document, the first file name in the <File Name> drop-down will be selected and the <Result> will be updated to the new expression result automatically.

To edit an expression:

1. Select the ✎ icon to open the Expression Editor dialog.
2. Edit the expression
3. Click **OK** to save the expression.

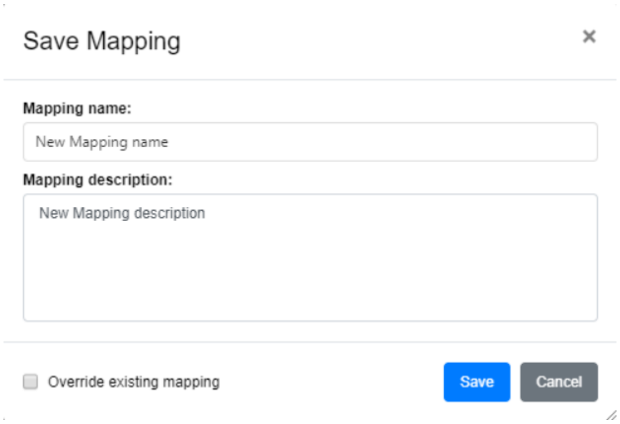
5.3.7 Saving Mapping

When you click the **Save Mapping** button located to the right of the Mapping Name drop-down list, the Publish Measurements tool will save the current mapping definition to the metastore service.

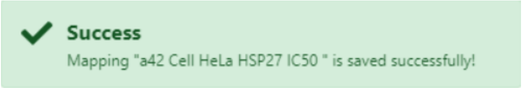
5.3.7.1 Saving a New Mapping

To save a new mapping:

1. Click **Save Mapping** button. The Save Mapping dialog appears.



2. Specify a Mapping Name and a description (optional) for the new mapping.
3. Click **Save**. A new mapping is created in the metastore service, and a message is displayed indicating that the mapping is saved successfully.


✓ **Success**

Mapping "a42 Cell HeLa HSP27 IC50 " is saved successfully!

5.3.7.2 Saving an Existing Mapping

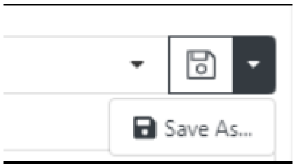
If the current mapping is an existing mapping, clicking the **Save Mapping** button will update mapping in the metastore service with the current mapping definition.

Saving as a New Mapping

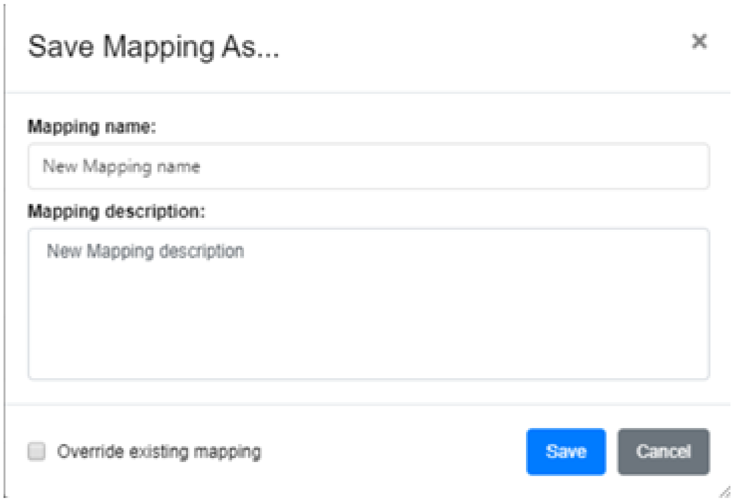
If the current mapping is an existing mapping, you can click the **Save As** button to create a new mapping.

To save as a new mapping:

1. Click the **Save As** button.



The Save Mapping As dialog appears.



2. Specify a Mapping Name and a description (optional) for the new mapping.
3. Click **Save**. A new mapping is created in the metastore service and a message is displayed indicating that the mapping is saved successfully.

5.3.7.3 Mapping Save Status Bar

The information bar located above the Validate and Publish buttons displays the saving status for the current map.

Note: Mapping must be saved before publishing. The **Publish** button is disabled until the current mapping is successfully saved.

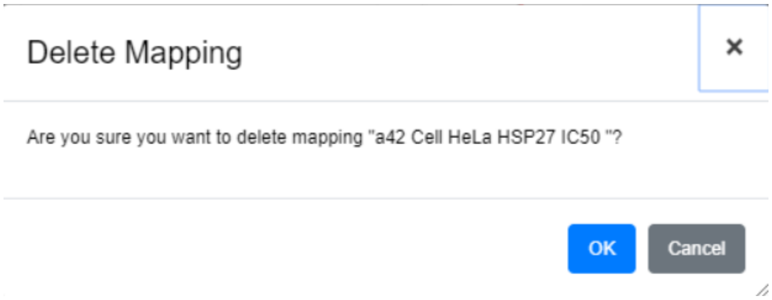
5.3.8 Delete a Mapping

To delete the selected mapping:

If the current mapping is not <New Mapping>, when hovering mouse on the Mapping name drop-down, the 🗑 icon is displayed.


Mapping name: a42 Cell HeLa HSP27 IC50

1. Click the 🗑 icon to delete the selected mapping. A message will appear prompting you to confirm the deletion.



Are you sure you want to delete mapping "a42 Cell HeLa HSP27 IC50 "?

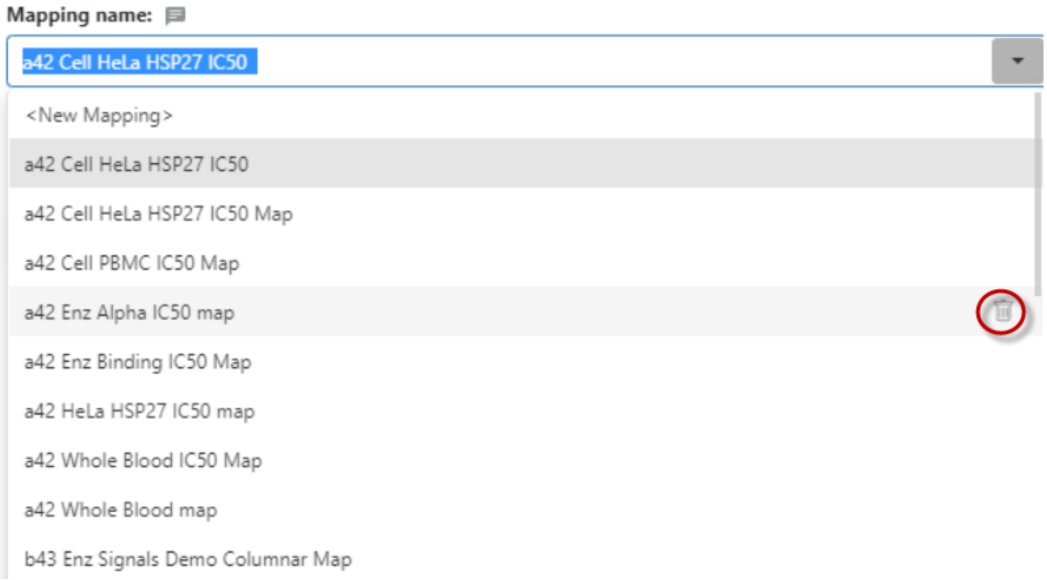
2. Click **OK** to delete the mapping.

The mapping is deleted from the metastore service and no longer appears in the Mapping name drop-down list box.

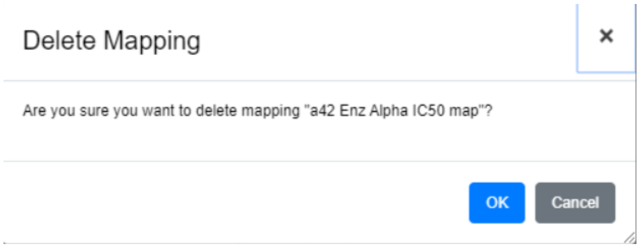
To delete other mappings from Mapping Name drop-down list box:

1. Click the Mapping name drop-down list box to expand the existing map list.

2. Hover the mouse on an existing mapping to be deleted. The 🗑 icon is displayed.



3. Click the 🗑 icon to delete the selected mapping. A message will appear prompting you to confirm the deletion.



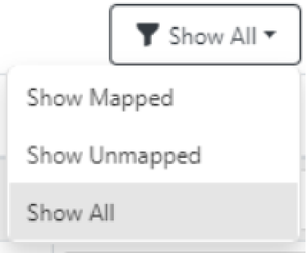
Are you sure you want to delete mapping "a42 Enz Alpha IC50 map"?

4. Click **OK** to delete the mapping.

The mapping is deleted from the metastore service and no longer appears in the Mapping name drop-down list box.

5.3.9 Viewing the Table Mapping

Clicking on the **Show All** button gives you the option to Show Mapped or Show Unmapped measurement type attributes. You can also select to Show All (mapped and unmapped attributes).



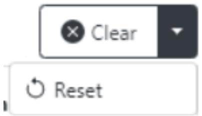
Option	Description
Show Mapped	Only the measurement type attributes with a mapped data table column or expression are visible. The measurement type attributes set to <Undefined> value are filtered out.
Show Unmapped	Only the measurement type attributes set to <Undefined> value are displayed.
Show All	Both mapped and unmapped measurement type attributes are displayed.

5.3.10 Clearing Mapping

Clicking the **Clear** button will set the mapping for all measurement type attributes to <Undefined>.

5.3.11 Resetting Mapping

If the current mapping is from the metastore service, clicking the **Reset** button will reset the map definition to the definition currently stored in the metastore service. For a <New Mapping>, the **Reset** button works in the same manner as the **Clear** button.



5.4 Validating Data

Before publication, it is necessary to validate the selected publishing data based on the measurement type attribute data type.

5.4.1 Mapping Rules

There are four rules defined for the measurement type attribute mappings.

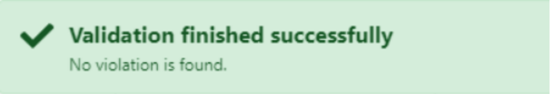
Rule	Message	Measurement Type Attribute Data Type
Missing required value	A value is required.	A measurement type attribute without a null constraint
String in a Number	A number is required.	A measurement type attribute requiring a number value
Invalid date value	A date value is required.	A measurement type attribute requiring a date value
Duplicated values for unique	A Spotfire data table column with unique values is required.	A measurement type attribute with a unique constraint

5.4.2 Validation Results

To validate the mapping for the selected published data:

1. Click the **Validate** button to validate the selected publishing data.

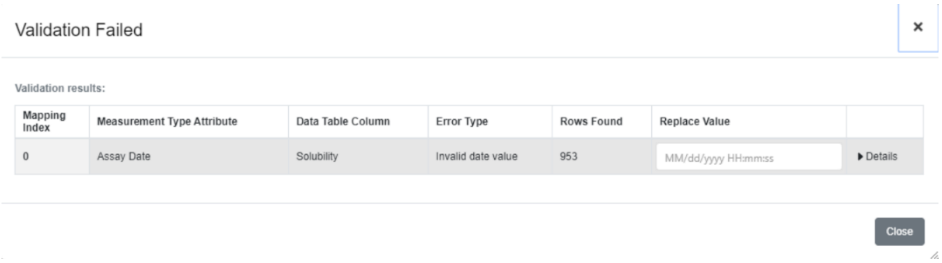
If there are no violations, you will be notified that validation finished successfully.



✓ **Validation finished successfully**

No violation is found.

If the validation process finds violations, you will be presented with a Validation Failed dialog, outlining the violations, similar to the example shown below.



Validation Failed

Validation results:

Mapping Index	Measurement Type Attribute	Data Table Column	Error Type	Rows Found	Replace Value	
0	Assay Date	Solubility	Invalid date value	953	MM/dd/yyyy HH:mm:ss	▶ Details

The following table describes the Validation results table.

Option	Description
Mapping Index	The index of the data table that is validated. 0 indicates that the current validation result is for the parent table, whereas 1 indicates that the current validation result is for the details table.
Measurement Type Attribute	The measurement type attribute displaying a violation.
Column	The name of the Spotfire data table column.

Error Type	The error type is displayed.
Rows Found	The number of rows found with the violation.
Replace Value	Input a replace value for the violation rows in the measurement type attribute.
Details	Show/hide violation details.

To show/hide violation details:

1. Click the **Details** button to expand the page to display the violation details. Click the **Details** button to collapse the details information.

5.4.3 Resolving Violations

You can choose to ignore the rows with errors at this time, or you can resolve the violations using the Replace Value field.

When you leave the Replace Value text box, the new replace value is immediately validated. An error message will appear in red text if there is still a violation with the replace value.

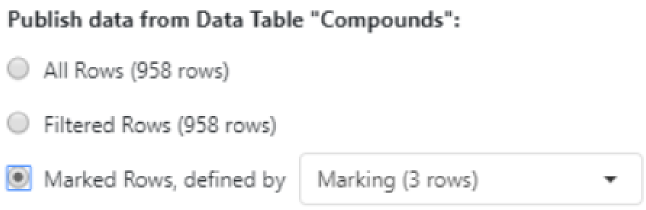
Note: Should you choose to ignore the rows with errors at this time, you will be prompted again to resolve any violations when publishing measurements.

5.5 Publishing Data

The Publish Measurements tool allows you to select the rows in the selected data table and publish measurements using the specified measurement type map to a file share location.

5.5.1 Selecting Rows for Publishing

The Publish Measurements tool provides three different options for selecting rows in the selected data table for publication.



Publish data from Data Table "Compounds":

○ All Rows (958 rows)

○ Filtered Rows (958 rows)

● Marked Rows, defined by Marking (3 rows)

The descriptions for option are listed in below table:

Option	Description
All Rows	All the rows in the selected data table will be published.
Filtered Rows	Only the result rows of the active filter will be published.
Marked Rows	Only the rows which are marked in the selected marking will be published.

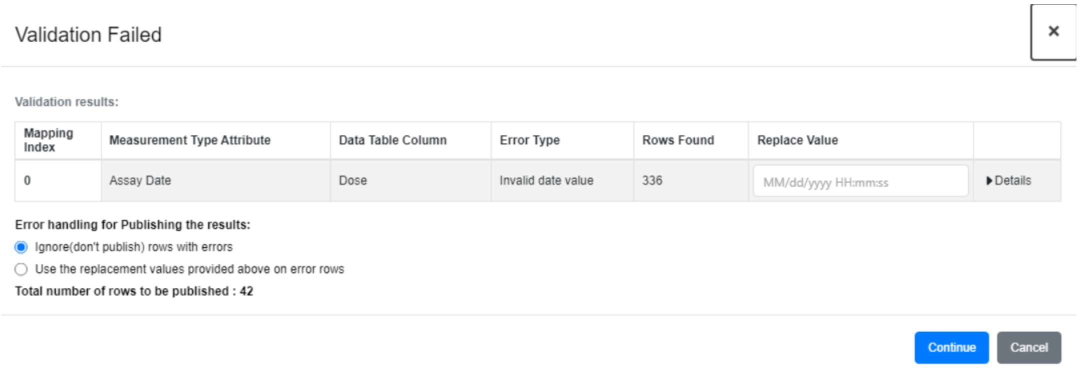
Selecting Marking for Publish

If you choose the “Marked Rows” option, the Marking drop-down will be enabled. You can choose a marking among all the markings in the document.

By marking rows in the “Measurements (TableName)” Table plot, you can select rows for publication.

5.5.2 Error Handling

If violations are identified in the selected publish rows, the Validation Failed dialog will appear listing the validation results, similar to the example shown below.



Validation Failed

Validation results:

Mapping Index	Measurement Type Attribute	Data Table Column	Error Type	Rows Found	Replace Value	
0	Assay Date	Dose	Invalid date value	336	MM/dd/yyyy HH:mm:ss	▸Details

Error handling for Publishing the results:

● Ignore(don't publish) rows with errors

○ Use the replacement values provided above on error rows

Total number of rows to be published : 42

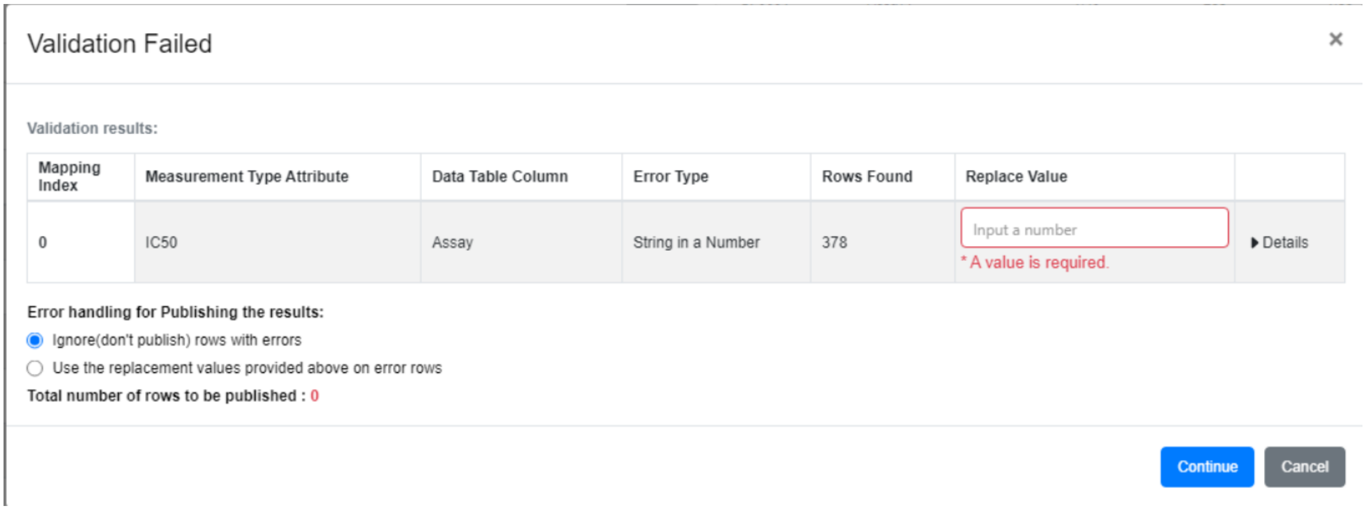
A row indicator identifies the number of rows to be published. Note that the number of rows to be published will be listed for both parent and child tables if applicable.

From here, you can select how to handle the identified violations.

Option	Description
Ignore (don’t publish) rows with errors	The publication job will ignore all rows with errors.
Use the replacement values provided above on errors rows	The specified replacement values will be used when publishing.

Note: If you define one data table column to map to multiple measurement type attributes, the publication job will only output one column in the CSV table and all violations in the column will be populated with the replacement value.

If the total number of rows to be published is 0, and you click the **Continue** button, you will be prompted to confirm if you want to continue with the publication.



Validation Failed

Validation results:

Mapping Index	Measurement Type Attribute	Data Table Column	Error Type	Rows Found	Replace Value	
0	IC50	Assay	String in a Number	378	Input a number * A value is required.	▸ Details

Error handling for Publishing the results:

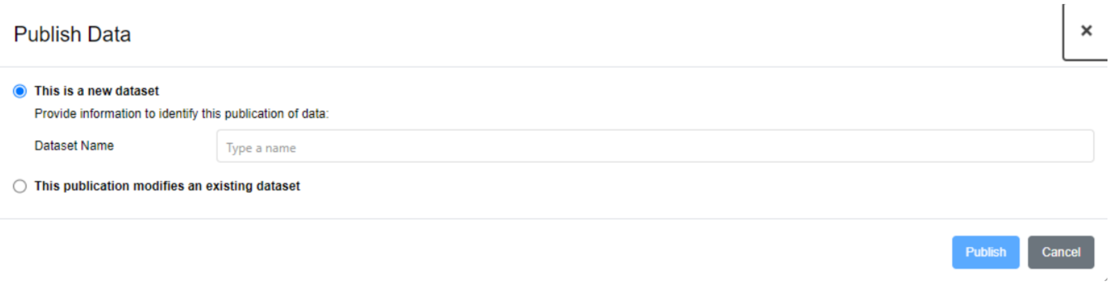
● Ignore(don't publish) rows with errors

○ Use the replacement values provided above on error rows

Total number of rows to be published : 0

5.5.3 Publishing

If there are not any violations, clicking the **Publish** button will open the **Publish Data** dialog directly. However, if there are violations, you need to handle the errors in **Validation Failed** dialog and then click **Continue** to proceed with the publication process.



Publish Data

● This is a new dataset

Provide information to identify this publication of data:

Dataset Name: Type a name

○ This publication modifies an existing dataset

From the Publish Data dialog, you can create a new dataset for the publication or modify an existing dataset. By default, creating a new dataset is selected.

Refer to Appendix D for information on importing images into Spotfire.

5.5.3.1 Publishing to a New Dataset

To publish data to a new dataset:

1. Select the “This is a New dataset” option.
2. Provide information to identity this publication of data by entering a Dataset Name. .
3. Click the **Publish** button.

A message is displayed indicating that the table has been successfully published to the dataset.

5.5.3.2 Publishing to an Existing Dataset

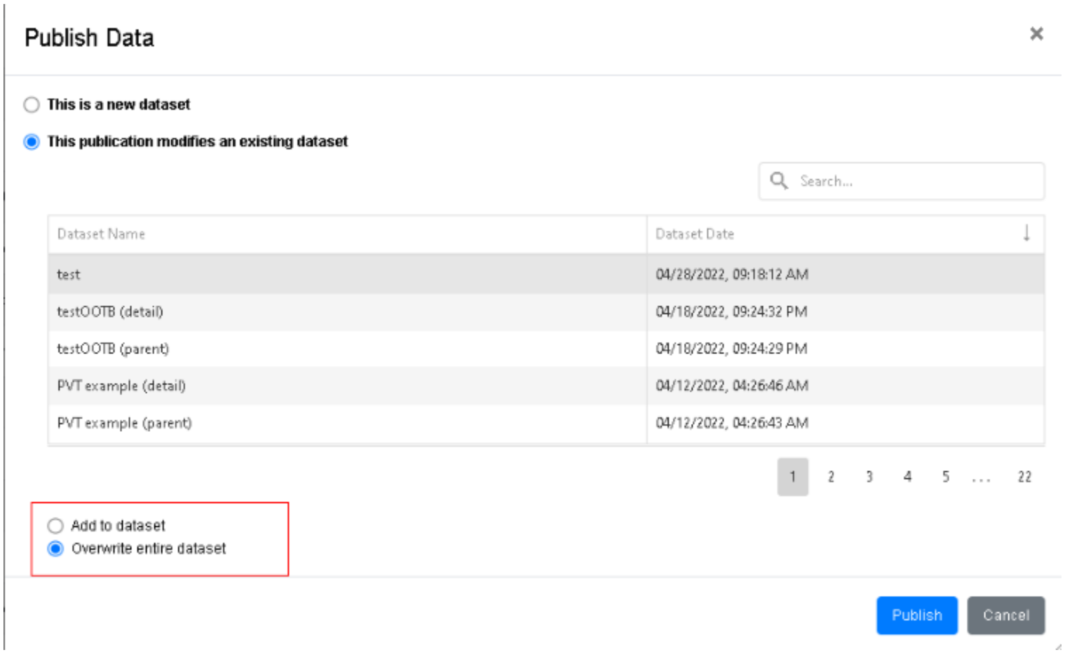
To publish to an existing dataset:

Note: This option will be greyed out if there are no existing datasets under the selected SDF project.

1. Select the “This publication modifies an existing dataset.”

Existing datasets under the selected SDF project are displayed in a table with the Dataset Name and Dataset Date.

2. Select the dataset to publish to.



Publish Data

○ This is a new dataset

● This publication modifies an existing dataset

Dataset Name	Dataset Date
test	04/28/2022, 09:18:12 AM
testOOTB (detail)	04/18/2022, 09:24:32 PM
testOOTB (parent)	04/18/2022, 09:24:29 PM
PVT example (detail)	04/12/2022, 04:26:46 AM
PVT example (parent)	04/12/2022, 04:26:43 AM

○ Add to dataset

● Overwrite entire dataset

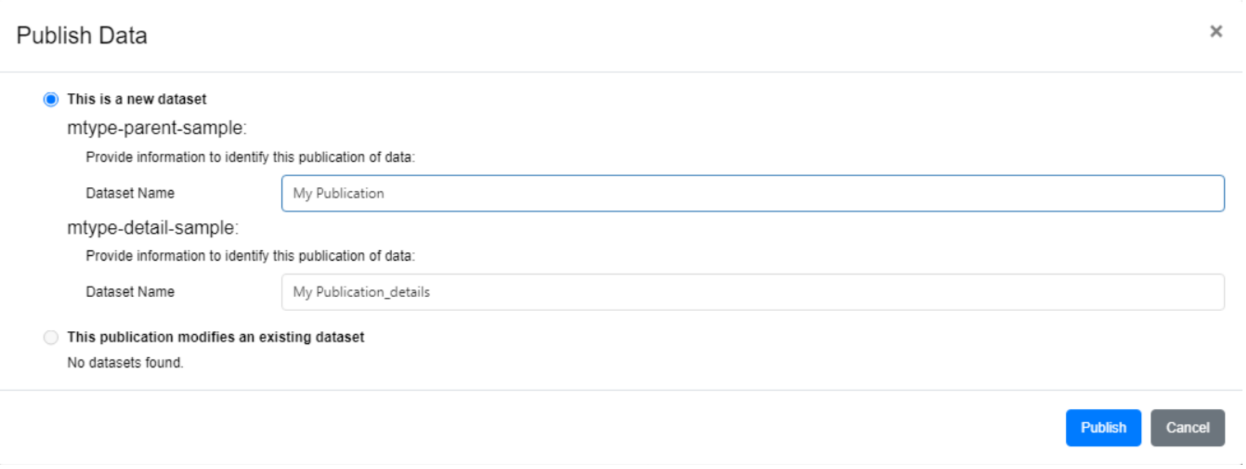
3. Select the method to publish to an existing dataset. The following options are available.

Option	Description
Add to dataset	Appends the publishing measurement data to an existing dataset. **Important Note**: If the mapping used for the publication differs from the mapping that was used by the selected dataset, all files in the selected dataset will be reinterpreted with the new mapping.
Overwrite entire dataset	The existing dataset will be overwritten by this publication. This is the default selection.

Note: To preserve dataset consolidation between Signals Inventa and Signals Data Factory, the dataset name assigned here will be the dataset name that is displayed in the Signals Data Factory allowing for quicker identification and retrieval of datasets in the Signals Data Factory.

Note: If “Also publish detailed measurement type of current measurement type” check box is checked, this means that both the parent and detail measurement types are going to be published. In such case:

If “This is a new dataset” option is chosen, the data of these two measurement types will be published into two different datasets in Signals Data Factory. Users can enter a DataSet Name for the parent measurement type. By default, the child Dataset name will autopopulate with the “parent Dataset Name” plus the suffix “_details”. Users have the option to rename the child Dataset Name.



Dataset Name: My Publication

Dataset Name: My Publication_details

No datasets found.

If “This publication modifies an existing dataset” is chosen, the user can choose the parent and child dataset from the list to modify. The ‘Add to dataset’ and ‘Overwrite an existing dataset’ options are applied to BOTH the parent and child measurement type.

4. Click the **Publish** button.

A message is displayed indicating that the table has been successfully published to the dataset.

6 Global Search

After data is published to the Signals Data Factory through Signals Inventa, the Global Search interfaces allows you to:

- Create complex nested queries and interrogate any subset of the stored data of interest.
- Explicitly set the scope of a query to be Compound, Batch, or Measurements, which results in much more precise control over the results set returned
- Query for Structure, any compound attribute, and any assay or measurement, and query over an expanded set of comparison operators.
- Include multiple chemistry search criteria to more precisely find the subset of compounds, batches or measurements of interest.
- Control system performance directly by choosing estimated vs. precise query result counts at different levels of precision.
- Save queries for easy re-use. Saved searches can be public or private
- Run the SAR Analysis App directly from the Global Search page

Global Search uses the Compounds, Batches and Assay Endpoint Results tables from Signals Data Factory to provide the search capabilities.

6.1 Accessing the Global Search tool

The Global Search is accessed through the main Spotfire Interface. You will be required to login to the Signals Data Factory using your SSO credentials before you can access Global Search if you have not already been authenticated or if your session has expired.

Note: If the SDF ApiKey Spotfire preference has been set, you will not be required to logon. Refer to Setting the SDF ApiKey section for further information.

Note: If you are using Safari web browser, please make sure that it won't block the pop-up dialog from Signals Data Factory domain. To enable the pop-up dialog from Signals Data Factory:

1. In Safari, select **Preferences** menu.
2. In the **Preferences** dialog, choose **Websites** tab.
3. In the **Configured Websites** list, make sure that Signals Data Factory web page has been set to **Allow.**

To access the Global Search tool:

In Spotfire Analyst Client:

1. Select from the main menu to open the Global Search page. Alternatively, you can open the Visualization types flyout and click the **Global Search** item to open the Global Search page.

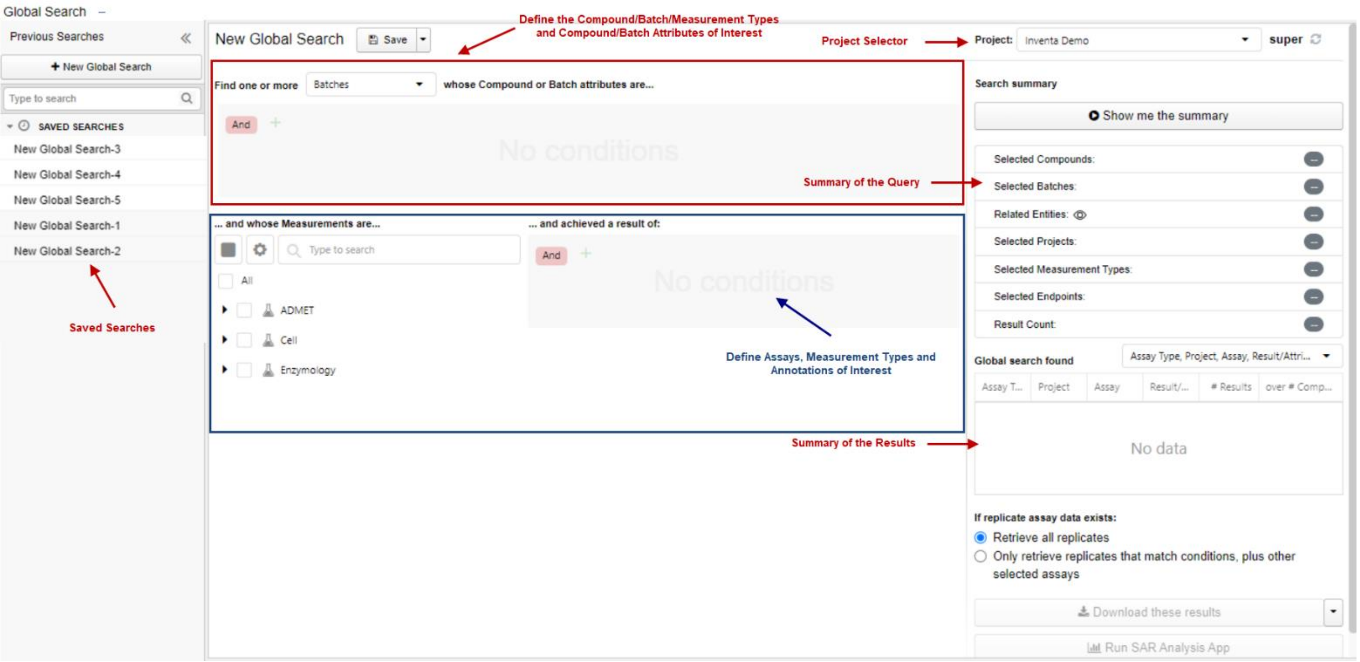
In Web Player:

1. Open data in Spotfire.

2. Select **Tools > Signals Inventa > Global Search** from the main menu to open the Global Search page.

   Alternatively, you can open the Visualization types flyout and click the **Global Search** item to add a Global Search page.

A Global Search page is displayed, similar to the example shown below.



The top right corner of the displays the name of the logged in user. A Project Selector drop down allows you to select the project to use for the Global Search. By default, the Global Search opens with the project defined in the Spotfire preference. Refer to the Setting the Signals Data Factory Project Name preference for more information. You have the option to hide the Project Selector through a Spotfire preference. Refer to the Show SDF Project Selector preference section for information on setting this preference.

The re-sizable left side panel lists all previously saved searches.

The center panel allows you to define the Compounds/Batches/Measurements and Assay/Measurement Types and Annotations of interest. Each of these elements contributes to an intersection that yields a unique list of compounds/batches/measurements and assays results to be included in the resulting SAR analysis.

Note: Global Search uses the Signals Data Factory custom security, so you will only be able to select the compounds that you have permission to see. Administrative users can limit the visibility of compounds to specific user groups by using the Advanced Security feature provided by Signals Data Factory. For more information about how to setup the Advanced Security, please refer to Advanced Security section in this documentation.

Note: Global Search uses the Signals Data Factory custom security, so you may not be able to view all measurement types in the hierarchy tree if you do not belong to a group that has View/Search permission to a measurement type. For more information about how to setup the measurement type permissions, please refer to Measurement Type - Security Settings section in this documentation.

Note: Global Search uses the Signals Data Factory custom security, so you may not be able to view all of the assays or annotations in the hierarchy tree or in the query builder. . For more information about how to setup the Advanced Security, please refer to Advanced Security section in this documentation.

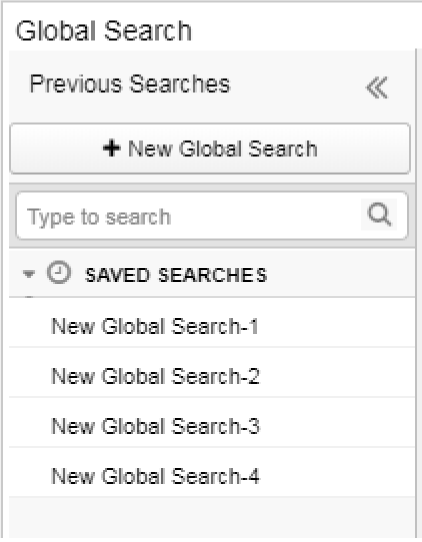
The right hand side of the panel presents the user with feedback about the search criteria and the set of compounds and results that will be returned by the search according to the user's permissions.

6.2 Previous Searches

From the Previous Searches panel, you can initiate a new global search, as well as see a list of your saved searches.

Saved searches can be selected and re-used. The search criteria and results will load once selected.

A Search field allows you to type ahead to search for the name of a previous search.



To expand/collapse Saved Searches list:

Above, the expanded view is shown. To collapse the Saved Searches, click the ▾ button. Alternatively,click on the ▸ button to expand the list.

To expand/collapse Previous Searches panel:

1. To increase the size of the query and result panel, you can choose to collapse the Previous Searches sidebar by clicking on the « button.
2. Click on the 🔍 button to expand the Previous Searches panel.

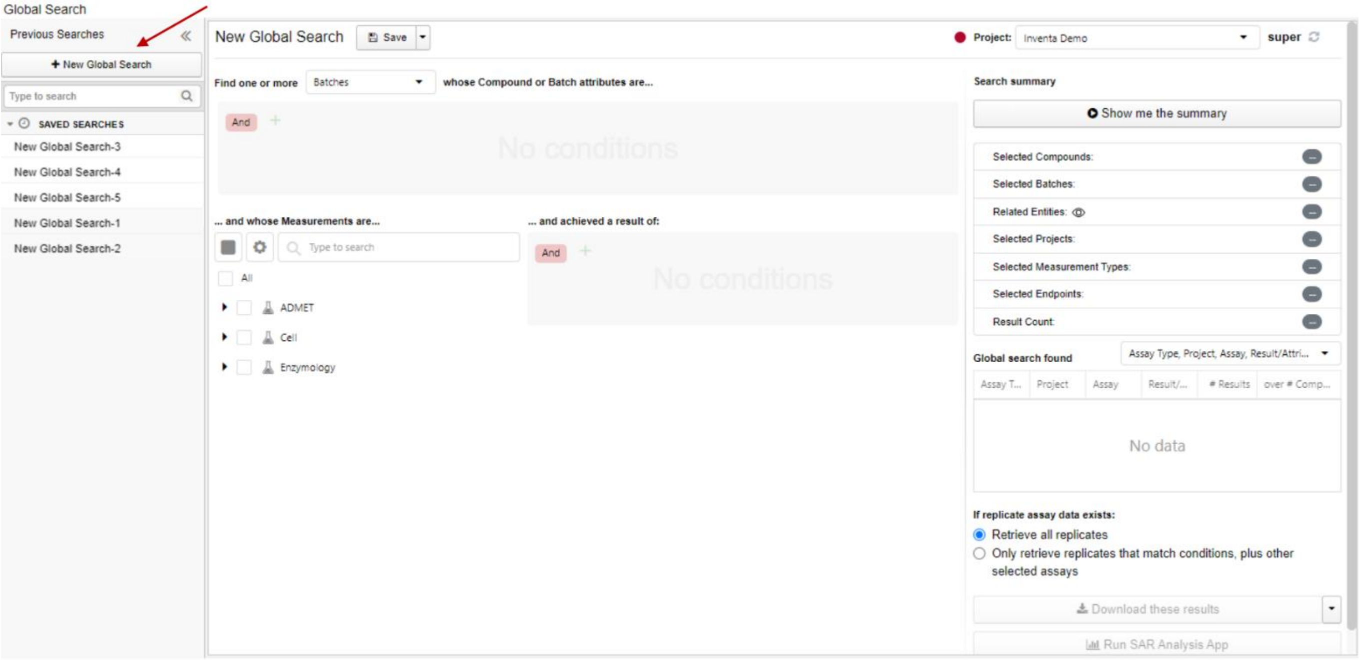
To delete a saved search:

1. Hover the cursor over the Saved Search name and click the 🗑 Delete button that appears. You will be prompted to confirm the deletion.

6.3 Performing a New Global Search

To initiate a new global search:

Click on the **+New Global Search** button to clear the previous search (if applicable).



A blank panel is now available for you to define a new search. By default, the search will be named ‘New Global Search’.

6.3.1 Reload

The Reload button is located in the right hand top corner of the page.

Clicking the ↻ Reload button will reload the data in the:

- Saved Searches list
- Chemical Compound Properties list
- Assay Hierarchy tree

6.4 Search for Compounds, Batches or Measurements of Interest

The ‘Find one or more <drop-down list> where Compound or Batch attributes are’ allows you to explicitly set the scope of a query to be Compound, Batch, or Measurements resulting in more precise control over the results set returned.

The default selection in the 'Find one or more <drop-down list> where Compound or Batch attributes are' can be set as a Spotfire preference via the Administration Manager. Refer to the section Setting the Default Search Scope in Global Search.

Using the filter builder widget, you can draw a query structure for the compound and/or define conditions for both compound and batch. The chemical structure and conditions will be used to perform a search on the compounds or batches.

The filter expressions are displayed as a tree structure where nodes represent simple filter conditions. Each condition consists of a data field, a comparison operation and a value. A logical operation combines conditions into groups.

The data field is a list of attribute names from the Compounds and Batchestables in Signals Data Factory. Compound attributes will be listed ahead of Batch attributes in the list. If applicable related entity tables are listed as well. Refer to the Search by Related Entity section for more information on related entities.

There is a structure field name allowing you to search by structure. Refer to the Search by Structure section for more information.

Note: This list is not fixed; it varies in different user scenarios, depending on what attributes have been defined for both Compound and Batch entities in the Signals Data Factory.

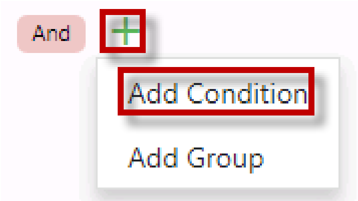
Note: The source entity name (e.g. Compound, Batch) to which the attribute is associated, is displayed in brackets as a prefix to the attribute name. This allows for you to easily identify which entity an attribute describes.

Note: Some attribute names may be followed by an asterisk (*). This indicates that a related entity table is linked to this field an additional information related to the attribute is available. Refer to the section Viewing Entity Relationships section for more information.

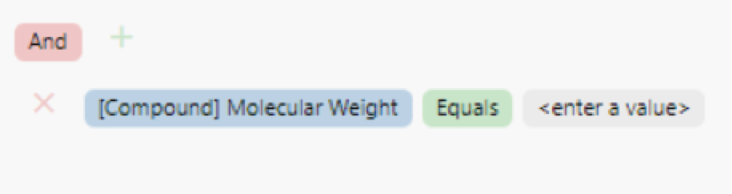
[Batch] Batch Number Is not blank
And +
[Batch] MolWeight Is less than 777
[Batch] Purity Equals 95

To add a condition:

1. Select **And**, **Or, Not And or Not Or** logical operator
2. Click on the + icon and select **Add Condition**.

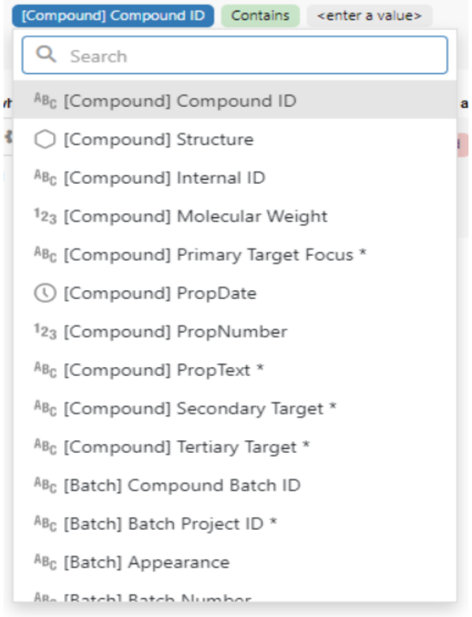


A condition is added to the filter builder.

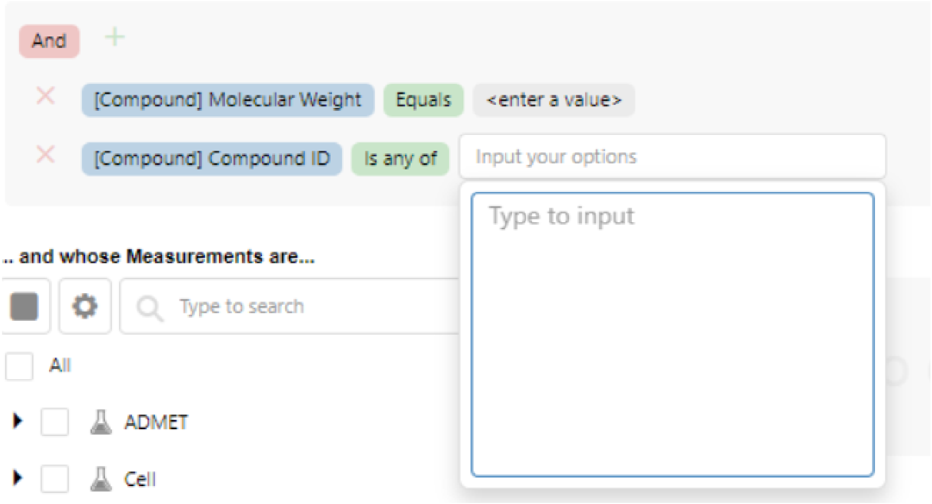


Clicking on the Data Field and Operation allows you to select the data field name and comparison operation from a list. Depending on the data field name selected, the comparison operators may vary.

A Search field allows you to type ahead to search for the data field name. A value can be entered in the Value field or you can use the type ahead to search for the value.



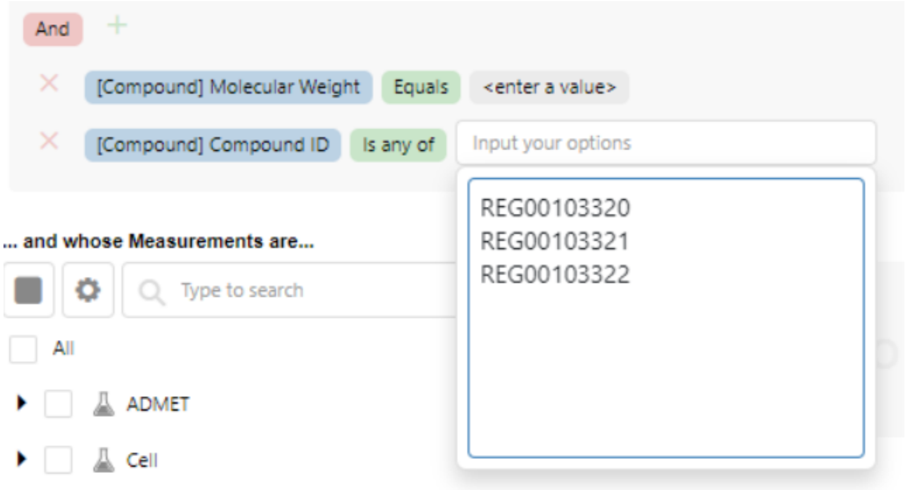
In the case where you want to input a list of values (e.g. list of compounds IDs), you will need to either select the ‘Is any of’ which is equivalent to an IN operation, or ‘Is all of’ which represents the operation that matches the field with all of the values specified



You can enter the values in the Type to input box. Accepted deliminators include comma, vertical bar, space or line break.

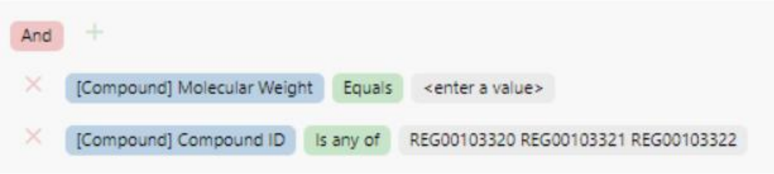
Note: For the ‘Is any of’ operator, you are limited to input no larger than 2.3MB text data (around 25,000 items approximately) in the input box. If the text data exceeds this limit, a warning message will appear and the operation will be cancelled. You will need to shorten the text in the input box

Note: For the ‘Is all of’ operator, a maximum of 100 items can be entered in the input box. As the ‘Is all of’ operation requires increased server resources, the amount of time it takes to provide the summary result or download data is increased. In certain cases, a failure may occur due to a time-out errorIf such an error occurs, reduce the number of items entered in the value input box



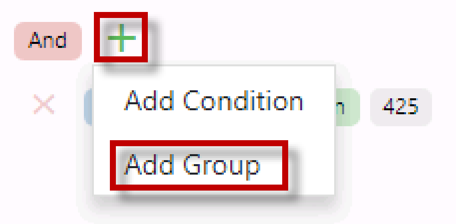
REG00103320
REG00103321
REG00103322

Once the values are entered, these will be displayed in the Values field, similar to the example shown below.

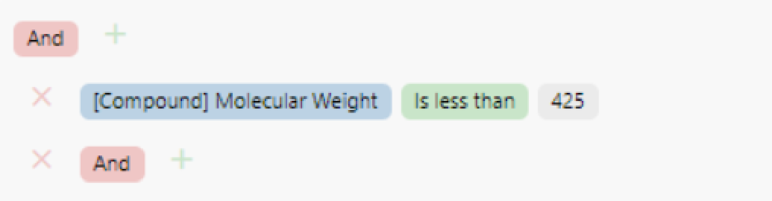


To add a group to the filter:

1. Select **And**, **Or, Not And or Not Or** logical operator.
2. Click on the + icon and select **Add Group**.

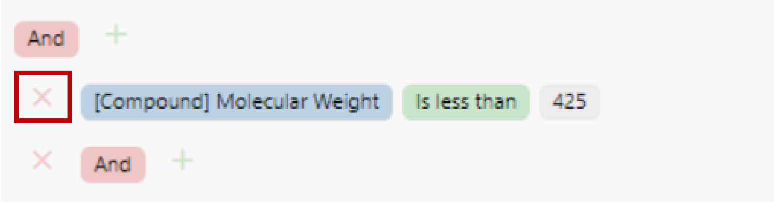


A Grouping query is added allowing you to group conditions.



To remove a condition:

1. Click on the × icon preceeding the condition to remove it from the filter.



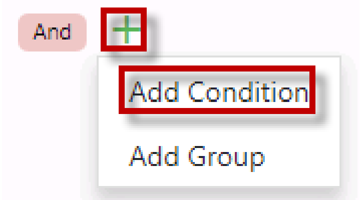
6.4.1 Search by Structure

Using the Structure data field, you can query a chemical structure.

Note: You can add multiple ‘Structure’ conditions using the filter builder widget.

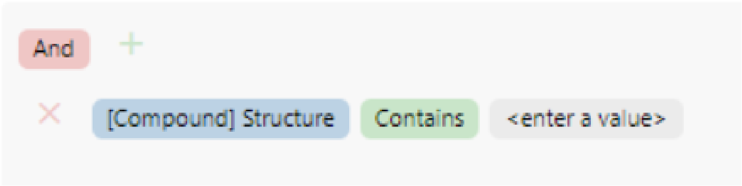
To define a structure query:

1. Select **And**, **Or, Not And** or **Not Or** logical operator
2. Click on the + icon and select **Add Condition**.



A condition is added to the filter builder.

3. Click on the Structure data field.



When the Structure column is selected, the operation field has the following options:

Contains – substructure search

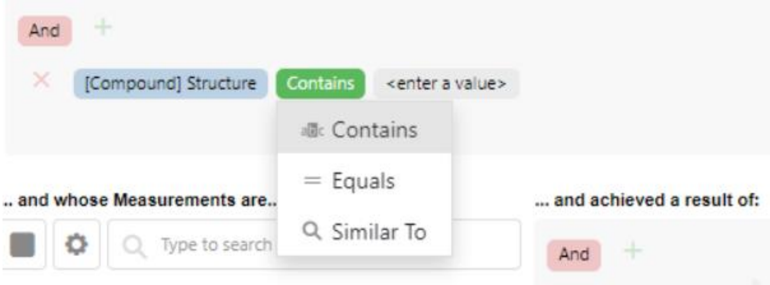
Equals – full structure search

Similar to – similarity search

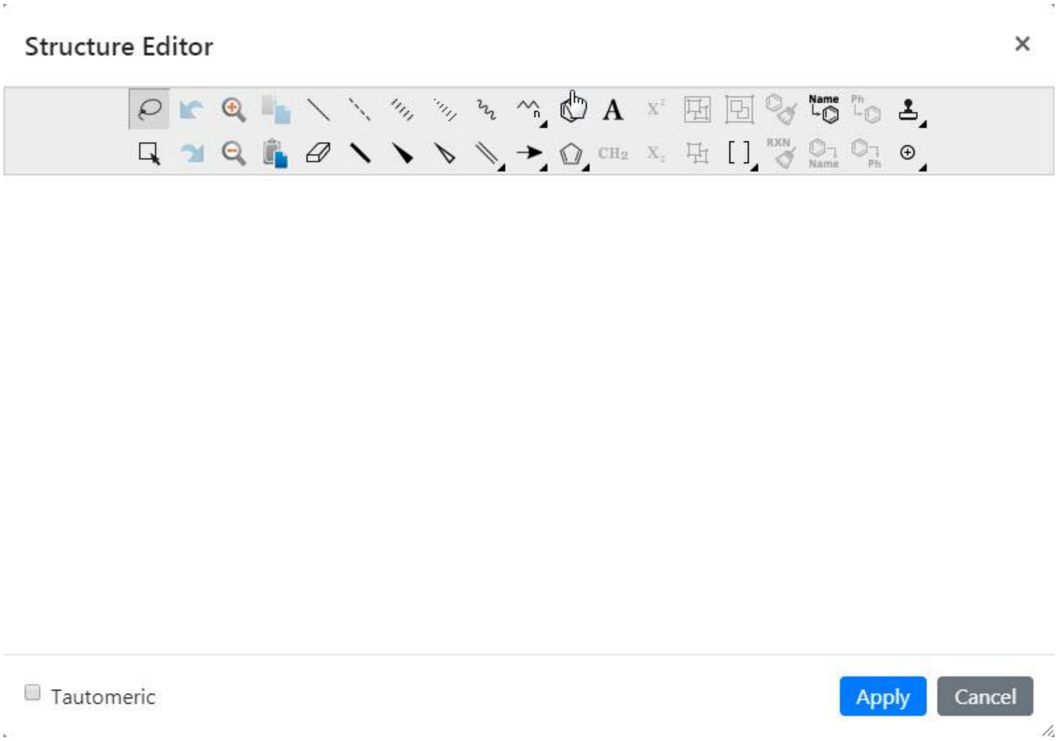
To perform a Substructure Search:

A Substructure search finds structures containing a common structural component, plus any additional attachments at the open positions. Substructure searches are useful if you have a general idea of the types of compounds you are looking for, but do not have an accurate description of the target compound.

1. Select the operation ‘Contains’,



2. Click on the <enter a value> parameter. The ChemDraw JS Structure Editor opens.



Note: The Structure condition supports the ChemDraw JS Editor. Signals Inventa will locate this application via a URL which is defined as a preference in Spotfire. Please refer to the ‘Setting the ChemDraw JS URL Preference’ section of Lead Discovery User Guide for more details.

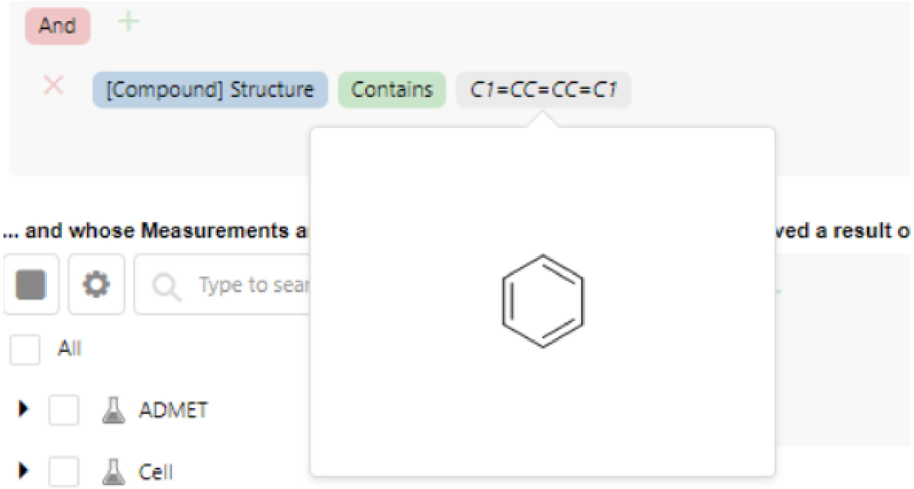
3. Draw the query structure in the Structure Editor window using appropriate tools.

Tautomers are isomers of a compound which differ only in the position of the protons and electrons. The carbon skeleton of the compound is unchanged. Substructure search types allow you to optionally filter for tautomers of the query structure.

4. To filter for tautomers, enable the Tautomeric checkbox.

5. Click **Apply**.

The SMILES representation of the structure is displayed in the Condition value. If you hover over the condition value, a thumbnail of the structure is displayed, similar to the example shown below.



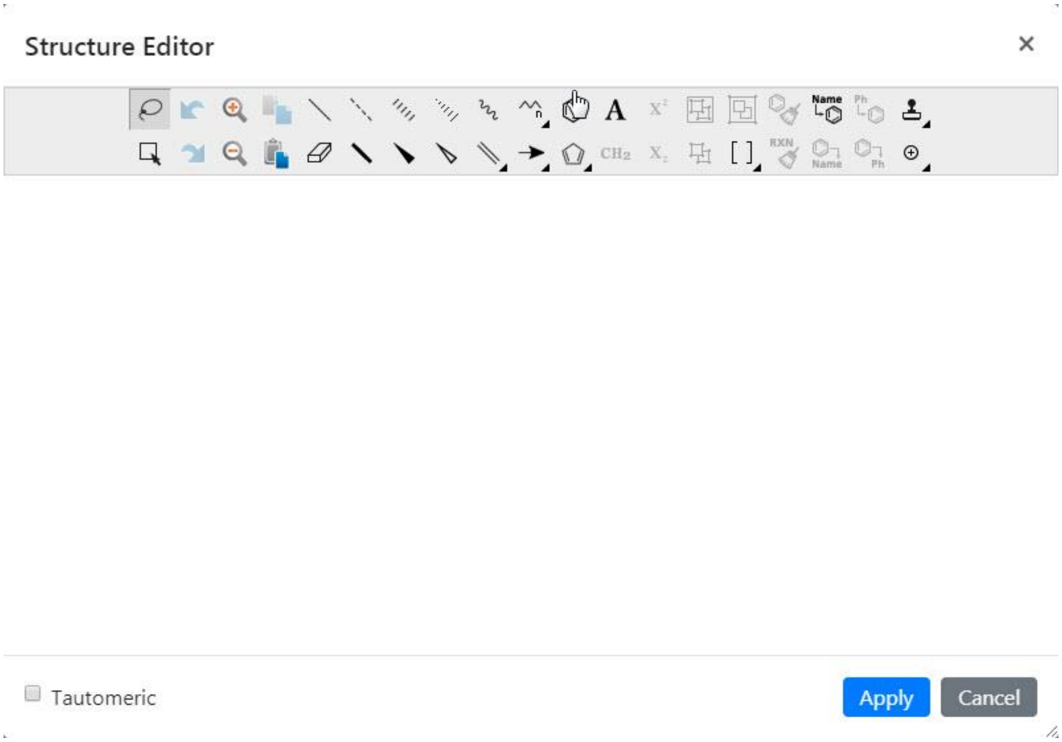
Clicking Apply initiates the search against Signals Data Factory.

To perform a Full Structure Search:

A Full structure search finds a particular structure.

1. Select the operation ‘Equals’,

2. Click on the <enter a value> parameter. The ChemDraw JS Structure Editor opens.



Note: The Structure condition supports the ChemDraw JS Editor. Signals Inventa will locate this application via a URL which is defined as a preference in Spotfire. Please refer to the 'Setting the ChemDraw JS URL Preference' section of Lead Discovery User Guide for more details.

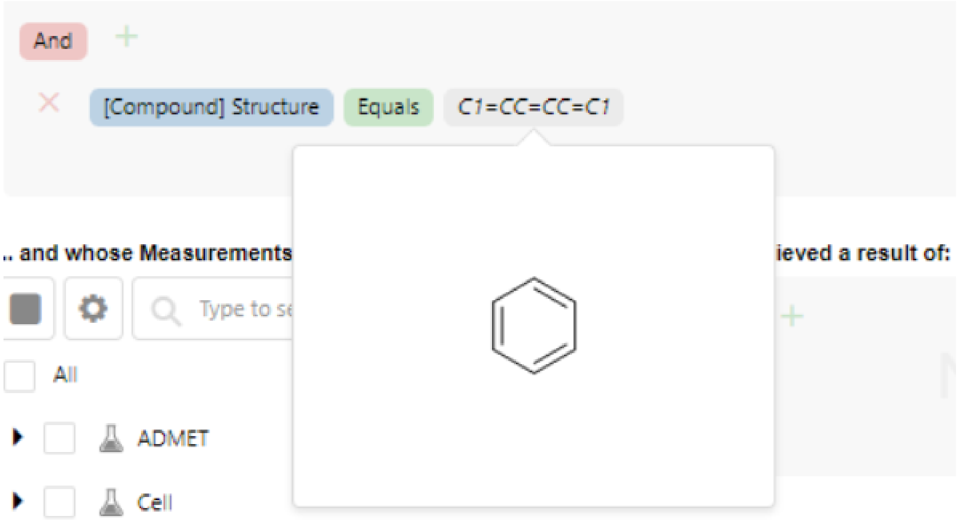
3. Draw the query structure in the Structure Editor window using appropriate tools.

Tautomers are isomers of a compound which differ only in the position of the protons and electrons. The carbon skeleton of the compound is unchanged. Substructure search types allow you to optionally filter for tautomers of the query structure.

4. To filter for tautomers, enable the Tautomeric checkbox.

5. Click **Apply**.

The SMILES representation of the structure is displayed in the Condition value. If you hover over the condition value, a thumbnail of the structure is displayed, similar to the example shown below.

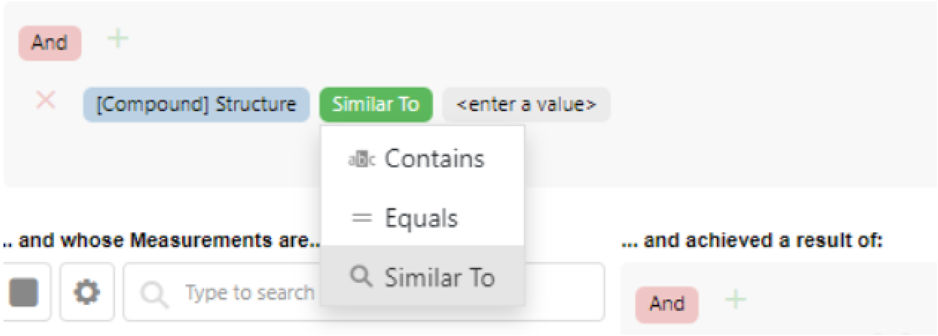


Clicking Apply initiates the search against Signals Data Factory.

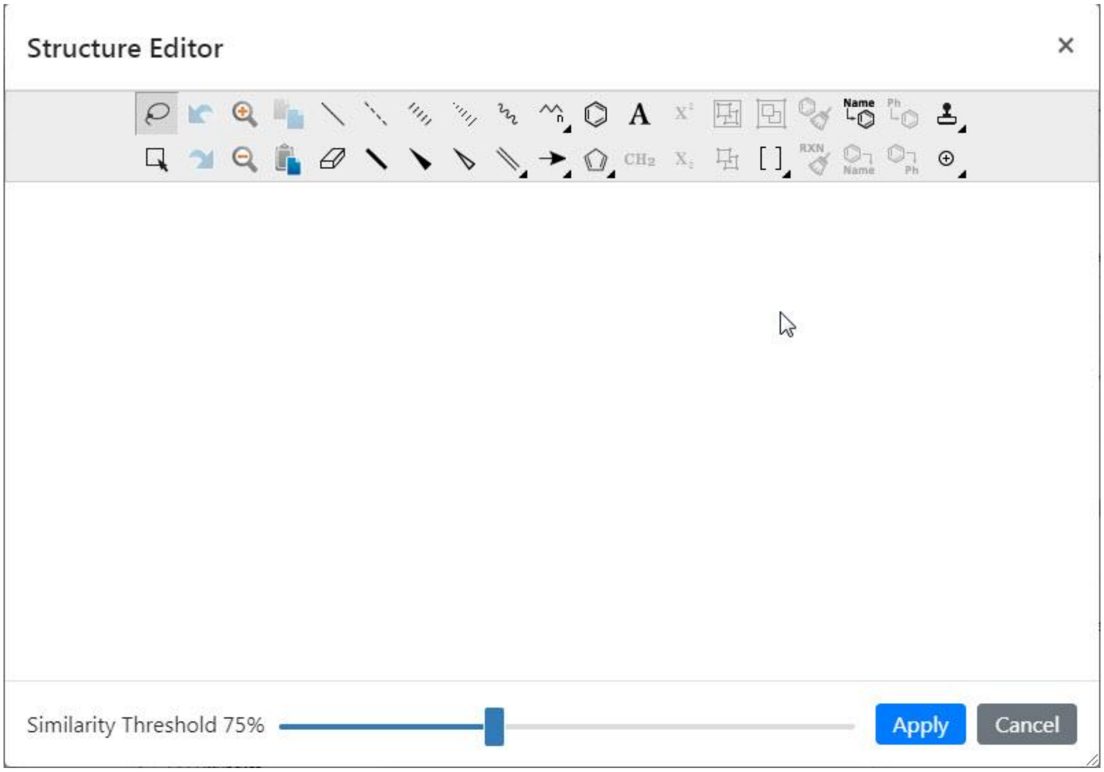
To perform a Similar Structure Search:

Similarity searches find structures having features similar to the query structure.

1. Select the operation ‘Similar To’.



2. Click on the <enter a value> parameter. The ChemDraw JS Structure Editor opens.



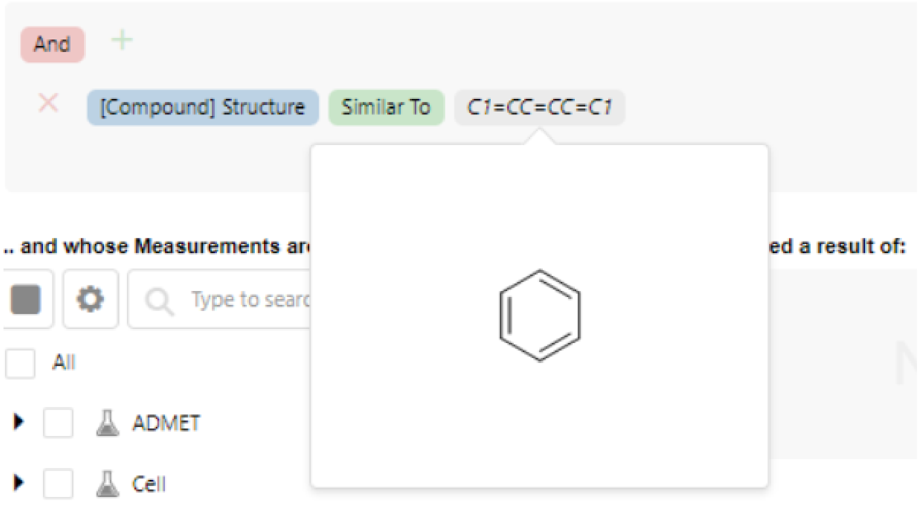
Note: The Structure condition supports the ChemDraw JS Editor. Signals Inventa will locate this application via a URL which is defined as a preference in Spotfire. Please refer to the 'Setting the ChemDraw JS URL Preference' section of Lead Discovery User Guide for more details.

3. Draw the query structure in the Structure Editor window using appropriate tools.

By default, a similarity search is performed based on a 75% - 100% range of similarity. You can adjust the range of similarity (from 60 to 100%) using the slider.

4. Click **Apply**.

The SMILES representation of the structure is displayed in the Condition value. If you hover over the condition value, a thumbnail of the structure is displayed, similar to the example shown below.



Clicking Apply initiates the search against Signals Data Factory.

To edit a structure:

1. Click on the SMILES representation of the structure to open the Structure Editor.
2. Make the necessary modifications to the structure
3. Click on the **Apply** button. A new search is initiated.

6.4.2 Search by Related Entity

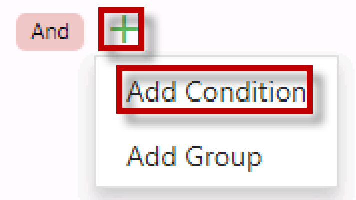
Signals Data Factory supports the addition of custom entities (or related entities). They allow you to associate entity tables to your core entity (e.g. Compound, Batch) tables and then leverage those relationships while querying data. For example, a compound entity could have a related entity associated with it which describes more details about the compounds. You can specify a search condition based on the associated entities.

Note: Refer to the Entities and Attributes section in **Appendix B: Signals Data Factory** for information on defining custom entities and relationships.

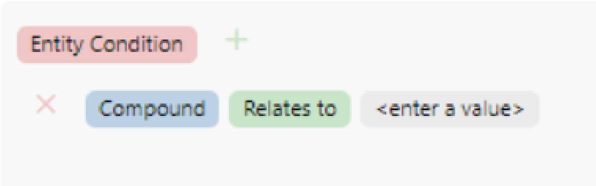
Using an Entity Condition, you can include related entity tables in your search.

To add an entity condition:

1. Select **Entity Condition** from the logical operator drop down list.
2. Click on the + icon and select **Add Condition**.



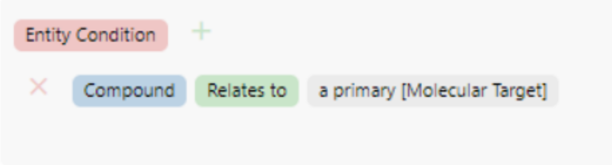
A condition is added to the filter builder. In the case of an Entry Condition, the operator ‘Relates to’ is static.



Compound Relates to <enter a value>

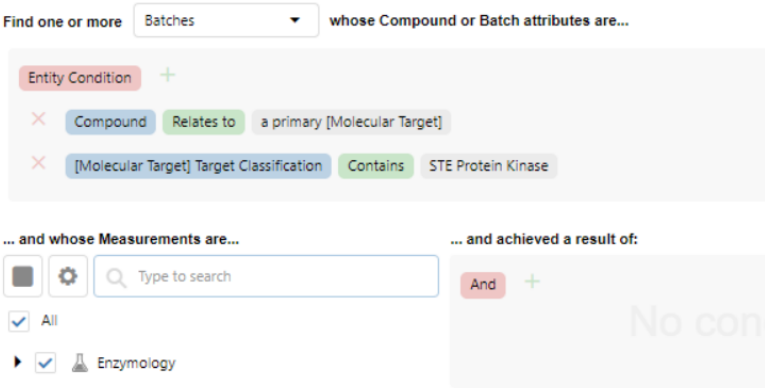
A Search field allows you to type ahead to search for the relationship. A value can be entered in the Value field or you can use the type ahead to search for the relationship.

3. Select the relationship.



Compound Relates to a primary [Molecular Target]

Using the filter builder widget, you can stack other And/Or conditions similar to the example shown below.



Find one or more Batches whose Compound or Batch attributes are...

Compound Relates to a primary [Molecular Target]

[Molecular Target] Target Classification Contains STE Protein Kinase

☑ All

☑ Enzymology

In the ‘And’ condition shown above, all columns from the related entity table (e.g. Molecular Target) are available for selection. Here, Target Classification is a column in the Molecular Target related entity table. The related entity name (e.g. Molecular Target) to which the attribute is associated, is displayed in brackets as a prefix to the attribute name (e.g. Target Classification). This allows for you to easily identify which entity an attribute describes.

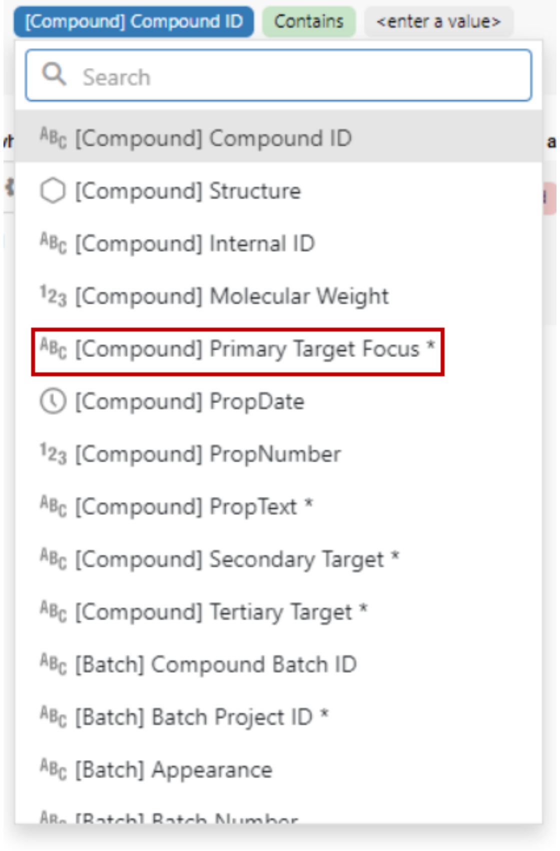
In the example shown above, the search will query for batches that were tested in Enzymology assays where their target is an STE protein kinase.

Global search queries can also contain multiple conditions across multiple related entities similar to the example shown below.

And
Entity Condition
Batch Relates to a [Discovery Project]
[Discovery Project] Disease Relevance Is any of Osteosarcoma Schizophrenia
Entity Condition
Compound Relates to a primary [Molecular Target]
[Molecular Target] Sequence Contains IS*P
[Compound] Molecular Weight Is less than or equal to 400

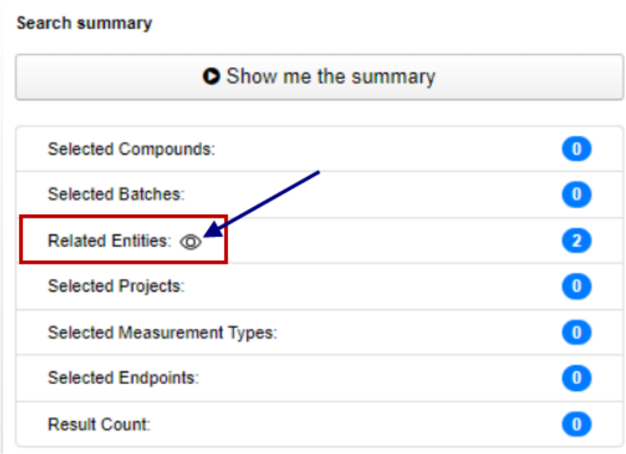
6.4.3 Viewing Entity Relationships

When adding conditions, using the filter builder widget, you will note that some attribute names may be followed by an asterisk (*). This indicates that a related entity table is linked to this field and additional information related to the attribute is available.



[Compound] Compound ID Contains <enter a value>

For example, a relationship exists where [Compound] Primary Target Focus is mapped to a related entity table. To gain insight into this relationship and see which table it is linked to, you can click on the 👁 icon next to the Related Entities in the Search Summary gird.



Search summary

Selected Compounds: 0

Selected Batches: 0

Related Entities: 👁 2

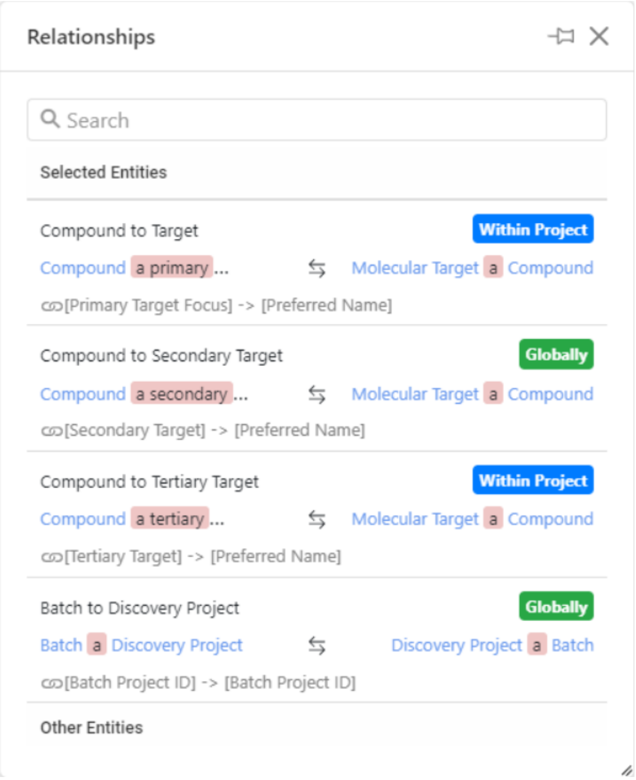
Selected Projects: 0

Selected Measurement Types: 0

Selected Endpoints: 0

Result Count: 0

This will open the Relationships window.



Relationships

Selected Entities

Compound to Target — Within Project

Compound a primary ... ⇆ Molecular Target a Compound

[Primary Target Focus] -> [Preferred Name]

Compound to Secondary Target — Globally

Compound a secondary ... ⇆ Molecular Target a Compound

[Secondary Target] -> [Preferred Name]

Compound to Tertiary Target — Within Project

Compound a tertiary ... ⇆ Molecular Target a Compound

[Tertiary Target] -> [Preferred Name]

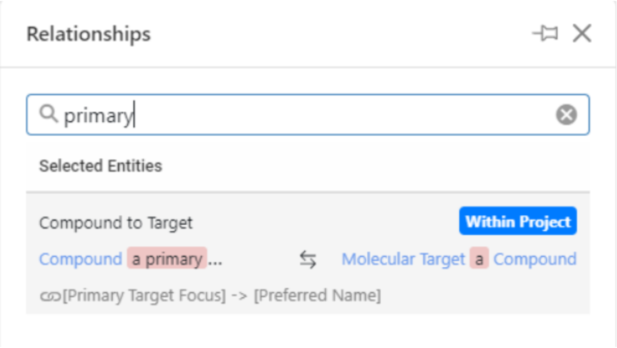
Batch to Discovery Project — Globally

Batch a Discovery Project ⇆ Discovery Project a Batch

[Batch Project ID] -> [Batch Project ID]

Other Entities

From here, you can search for the relationship and discover that in this example, Compound is linked to the Primary Target table. The Relationships window is a means for you to find out more information about the data field in question. This window can be pinned for your reference.



Relationships

primary

Selected Entities

Compound to Target

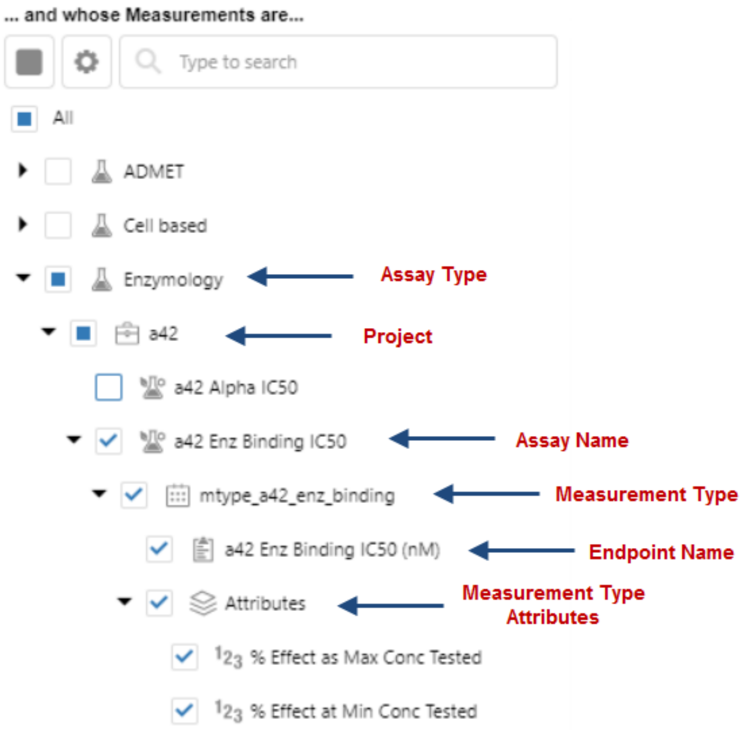
Within Project

Compound a primary ... ⇆ Molecular Target a Compound

[Primary Target Focus] -> [Preferred Name]

6.5 Search for Assays and Annotations of Interest

In this section (…and whose Measurements are…), you can search for assays, annotations, and result types of interest. These are organized into a hierarchy defined by the metadata of the underlying Signals Data Factory that stores these results and is managed by your data administrator.



The levels of the hierarchy are:

- **Assay General Type** - this is a general organization column, but most commonly is used to organize the assays into general classes to make them easier to find.
- **Biology Project** - this is a general organization column, but most commonly is used to group assays into the project that they primarily support.
- **Assay** – this is the name under which the assay results were published.

- **Measurement Type** – this is a category of measurements that are similar.
- **Result Name** – this is the name of assay result (e.g. Assay 1 IC50 (nM)) belonging to the measurement type
- **Measurement Type Attribute –** this is the name of the attribute belonging to the measurement type

Note: The hierarchal tree displays measurement types that are linked to both Compounds and Batches.

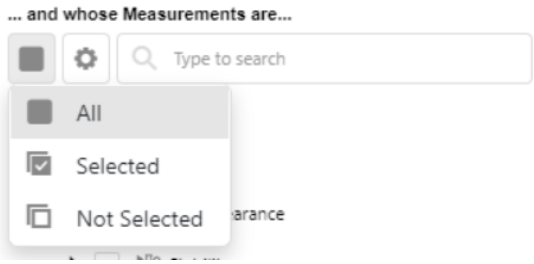
Note: In the case where data is loaded directly into the Assay Endpoints Results table and measurement types are not defined, the resulting node in the assay hierachal tree is labelled 'Endpoints' by default. The **Undefined Measurement Type Display Name** Spotfire preference allows you to specify a display name if you choose not to use the default name.

In the case, where there is a mix of some and no measurement types, the resulting node in the assay hierarchal tree is labelled 'Other Endpoints' by default. The **Undefined Measurement Type Display Name** preference allows you to specify a display name if you choose not to use the default name. For example, the node will be labelled "Other {preference value}".

Refer to the section Setting the Undefined Measurement Type Display Name for more information.

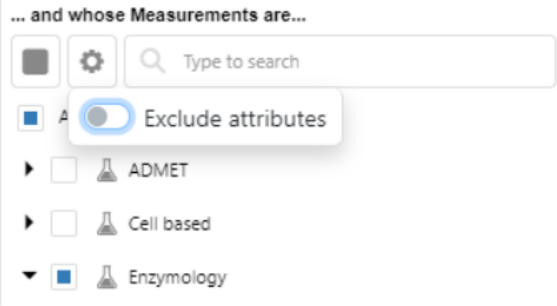
Displaying Hierarchies

To aid in the selection of assays, you can choose to display 'All' hierarchies, only those hierarchies that have been 'Selected', or those that have are currently 'Not Selected'.



Exclude Attributes

An Exclude attributes toggle is available for you to exclude measurement attributes from being downloaded when the global search results are downloaded into Spotfire.

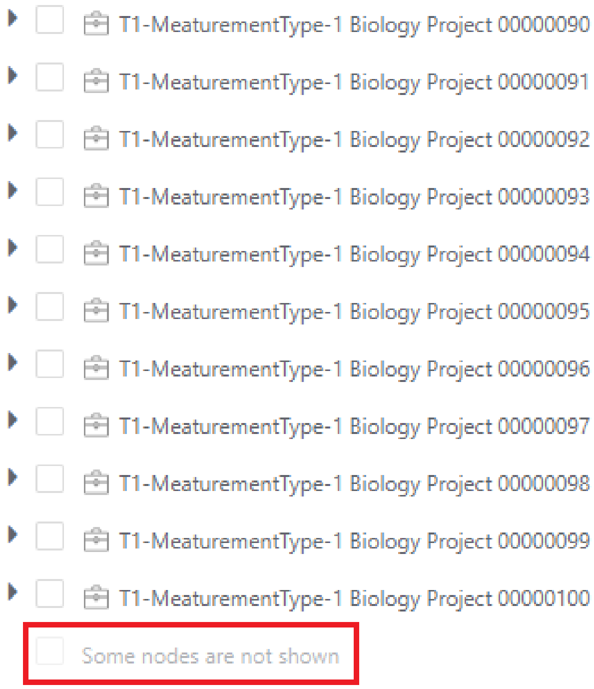


Depending on how the Spotfire preference is set, the attributes may be included in the download by default. Using this toggle, you can override this preference. Refer to the section Setting the Include Attributes by Default in Global Search for further information.

Search

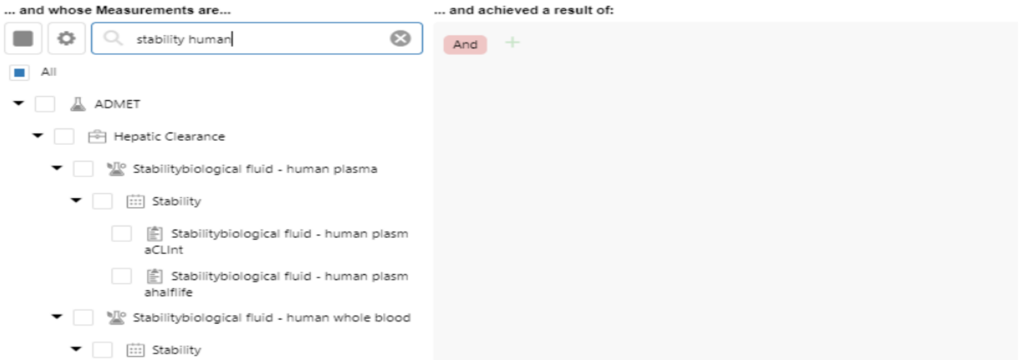
Here, you can perform a type-ahead search to look for results of interest. As you type, the hierarchy will be dynamically filtered, and the hierarchy sections opened to display results that match the input text.

Note: When expanding a parent node, a maximum of 100 child nodes will be shown with accompanying text to indicate 'Some nodes are not shown', similar to the example shown below. It is recommended that you enter a query string for searching to help you find the precise target nodes for selection.



▸ ☐ T1-MeaturementType-1 Biology Project 00000090
▸ ☐ T1-MeaturementType-1 Biology Project 00000091
▸ ☐ T1-MeaturementType-1 Biology Project 00000092
▸ ☐ T1-MeaturementType-1 Biology Project 00000093
▸ ☐ T1-MeaturementType-1 Biology Project 00000094
▸ ☐ T1-MeaturementType-1 Biology Project 00000095
▸ ☐ T1-MeaturementType-1 Biology Project 00000096
▸ ☐ T1-MeaturementType-1 Biology Project 00000097
▸ ☐ T1-MeaturementType-1 Biology Project 00000098
▸ ☐ T1-MeaturementType-1 Biology Project 00000099
▸ ☐ T1-MeaturementType-1 Biology Project 00000100
☐ Some nodes are not shown

Split query strings separated by whitespaces can also be used to search for results as illustrated in the example below.



stability human

■ All
▾ ☐ ADMET
  ▾ ☐ Hepatic Clearance
    ▾ ☐ Stabilitybiological fluid - human plasma
      ▾ ☐ Stability
        ☐ Stabilitybiological fluid - human plasmaCLInt
        ☐ Stabilitybiological fluid - human plasmahalflife
    ▾ ☐ Stabilitybiological fluid - human whole blood
      ▾ ☐ Stability

From the hierarchy tree, you can check the checkbox next to any item of interest. Checking the box next to an item automatically selects the boxes for all subordinate items.

Any leaf node that is checked in the hierarchy tree automatically becomes available to be set as an assay/measurement criterion in the Conditions panel (…and achieved a result of:)

Note: Checking the ‘All’ checkbox will select all nodes in the assay hierarchy.

6.6 Adding Conditions to an Assay or Measurement Query

Here you can limit the returned compounds/batches/measurements with their assay results by assay and assay result conditions and/or measurement type results by assay and attribute conditions.

Similar to the Compound Search, described previously, using a filter builder, conditions can be added to the assay and/or measurement query for further definition. Refer to Search for Compounds/Batches/Measurements of Interest for details on using the filter builder.

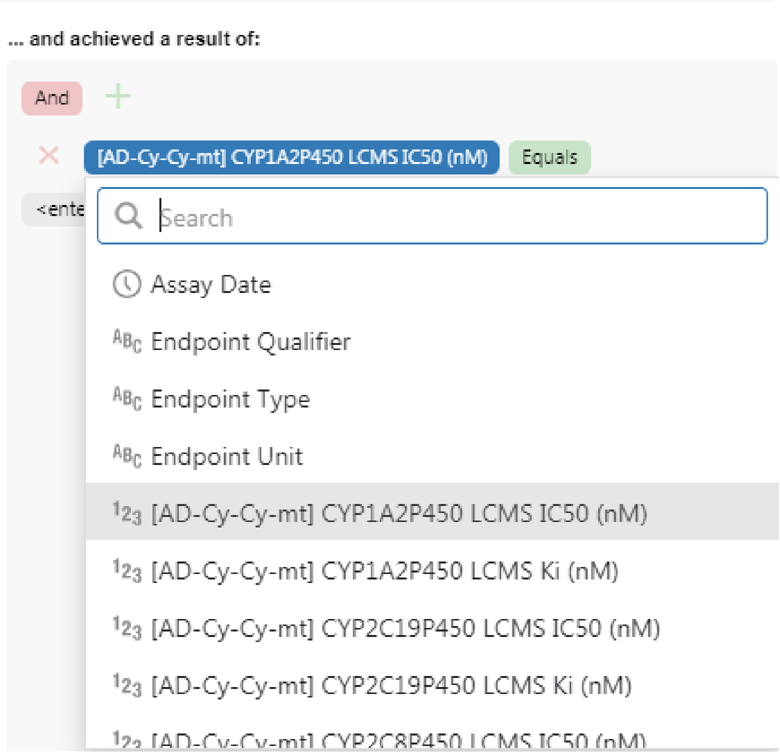
Clicking on the Data Field and Operation allows you to select the data field name and comparison operation from a list.

The “Is any of” and “Is all of” conditions are useful for the following cases:

For example, when a user specifies "IS ANY OF" -> "Batch Project 1, Batch Project 2", this means that the compounds that are in Batch Project 1 OR Batch Project 2 will be returned.

In the case where some compounds belong to multiple batch projects, the “Is all of” operator returns the compounds that belong to both Batch Project 1 AND Batch Project 2.

A Search field allows you to type ahead to search for the data field name. A value can be entered in the Value field, you can also use the type ahead to search for the value.



In addition to the logical operators in the filter builder, there are two additional group operators available for the assay query called the “Assay Condition” group operator and the “Measurement Condition” group operator.

Assay Condition

An “Assay Condition” group operator can contain multiple annotative attribute criterias but only one result criteria. All of the conditions specified under the “Assay Condition” group are concatenated by AND operator logically.

For the And, Or, Not And and Not Or operators, they can only hold one type of criteria, either annotative attribute criteria or result criteria. This means that if you choose an annotative attribute for the first criteria, you will not be able to choose a result criteria for the other operators.

Once the logical/group operator has been determined, you can create the criteria starting from the data field. The data field is a list of annotative attributes from the measurement types or results that are currently selected in the hierachy tree. Any deselection of the annotative attribute or the result will trigger removal from the data field list.

Note: The prefix for each field name is the first two letters of the parents for the result name (i.e. the path)

Note: Annotative attributes in the data field list won’t have a prefix on their names

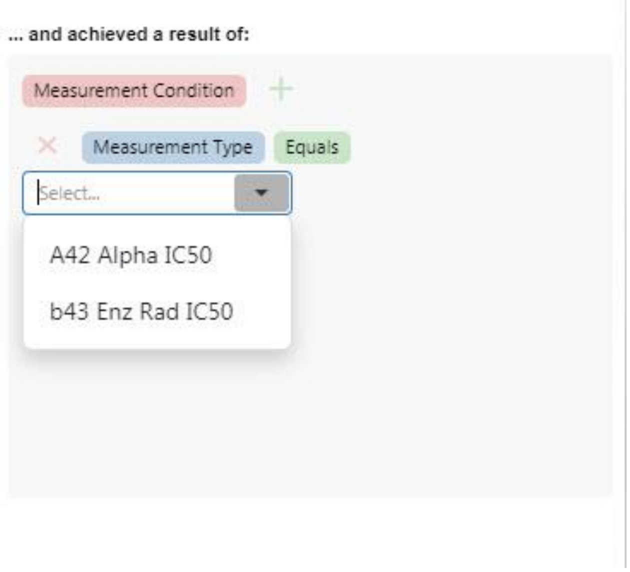
Note: When expanding the drop-down, a maximum of 100 child nodes will be shown. It is recommended that you enter a query string for searching to help you find the precise target result names.

Result conditions will be dynamically updated according to the hierarchy. For example, any condition with a field selected in the hierarchy tree will be removed once the associated result name is deselected in the tree.

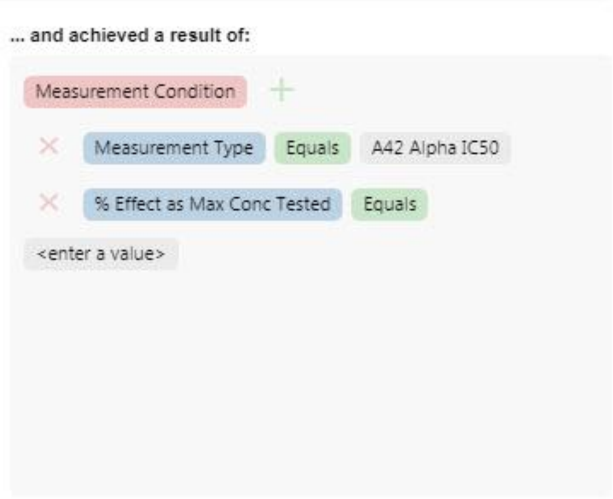
Measurement Condition

A “Measurement Condition” group operator can contain multiple measurement attribute criterias All of the conditions specified under the “Measurement Condition” group are concatenated by AND operator logically.

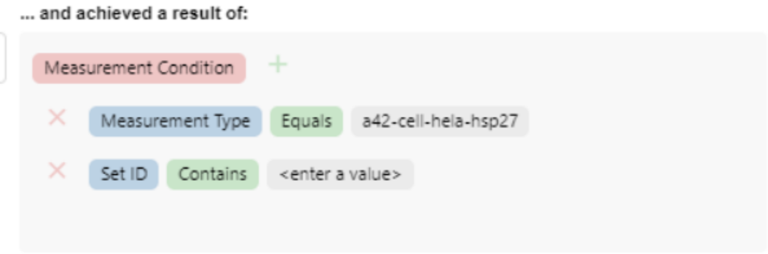
Once the logical/group operator has been determined, you can create the criteria starting from the data field. The first data field in the condition is always Measurement Type. The value field will list the available measurement types that are selected in the assay tree. If no Measurement Type is selected, the “Measurement Type” operator will be disabled.



Once the measurement type has been defined in the first condition, additional conditions can be added. The data field is a list of measurement type attributes that are currently selected in the hierachy tree for the measurement type specified in the first condition. Any deselection of the measurment attribute will trigger removal from the data field list.



Note: You can search for the dataset that you used for publishing the measurement data in the measurement condition by specifying the Set ID (dataset ID) as a condition in the Measurement Condition filter.


... and achieved a result of:

Measurement Condition +

× Measurement Type Equals a42-cell-hela-hsp27

× Set ID Contains <enter a value>

If you select a second measurement type from the value drop down list, the current conditions will be cleared, and the data field will now contain the measurement type attributes for the newly selected measurement types.

Note: When expanding the drop-down, a maximum of 2,000 child nodes will be shown. It is recommended that you enter a query string for searching to help you find the precise target measurement attribute.

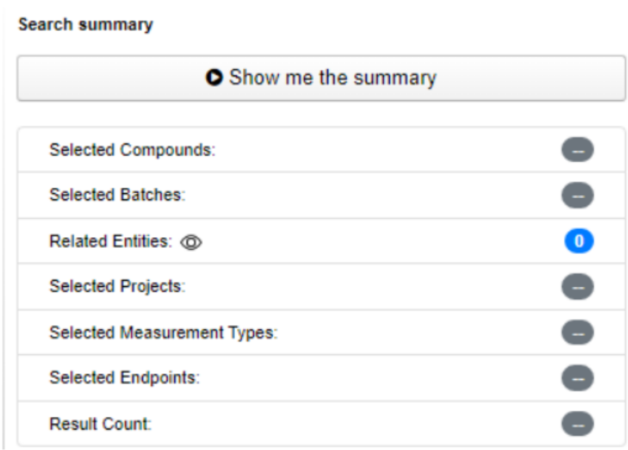
Result conditions will be dynamically updated according to the hierarchy. For example, any condition with a field selected in the hierarchy tree will be removed once the associated measurement attribute is deselected in the tree.

Technical Note: It is possible build advanced queries that define criteria for both the Assay Endpoint Results (AER) table and individual Measurement Tables. Criteria is applied to the AER table when an Endpoint is selected from the Global Search tree, when a results criteria for an Endpoint is specified, or when an “Assay Condition” is defined. Criteria is applied to individual Measurement Tables when an Attribute is selected from the Global Search tree or when a results criteria for a “Measurement Condition” is set. Global Search will always attempt to perform a join query, whereby Measurement Table results will be filtered based on corresponding records in the AER table. In this scenario, every row in a Measurement Table will have a corresponding record in the AER table. When queries are sufficiently broad with large numbers of Measurement Results, they join limit may be exceeded. Global Search will perform a non-join query instead and notify the user. In this case, it is possible to return Measurement Table rows that do not have a corresponding record in the AER table. The specified AER criteria is still applied to the AER table, and the specified measurement criteria is applied to the appropriate Measurement Tables, but the Measurement rows are not then filtered by corresponding AER rows. If this occurs, users will receive a notification upon data download.

6.7 Get the Summaries of the Query to be performed

In the sections on the right-side of the page, you can access feedback about the search criteria and the set of compounds/batches/measurements and results that will be returned by the search. This panel is resizable.

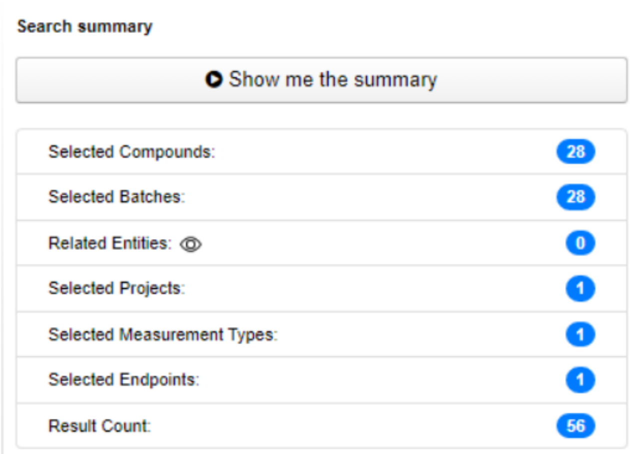
Search Summary


Search summary

Selected Compounds: –
Selected Batches: –
Related Entities: 0
Selected Projects: –
Selected Measurement Types: –
Selected Endpoints: –
Result Count: –

Click on the **Show me the summary** button to see the data. You have the option hide the **Show me the summary** button and automatically load the Search summary results right after you have modified the compound or assay criterias. Refer to the section **Setting the Turn Off Summary Button in Global Search.**

This section provides a succinct summation of the search criteria outlining the numbers of selected compounds batches, projects, measurement types, endpoints as well as result counts returned by the search.

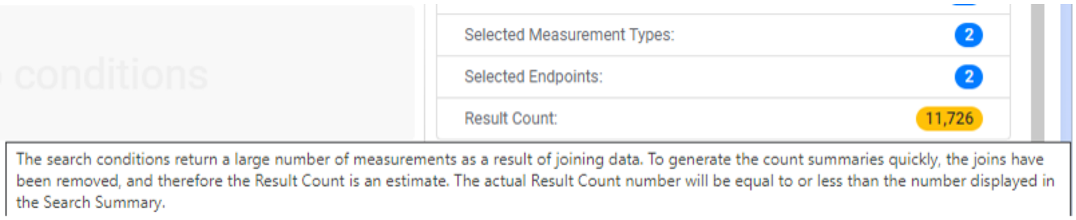

Search summary

Selected Compounds: 28
Selected Batches: 28
Related Entities: 0
Selected Projects: 1
Selected Measurement Types: 1
Selected Endpoints: 1
Result Count: 56

Note: The Select Measurement Types, Selected Endpoints and Result count values are the sum of the respective Batch and Compound values.

Note: The Summary does not include the Result Counts for Details Measurement Types.

There may be instances where the Result Count value is highlighted in a yellow badge. In this case, the search conditions return a large number of measurements as a result of joining data. To generate the count summaries quickly, the joins have been removed, and therefore the Result Count is an estimate. The actual Result Count number will be equal or less than the number displayed in the Search Summary. You can hover the mouse over the yellow badge to display an information message with more detail about the Result Count. There is a 'Search Maximum Join' adminstrative system configuration setting in Signals Data Factory.



conditions

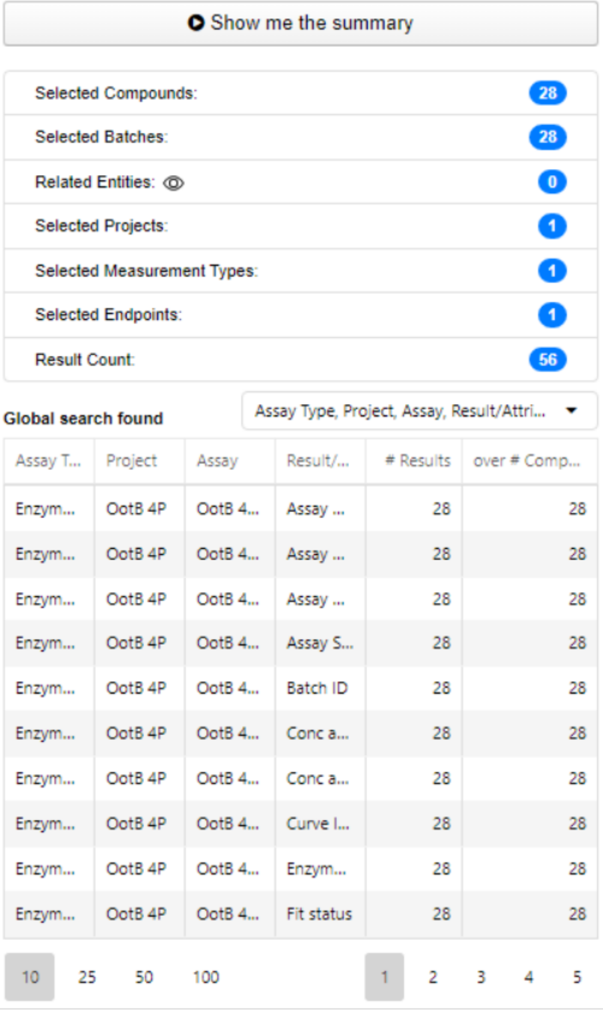
Selected Measurement Types:	2
Selected Endpoints:	2
Result Count:	11,726

The search conditions return a large number of measurements as a result of joining data. To generate the count summaries quickly, the joins have been removed, and therefore the Result Count is an estimate. The actual Result Count number will be equal to or less than the number displayed in the Search Summary.

Global Search Found

The Global Search grid displays all result names meeting the search criteria including the # Results and over # Compounds/Batches/Measurements for each.

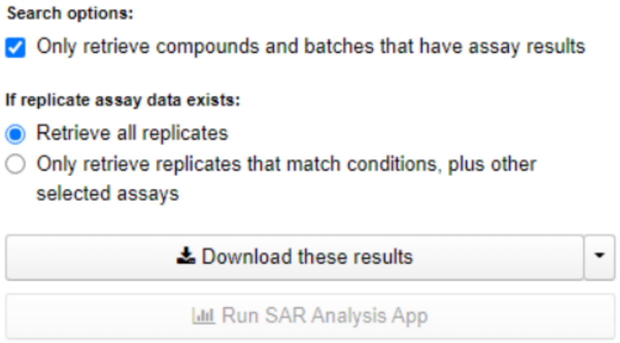
From the Global search found drop down list, you can select the hierarchy level (Assay Type, Project, Assay, Measurement Type, Result/Attribute name) to group the values displayed in the grid. At least one hierarchy level should be selected in this drop down, such that the **Global search found** table could display the aggregated numbers under that selected level. You can also choose multiple hierarchy levels by clicking on the check boxes for each item in this drop down.



Selected Compounds:	28
Selected Batches:	28
Related Entities:	0
Selected Projects:	1
Selected Measurement Types:	1
Selected Endpoints:	1
Result Count:	56

Global search found Assay Type, Project, Assay, Result/Attri...

Assay T...	Project	Assay	Result/...	# Results	over # Comp...
Enzym...	OotB 4P	OotB 4...	Assay ...	28	28
Enzym...	OotB 4P	OotB 4...	Assay ...	28	28
Enzym...	OotB 4P	OotB 4...	Assay ...	28	28
Enzym...	OotB 4P	OotB 4...	Assay S...	28	28
Enzym...	OotB 4P	OotB 4...	Batch ID	28	28
Enzym...	OotB 4P	OotB 4...	Conc a...	28	28
Enzym...	OotB 4P	OotB 4...	Conc a...	28	28
Enzym...	OotB 4P	OotB 4...	Curve I...	28	28
Enzym...	OotB 4P	OotB 4...	Enzym...	28	28
Enzym...	OotB 4P	OotB 4...	Fit status	28	28



Search options:

☑ Only retrieve compounds and batches that have assay results

If replicate assay data exists:

● Retrieve all replicates

○ Only retrieve replicates that match conditions, plus other selected assays

When applicable, you can specify the maximum number of rows (e.g. 10, 25, 50, 100) to be displayed on one page in the grid, as well as page through the grid to see results.

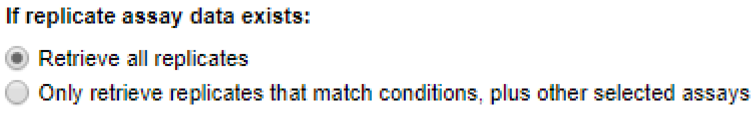
Search

You have the option to only retrieve compounds and batches that have assay results.

In the case where the ‘Only retrieve compounds and batches that have assay results’ checkbox is not enabled, the number of Compounds and Batches with no results is displayed directly below the grid.

If replicate assay data exists

You have the option to retrieve all replicates or only retrieve replicates that match conditions, plus other selected assays.



If replicate assay data exists:

● Retrieve all replicates

○ Only retrieve replicates that match conditions, plus other selected assays

For example, an assay condition has been defined as ‘[A-S-S] Solubility at pH 1.2 Solubility (um/ml) > 5’.

If ‘**Retrieve all replicates**’ is selected, all compounds which have the assay results ‘[A-S-S] Solubility at pH 1.2 Solubility (um/ml) > 5’ will be selected, and all assay result for these compounds will be returned, however, all compounds which contain the assay results ‘[A-S-S] Solubility at pH 1.2 Solubility (um/ml) <= 5 will also be returned.

If “**Only retrieve replicates that match conditions, plus other selected assays**’ is selected, only the assay results ‘[A-S-S] Solubility at pH 1.2 Solubility (um/ml) > 5’ will be returned.

6.8 Saving a Global Search

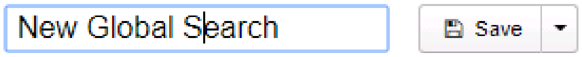
Global Searches can be saved as private or public and shared with specified groups.

Administrative users can save a search as public and can also limit who can see the search by sharing the search only with specific groups. A user will only see that search if he/she is a member of that group.

Non-administrative users cannot save a search as public. They can only save as a private search or share with a group that he/she is a member of.

To save a new global search:

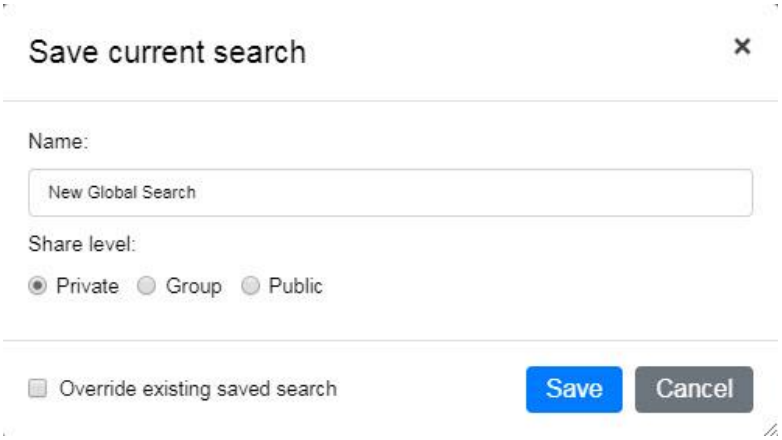
1. Single click on the name field to place the field in edit mode. Alternatively, you can click on the **Save** button to open the Save Current Search dialog.


New Global Search

2. Enter a unique name for the search.

You will be notified if the name already exists.

3. Click **Save**. The **'Save current search'** dialog opens.


Save current search

Name: New Global Search

Share level: ● Private ○ Group ○ Public

☐ Override existing saved search

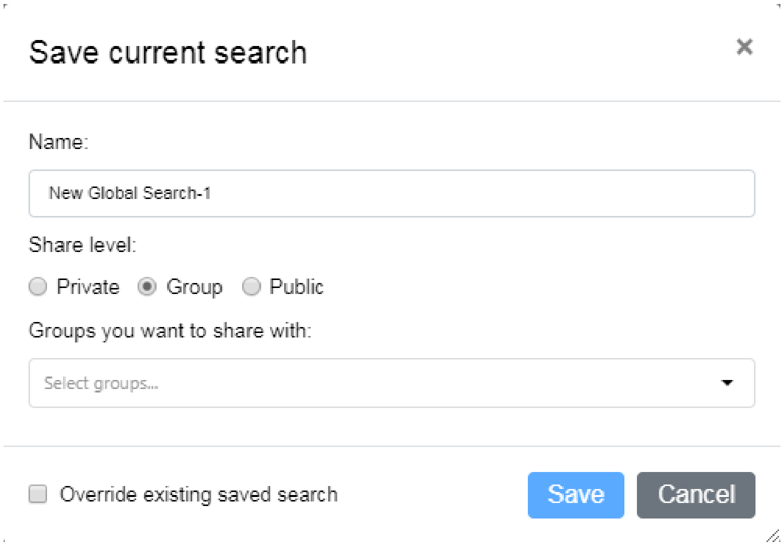
4. If not already done so, enter a unique name for the current search.

5. Specify the Share level for the search.

You can choose to make the search private, public or define which groups can see the saved search. A non-administrative user cannot save a search as public and this option will not be available.

Private – the saved search will only be visible to the current logged in user.

Group – the saved search will only be visible to users who belong to the selected group(s). Only groups that you are a member of will be available for selection.



Save current search

Name:

New Global Search-1

Share level:

○ Private ● Group ○ Public

Groups you want to share with:

Select groups...

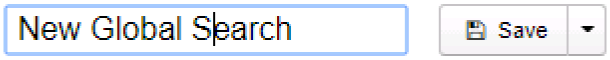
☐ Override existing saved search

Public – This option is only available for administrative users. The shared search will be visible to all users/groups.

6. Click on the **Save** button.

To re-name and save a global search:

1. Single click on the name field to place the field in edit mode.

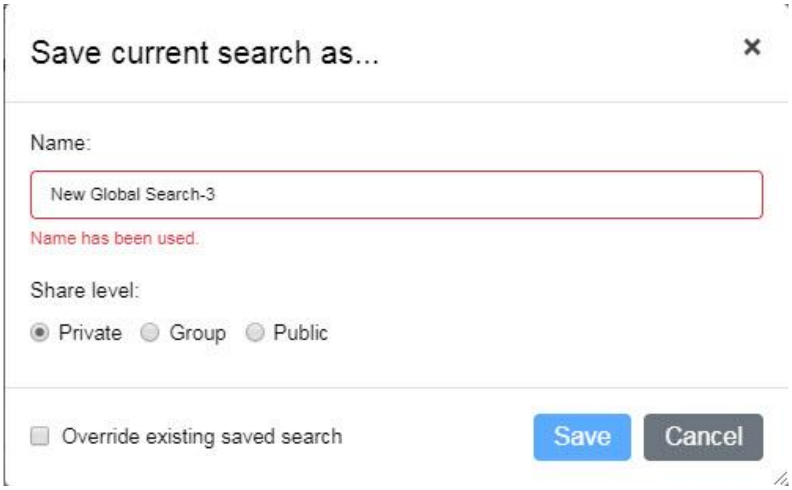


New Global Search

2. Enter a unique name for the search.
3. You will be notified if the name already exists.
4. Click **Save**..

OR

1. From the Save drop-down list, click **Save As**. The Save current search as dialog opens.



Name: New Global Search-3

Name has been used.

Share level: ● Private ○ Group ○ Public

☐ Override existing saved search

2. You will be notified that the name has been used. Enter a new unique name for the global search.
3. Specify the Share level for the search.

You can choose to make the search private, public or define which groups can see the saved search. A non-administrative user cannot save a search as public and this option will not be available.

4. Click on the **Save** button.

Editing a Saved Query

Public queries are read-only and can only be edited by the administrative user who saved the search.

A read-only search is identified by hovering the cursor over the Saved Search name. The locked 🔒 indicator identifies the public search as read-only.

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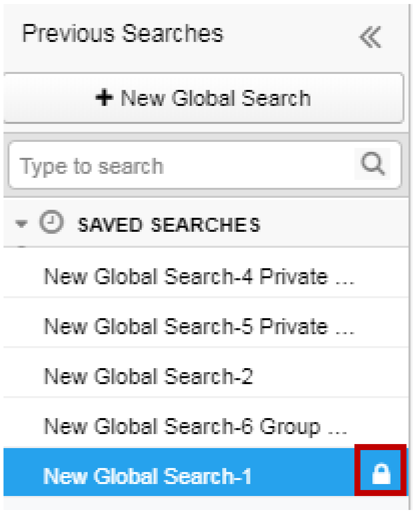


New Global Search-4 Private ...

New Global Search-5 Private ...

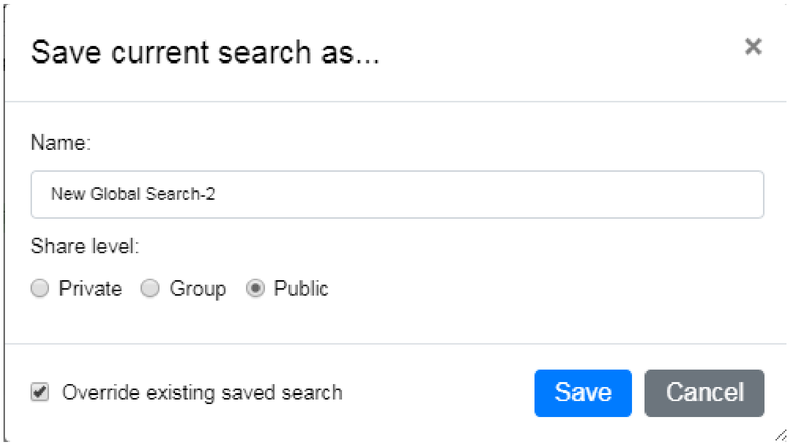
New Global Search-2

New Global Search-6 Group ...

New Global Search-1 🔒

To edit a saved query:

1. Make the updates to the saved search.
2. From the Save drop-down list, click **Save As**. The Save current search as dialog opens.



Save current search as...

Name: New Global Search-2

Share level: ○ Private ○ Group ● Public

☑ Override existing saved search

3. If applicable, make modications to the Share level.
4. Enable the **Override existing saved search** checkbox.
5. Click on the **Save** button.

Note: If modifications are made to a locked search, the search will be saved as a new search and the previous search will not be overwritten.

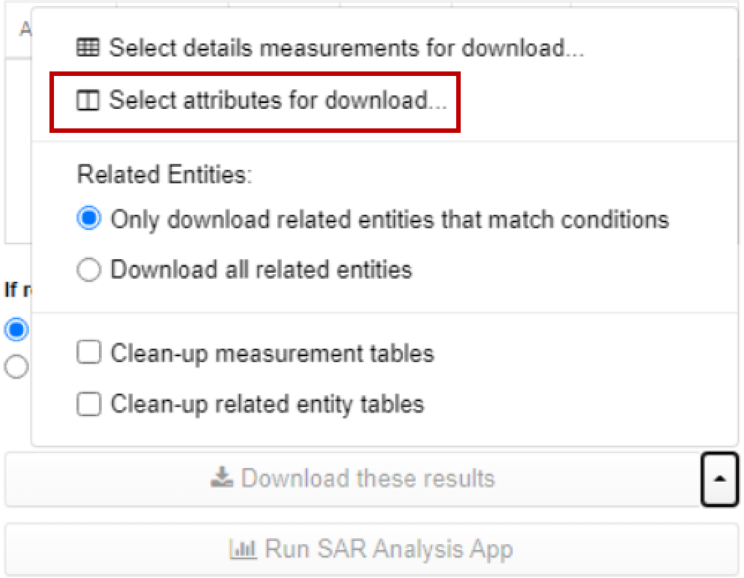
6.9 Downloading Assay Results into Spotfire

Once the Search criteria has been defined, the assay results can be downloaded into Spotfire. Clicking the **Download these results** button will download the data from Signals Data Factory and generate three Spotfire data tables; a ‘Compounds’ table if you have any compounds data, ‘Batch’ table if you have any batch data, a ‘Compound Assay Endpoint Results’ table that contains assay data for compounds and a ‘Batch Assay Endpoint Results’ table that contains assay data for batches. If applicable, related entity table(s) are also downloaded. In addition, one data table per measurement type (if at least one attribute is selected in the hierarchy tree) is also generated. Only the selected measurement type attributes are downloaded.

Selecting entity attributes for download

By default, all projects share a single attribute list and all entity attributes are retrieved for all queries. You can specify the entity attributes for retrieval.

From the **Download these results** drop-down button, selecting ‘Select attributes for download’ will open a ‘Select attributes for download’ window.



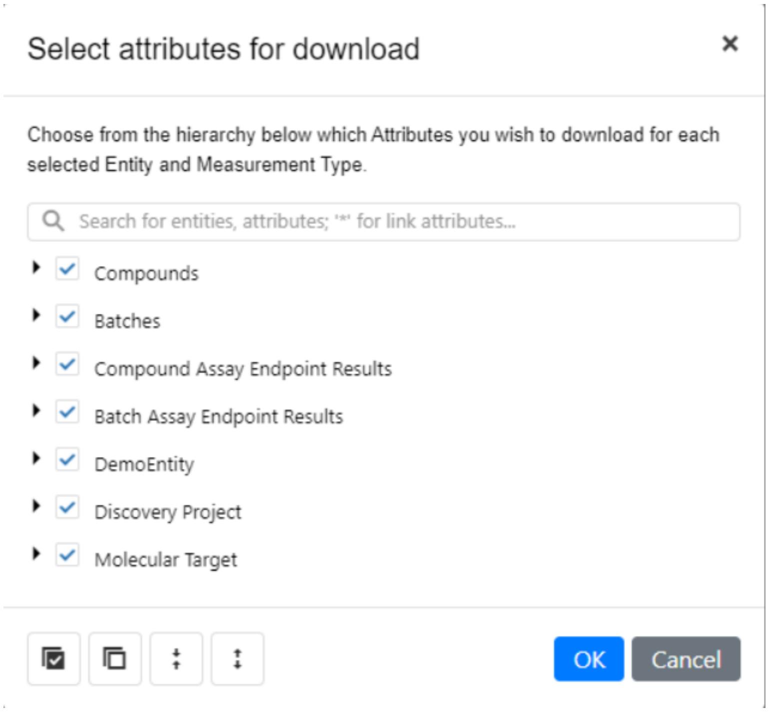
Related Entities:

● Only download related entities that match conditions

○ Download all related entities

☐ Clean-up measurement tables

☐ Clean-up related entity tables



Select attributes for download

Choose from the hierarchy below which Attributes you wish to download for each selected Entity and Measurement Type.

Search for entities, attributes; '*' for link attributes...

- ☑ Compounds
- ☑ Batches
- ☑ Compound Assay Endpoint Results
- ☑ Batch Assay Endpoint Results
- ☑ DemoEntity
- ☑ Discovery Project
- ☑ Molecular Target

Choose from the hierarchy which attributes you wish to download for each selected Entity and Measurement Type.

You can choose the Compound/Batch/Compound Assay Endpoint Results/Batch Assay Endpoint Results to download.

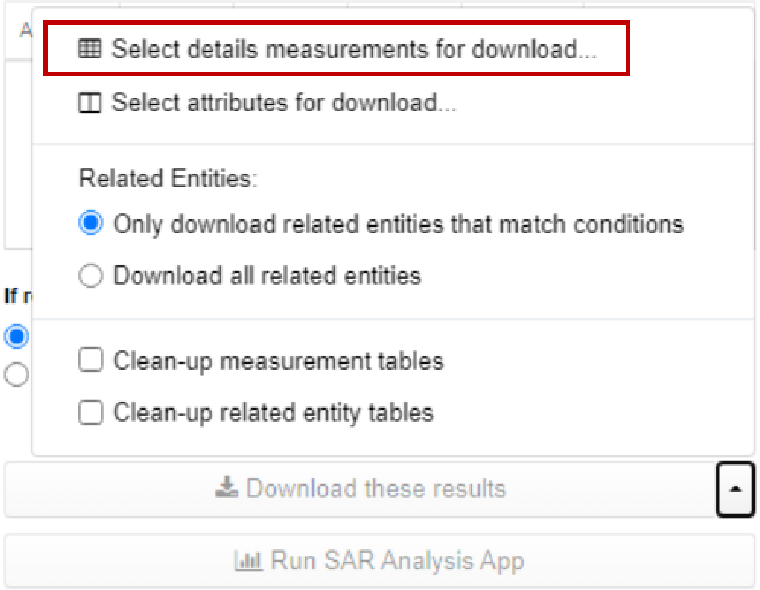
Related entities are also available for selection. Note that is you choose to 'Download all related entities' (see below) only the entities specified here will be downloaded into Spotfire.

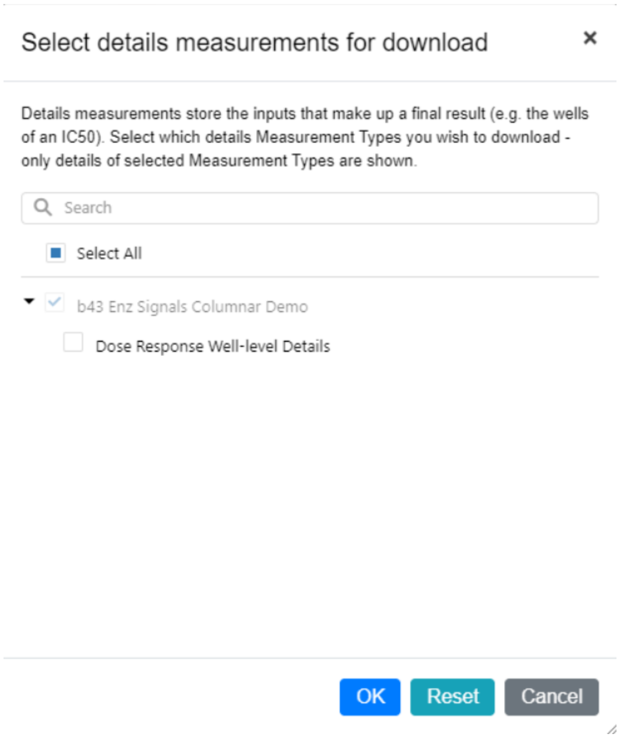
The selected entities will be saved as part of the Saved Search when the current search is saved.

Selecting detail measurements for download

If applicable, you can download detail measurement types for the measurement types selected in the hierarchy tree. Details measurements store the inputs that make up a final result (e.g. the wells of an IC50).

From the **Download these results** drop-down button, selecting 'Select details measurements for download' will open a 'Select details measurements for download' window.




Select details measurements for download

Details measurements store the inputs that make up a final result (e.g. the wells of an IC50). Select which details Measurement Types you wish to download - only details of selected Measurement Types are shown.

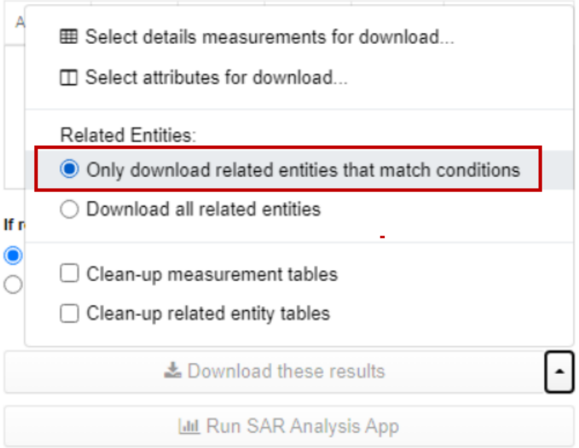
Select which details Measurement types you wish to download - only details of selected Measurement Types are shown.

Note: If you have selected a measurement type on the hierarchy tree which is associated with “details” measurements, and you want a Spotfire table relation to be established between the two measurement types, make sure the “details” measurement type is not selected in the hierarchy tree. If you select both parent and details measurements on the hierarchy tree, then you cannot change selections in the **Select details measurements for download** dialog, and there will be no table relationship established between the two downloaded tables.

Related Entities:

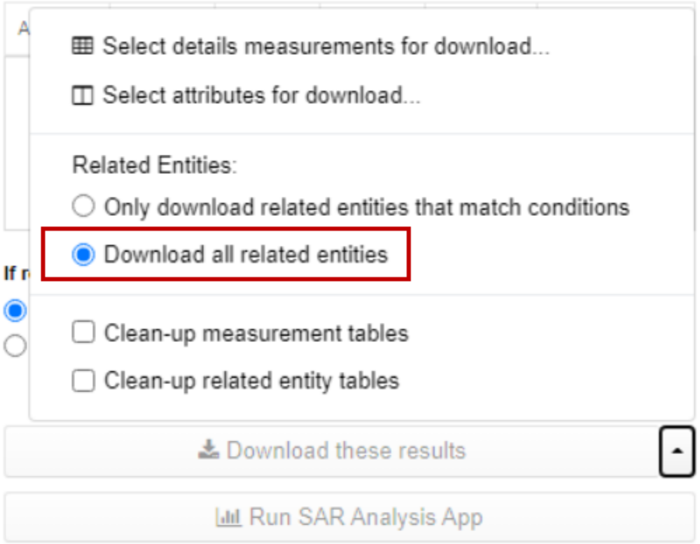
Only Download Related Entities that match conditions

If the ‘Only download related entities that match conditions’ option is selected then only those rows from the related entities table that meet the attribute conditions defined in the search criteria are downloaded. This means that all related entities that are either called by the Entity Condition statement or those that are implied using a hierarchal entity attribute are returned AND their rows are filtered based on conditions specified in the Global Search.



Download all related entities

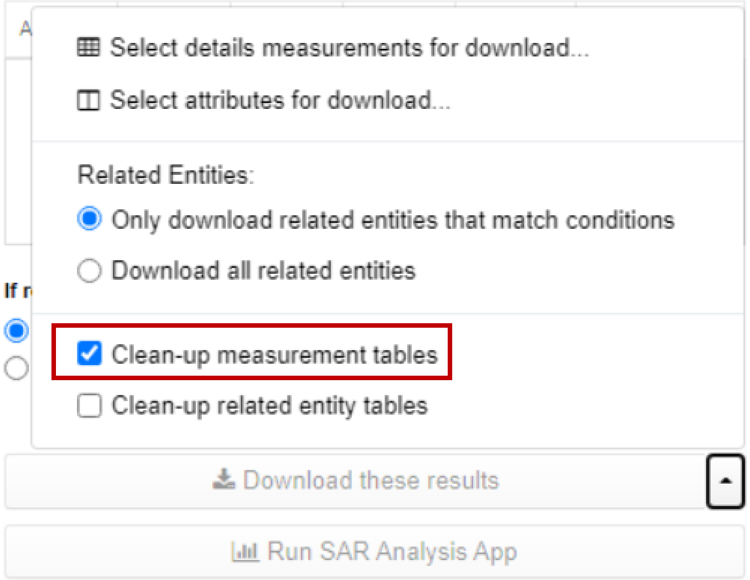
If the "Retrieve all related entities " option is selected, then all rows for all related entity tables are downloaded into Spotfire This allows you to do your own Spotfire joins and linkages (transformations).



Clean-up Measurement tables

In the case where the hierarchy selection state changes, you can remove measurement tables that are no longer required in the Spotfire document.

From the **Download these results** drop-down button, enable the Clean-up Measurement tables checkbox.

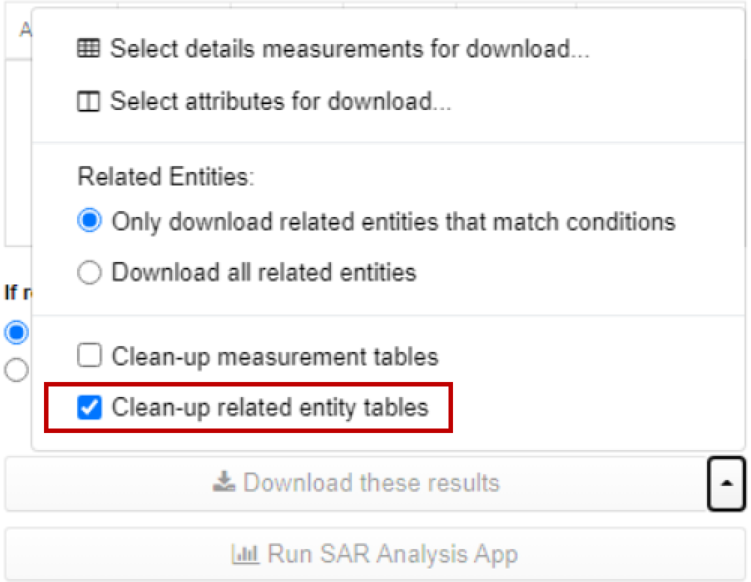


When this option is checked, the existing measurement type tables in Spotfire that are not selected as part of the current download will be removed from the Spotfire document.

For example, you have chosen and downloaded the assay data for measurement type A, and then you deselected measurement type A in the hierarchy tree, but selected measurement type B for download. If you checked "**Clean-up measurement tables**" option before clicking the **Download these results** button, then after download, the Spotfire data table that holds the data for measurement type A will be deleted from the Spotfire document.

Clean-up related entity tables

From the **Download these results** drop-down button, enable the Clean-up related entity tables checkbox.



Related Entities:

● Only download related entities that match conditions

○ Download all related entities

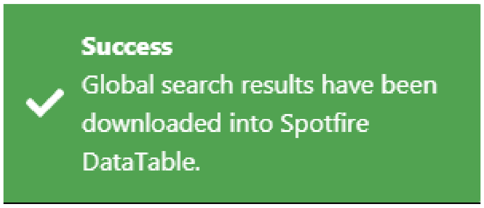
☐ Clean-up measurement tables

☑ Clean-up related entity tables

When this option is checked, the existing related entity tables in Spotfire that are not selected as part of the current download will be removed from the Spotfire document.

Downloading these results

Once the download is complete, a message will appear indicating that the global search results have been downloaded into a Spotfire data table(s).



✓ **Success**
Global search results have been downloaded into Spotfire DataTable.

Note: The **Download these results** button will be disabled if no results are returned from the search.

Note: The “Measurement Type” column of the downloaded Assay Endpoint Results table is now renamed to “Assay Type”, and a new “Measurement Type” column is added to the table but has a different meaning. If you open an existing Spotfire document that was saved in previous version of Signals Inventa, you may have to do the column mapping manually when you refresh or download the Assay Endpoint Results table.

Note: The dataset ID column (Set ID) column is included in the downloaded Measurement Type table to easily identify the dataset from which the measurement data came from.

6.10 Run SAR Analysis App

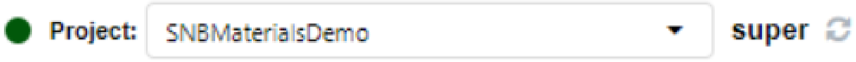
You can run the SAR Analysis App directly from the Global Search page by clicking the **Run SAR Analysis App** button. This option only becomes available after the global search results have been downloaded into a Spotfire data table(s).

If the SAR Analysis App already exists in the current document, the first occurrence of the app will be activated.

Refer to SAR Analysis App for detailed information.

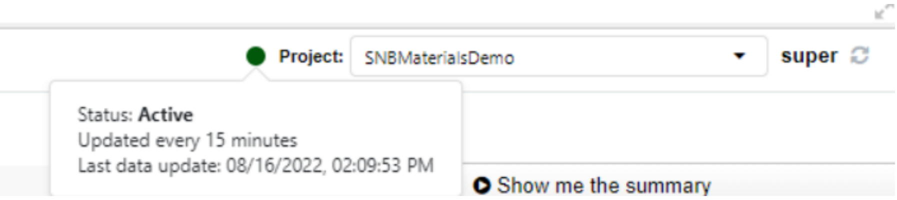
6.11 Signals Notebook Integration

To the left of the Project selector in the upper right corner of the Global Search panel, a status cue of the Signals Notebook material synchronization is displayed indicating the status of the Signals Notebook data stream to confirm that data is being properly ingested into Signals Inventa.



Project: SNBMaterialsDemo

By hovering over the visual cue, additional details on the Signals Notebook materials synchronization (last update, update frequency) is displayed so you can confirm that the data in Signals Inventa is current.



Project: SNBMaterialsDemo

Status: **Active**
Updated every 15 minutes
Last data update: 08/16/2022, 02:09:53 PM

Refer to Appendix E: Signals Notebook Integration.

Note: Currently Signals Notebook material synchronization is specifically available for Compound/Batch configured systems and is not available for other entity models.

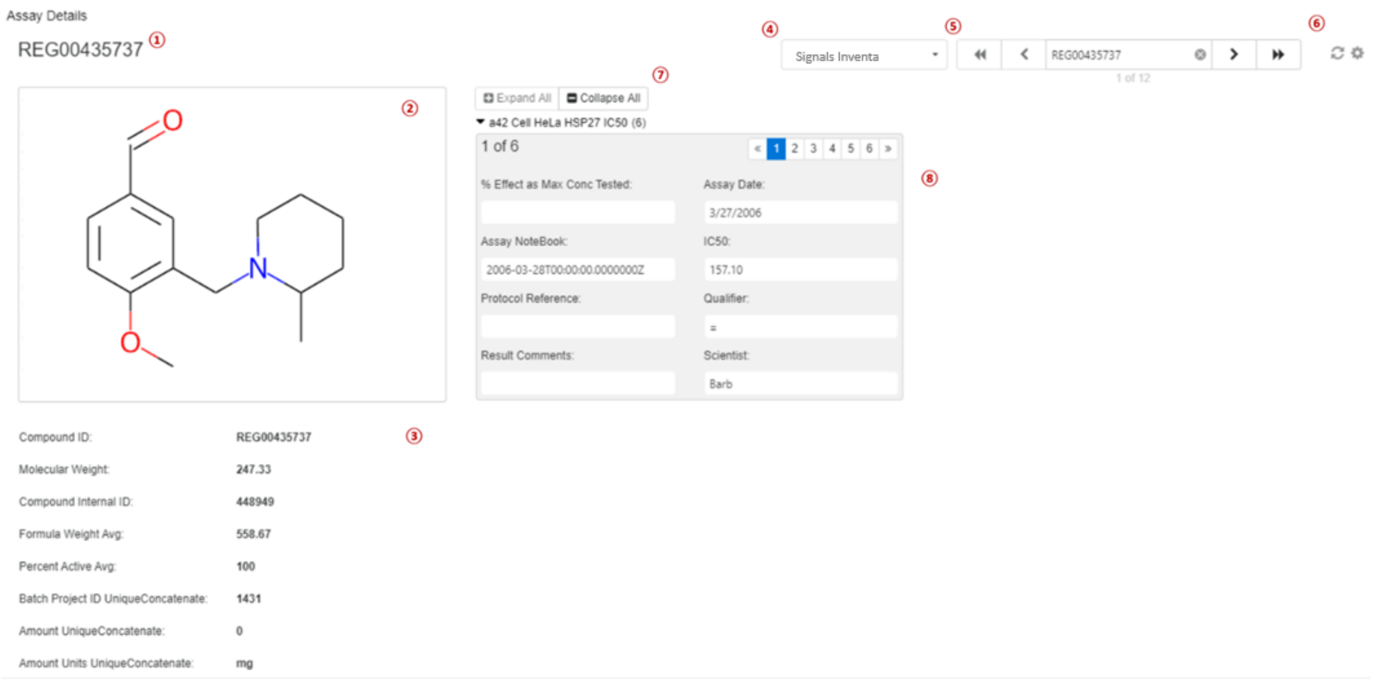
Note: If your company is not integrated with Revvity Signals Notebook, the streaming visual status icons are not visible on the Global Search panel.

6.12 Theme Support

The Global Search panel supports themes in Spotfire. You can either select the light or dark visual themes that are predefined or customize your own theme.

7 Assay Details

The Assay Details visualization displays the assay details data from different measurement types for a particular candidate (usually chemical compound). You are able to define how the assay data will be represented based on the measurement types, by using the Assay Details Layout definition page. Refer to Managing Assay Details Layout section for more information.



▾ a42 Cell HeLa HSP27 IC50 (6)

1 of 6

% Effect as Max Conc Tested:

Assay Date: 3/27/2006

Assay NoteBook: 2006-03-28T00:00:00.0000000Z

IC50: 157.10

Protocol Reference:

Qualifier: =

Result Comments:

Scientist: Barb

Compound ID:	REG00435737
Molecular Weight:	247.33
Compound Internal ID:	448949
Formula Weight Avg:	558.67
Percent Active Avg:	100
Batch Project ID UniqueConcatenate:	1431
Amount UniqueConcatenate:	0
Amount Units UniqueConcatenate:	mg

To view the Assay Details visualization:

1. Select **Tools > Signals Inventa > Open Assay Details** from the main menu to open the Assay Details page.

Refer to the Assay Details Properties section below for information in configuring the data to be dispayed on this page.

In the figure above:

1. **ID Column:** The column which represents the value from the Compound ID or Compound Batch ID column. This value will be used as the key value to retrieve the assay data for each measurement type. You can choose whether it is the Compound ID or Compound Batch ID that will be used as the ID column by changing the corresponding settings in the Assay Details Properties dialog.
2. **Box Column:** The column which contains the compound information. This information can be in a chemical structure format, for example, MOLFILE or SMILES, can be a BLOB which contains the image data, or a hyperlink which links to an image online. You can select the renderer for this Box Column to render the content and display in this square area.

3. **Simple Value Columns:** The columns from the data table which contains the ID Column and Box Column can be shown in this area, depending on the user selection. The data table that contains the ID Column and Box Column is called the Main Table, which is also the data source for the Assay Details visualization.

4. **Signals Inventa Project:** The currently selected project is displayed.

5. **Navigation Panel:** With this panel, you can navigate between each compound back and forth, or go to the first or last record in the Main Table. You can also navigate to a specific compound directly by typing the compound ID or compound batch ID value in the text box. The Navigation Panel will list the IDs that match the value in the text box as you type to assist in easily locating the compound you are interested in.

6. **Tool Buttons:** Assay details visualization has two tool buttons:

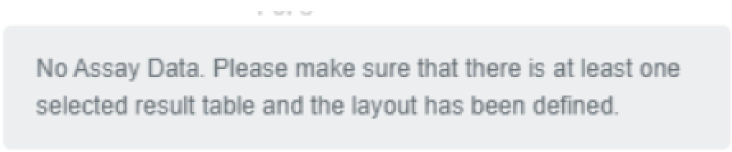
   a) **Refresh Button**: Each time the assay details layout is modified, Spotfire users can refresh the visualization by clicking this button, so that the latest layout will be displayed.

   b) **Properties Button**: Clicking this button will display the Assay Details Properties dialog. From here, you can perform additional configuration for the current assay details visualization.

7. **Collapse/Expand Buttons:** Use these buttons to collapse or expand all the assay details shown on the page.

8. **Assay Details Area:** Assay data for the selected measurement type is displayed here with the specified order, layout and format dependent on the properties defined in the Assay Details Properties window.

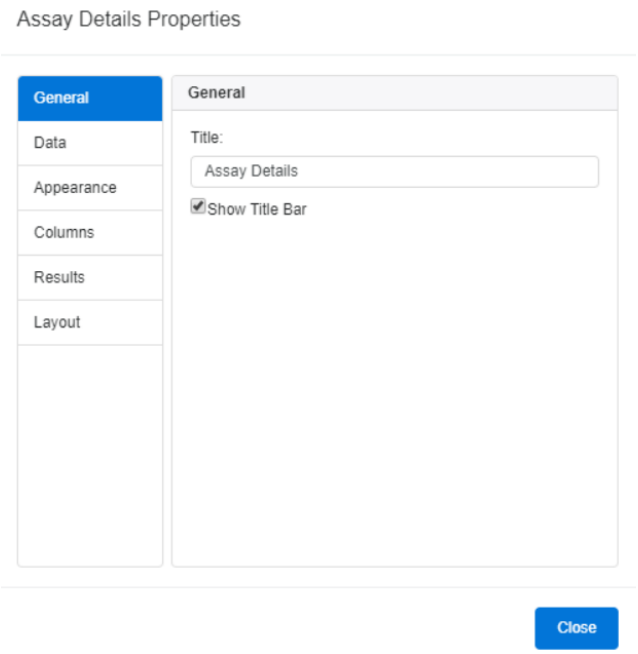
Note: Initially when the Assay Details visualization is opened, it will automatically choose the first table in the document as the Main Table. By default, the marking of the Main Table will be set to **(All)**, indicating that you are able to navigate each of the rows in the Main Table by using the Navigation Panel. You can also limit the navigation to only the rows that are selected by a specific marking. In addition, if no result measurement type has been chosen, or no layout has been defined for the chosen measurement type in the Assay Details Properties dialog, the following warning message will be shown. In this case, you need to define at least one layout for the measurement type in the Assay Details Layout configuration and make sure the measurement type is chosen in the Result tab under the Assay Details Properties dialog.



No Assay Data. Please make sure that there is at least one selected result table and the layout has been defined.

Assay Details Visualization Properties

To configure the Assay Details Visualization, click the cog icon (⚙) at the upper-right side of the page. This will open the Assay Details Properties dialog similar to the example shown below:



Assay Details Properties

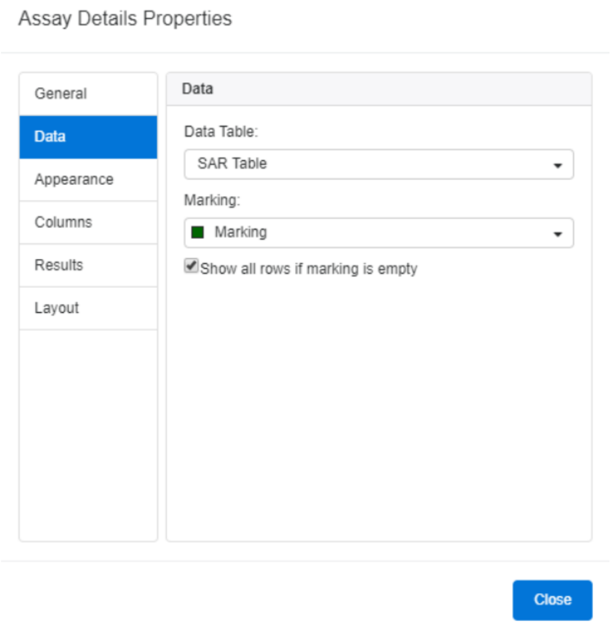
Title: Assay Details

☑ Show Title Bar

This dialog is very similar to the standard Spotfire visualization properties dialog in terms of the look-and-feel making it easy for you to change the settings for the current Assay Details visualization.

General Tab

This tab is very simple; it contains the basic settings for the current Assay details visualization, which includes the title of the visualization and whether the title bar should be displayed. Note that when you toggle the **Show Title Bar** checkbox, the visualization will refresh immediately without having to click the **Data Tab.**



Assay Details Properties

Data Table: SAR Table

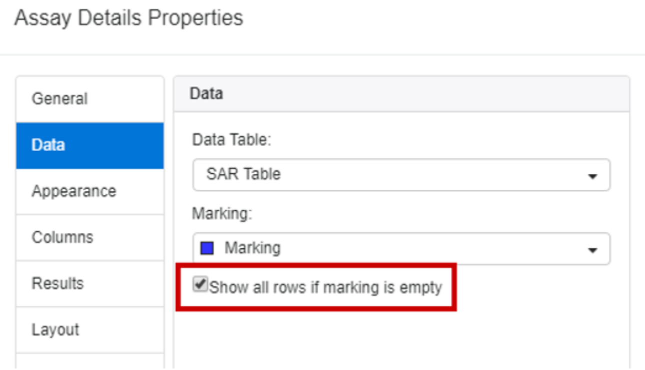
Marking: 🟩 Marking

☑ Show all rows if marking is empty

Within the Data Tab, you can choose which data table in the currently opened Spotfire document should be used as the Main Table to provide the ID Column, compound data as well as the compound properties information.

You can also choose the preferred marking to be used by the Assay Details visualization. Marked rows that belong to the selected marking will be displayed in the Assay Details visualization.

If the 'Show all rows if marking is empty' option is checked, and there is no row being selected under the specified marking (marking is empty), all rows will be bound to the Assay Details visualization.

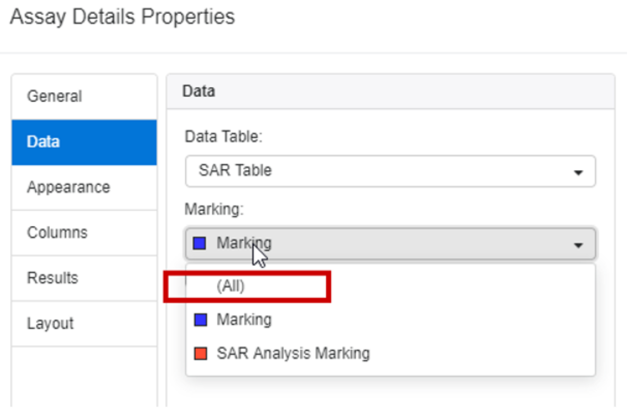


Data Table: SAR Table

Marking: Marking

☑ Show all rows if marking is empty

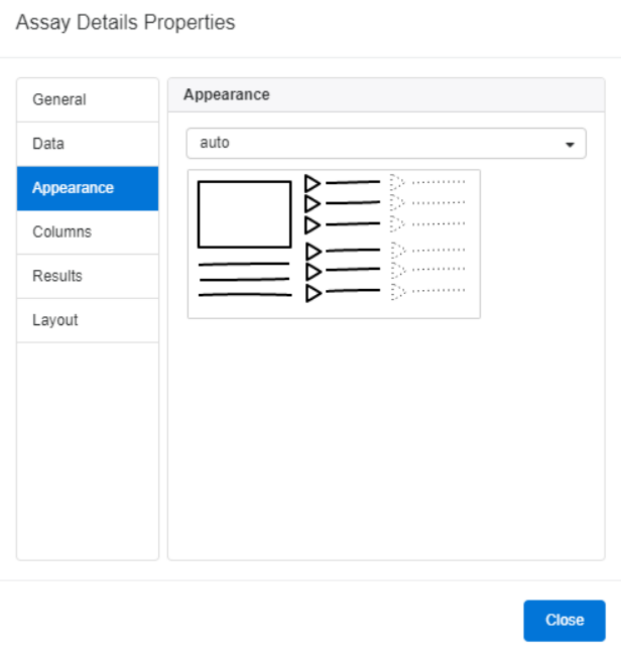
If the 'All' option is selected, all rows will be bound to the Assay Details visualization, regardless whether or not there is any marking applied on the selected table.



Data Table: SAR Table

Marking: Marking

Appearance Tab

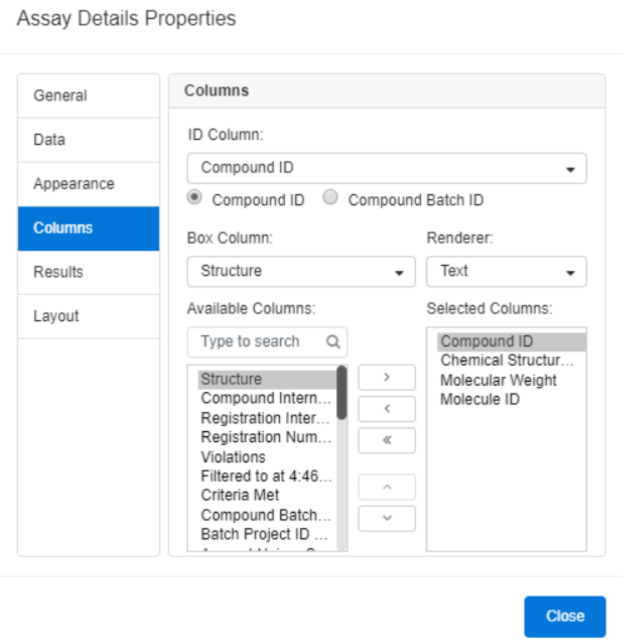


In the **Appearance** tab, you can choose the overall layout of the assay details visualization. There are four choices in the drop-down box:

1. **auto** – The number of columns shown in the assay details visualization will be adjusted automatically, depending on the screen resolution. A maximum of three columns will be displayed depending on resolution.
2. **1-column** – Assay Details visualization will only show one column, with the ID Column and Box Column be stacked on to the assay details area.
3. **2-columns** – Assay Details visualization will show two columns, with the ID/Box Column and assay details area showing side-by-side.
4. **3-columns** – There will be one column for the ID/Box Column and two columns displaying assay details.

When switching between the options, the preview picture is updated according to the selection and the selection will take effect immediately.

Columns Tab



Assay Details Properties

ID Column: Compound ID

● Compound ID ○ Compound Batch ID

Box Column: Structure

Renderer: Text

Settings under the Columns tab determine how the columns from the Main Table will be used in the Assay Details visualization. For example, you can choose a particular column as the Box Column, and specify a renderer for that column, so that it can be shown with a correct representation in the Box Column square area in the Assay Details visualization. More configuration options are available under this tab to control the display of the data columns from the main table.

1. **ID Column:** The column which represents the value from the Compound ID or Compound Batch ID column. This value will be used as the key value to retrieve the assay data for each measurement type. When defining the measurement mappings for measurement types, there are Compound ID and Compound Batch ID mapping fields that cannot be set as an empty value at the same time. You must specify the mapping between the measurement type and the assay endpoint results table for either Compound ID column or Compound Batch ID column, or both. Based on this mapping setting in the measurement type maps, you can select either the Compound ID or Compound Batch ID radio button here, to decide whether it is the Compound ID column or Compound Batch ID column from the measurement type that is going to be compared with the selected ID Column. This defines the key column to be used for retrieving the assay details from the backend services.

2. **Box Column:** The column whose content will be shown in the large square box in the Assay Details visualization. Typically, this column contains the chemical structure data, or it can be a column that holds the BLOB data which represents an image, or a hyperlink which links to an image online. Different content can be rendered into a human-readable representation via selected renderer at the right-hand side

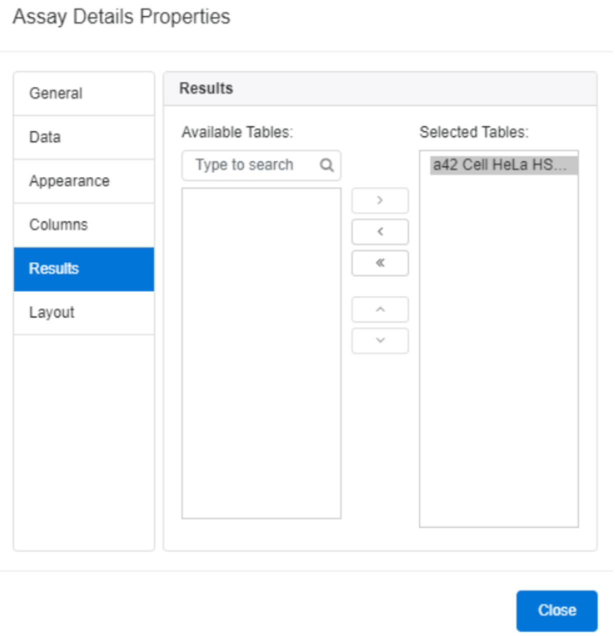
3. **Renderer:** This drop-down box lists all the available renderers that can be used for rendering the Box Column. The available renderers are retrieved from Lead Discovery Premium which is installed alongside Signals Inventa. Note that in the Assay Details Properties window, you are not able to configure the renderer settings. Those settings are configured and managed by Lead Discovery Premium. Assay details page will only use the default renderer settings, if there is any renderer setting options for the selected renderer.

4. **Available Columns:** All the columns in the selected table under the **Data** tab will be listed here as a candidate to be added into the **Simple Value Columns** area of the Assay Details visualization. You can add the columns to or remove them from the **Simple Value Columns** area by using the **Add**, **Remove** and **Remove All** buttons, to move the columns between **Available Columns** list and **Selected Columns** list.

5. **Selected Columns:** The columns listed in the **Selected Columns** list are placed into the **Simple Value Columns** area of the Assay Details visualization. You can adjust the order of the columns by clicking the **Move Up** and **Move Down** buttons.

Results Tab

Users can define the measurement types that contain the assay data to be shown on the Assay Details visualization. You can choose the measurements that you are interested in from within the **Results** tab of the Assay Details Properties window.

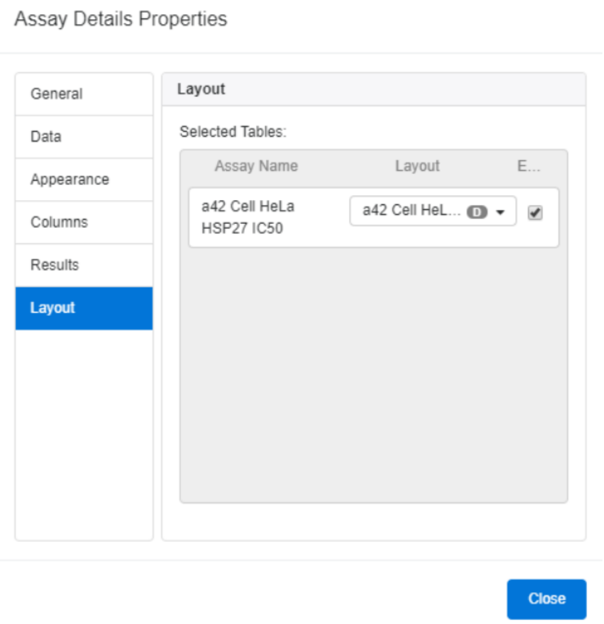


In the screen above, the **Available Tables** list will show all the measurement types which already have a layout defined. Users can choose the measurements that should be shown in the Assay Details visualization by moving them from the **Available Tables** list into **Selected Tables** list. You can also define the order of the measurements by clicking the **Move Up** and **Move Down** buttons.

Note that only the measurement types that have the assay details layout defined will be shown in the Available Tables list.

Layout Tab

With the Layout tab, you can choose the layout that is used for presenting the assay data for each selected measurement type. For each measurement type (also known as the assay), you can choose one layout from all available layouts; you can also define whether the content of the assay should be expanded or collapsed when it is first added to the Assay Details visualization.



Assay Name	Layout	E...
a42 Cell HeLa HSP27 IC50	a42 Cell HeL... D ▾	☑

1. **Assay Name:** This column shows the name of the assay (measurement type) that has been selected in the Results tab
2. **Layout:** For each assay (measurement type), there will be one or multiple pre-defined layout that will be listed in the Layout column here. You can choose the layout for the Assay Details visualization to present the assay details. For example, in the assay details layout definition, if you have defined a layout with the Table type, and you have selected that layout for the current assay, the data for that particular assay will be presented in the Table layout in the Assay Details visualization. The D icon at the right side represents that the current layout is the default layout
3. **Expand:** The check box determines if the display of the result data should be expanded when it is first added to the Assay Details visualization. Uncheck this check box to collapse the result data area. You can still expand/collapse the results in the Assay Details visualization by clicking the small triangle icon in front of each assay name, or expand/collapse all the results by clicking the **Expand All/Collapse All** buttons

In the Layout tab, you can also adjust the order of the assays to be shown by using drag-and-drop. The changes will take effect immediately.

8 Publish Measurements App

8.1 Accessing the Publish Measurements App

The Publish Measurements App is available in the Signals Apps store which is accessed through the main Spotfire Interface. You will be required to login to the Signals Data Factory using your SSO credentials before you can access this app if you have not been authenticated or if your session has expired.

Note: If the SDF ApiKey Spotfire preference has been set, you will not be required to logon. Refer to Setting the SDF ApiKey section for further information.

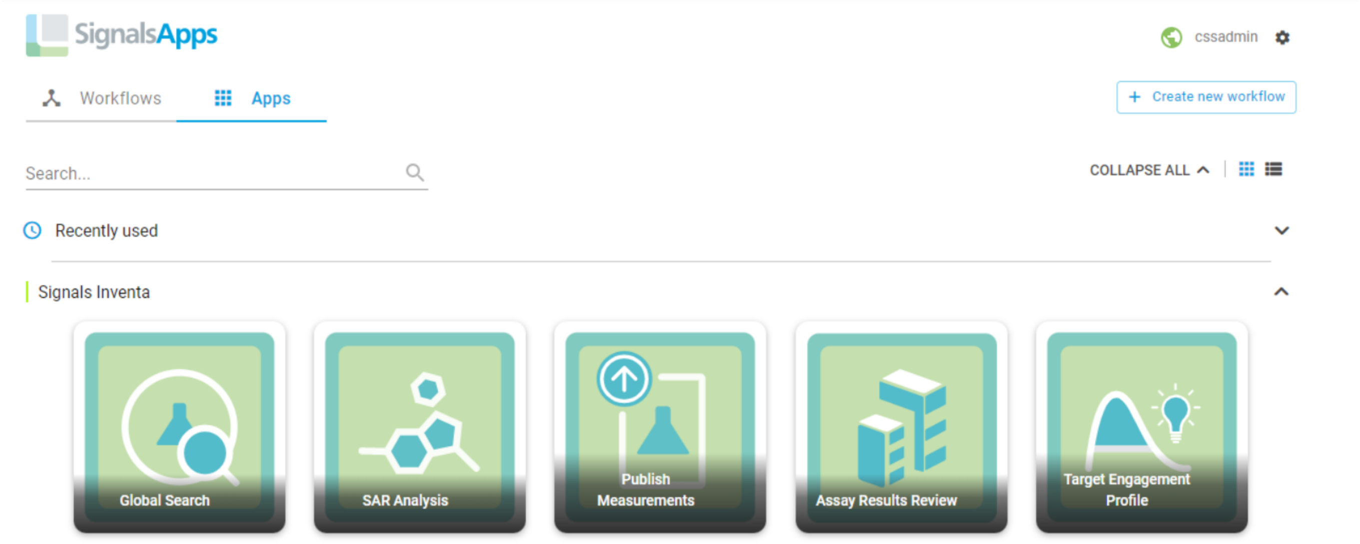
Note: If you are using Safari web browser, please make sure that it won't block the pop-up dialog from Signals Data Factory domain. To enable the pop-up dialog from Signals Data Factory:

1. In Safari, select **Preferences** menu.
2. In the **Preferences** dialog, choose **Websites** tab.
3. In the **Configured Websites** list, make sure that Signals Data Factory web page has been set to **Allow.**

To access the Publish Measurements App:

In Spotfire Analyst Client:

1. Select **Tools > Signals Apps**.



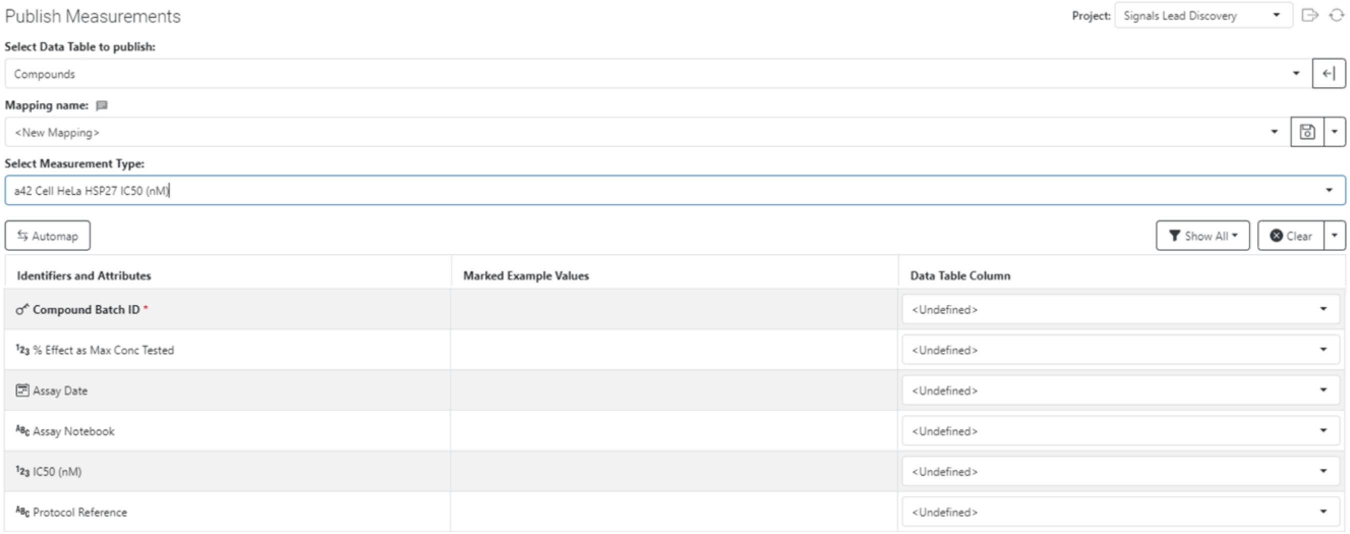
To launch the app, click anywhere on the **Publish Measurements App** card and it will be added to the document using the default app settings.

In Spotfire Web Player:

1. Open data in Spotfire.

2. Select **Tools > Signals Apps**.
3. To launch the app, click anywhere on the **Publish Measurements App** card and it will be added to the document using the default app settings.

A Publish Measurements page is displayed, similar to the example shown below.



Project: Signals Lead Discovery

Select Data Table to publish: Compounds

Mapping name: <New Mapping>

Select Measurement Type: a42 Cell HeLa HSP27 IC50 (nM)

Identifiers and Attributes	Marked Example Values	Data Table Column
Compound Batch ID *		<Undefined>
% Effect as Max Conc Tested		<Undefined>
Assay Date		<Undefined>
Assay Notebook		<Undefined>
IC50 (nM)		<Undefined>
Protocol Reference		<Undefined>

Please refer to the Publish Measurements Tool section of the main Signals Inventa User Guide for information on using Publish Measurements tool.

Note: You can change the name of the app by modifying the default settings. Click on the **Configure** button that will appear when you hover the mouse over the app card. The name of the added app page can be changed in the ‘Page Name’ field. It is recommended that you assign a unique name to the app page for clarity while working with the resulting Spotfire dashboard. Alternatively, you can change the page title by right clicking on the Publish Measurements page tab and selecting **Rename Page** from the pop-up menu.

Note: The Publish Measurements App supports Signals Apps workflows. Workflows is a feature that allows you to streamline the workflows by creating a document where you can string several Apps together, run different types of analysis with the same app, etc. If the Publish Measurements App has been added to a workflow, the “Select Measurement Type”, “Select Data Table to publish” and the “Mapping name” values will be kept when you reinitiate a document with the saved workflow. For more information about workflows, please refer to the Appendix A.

9 Global Search App

After data is published to Signals Data Factory through Signals Inventa, the Global Search app allows you to:

- Create complex nested queries and interrogate any subset of the stored data of interest.
- Explicitly set the scope of a query to be Compound, Batch, or Measurements, which results in much more precise control over the results set returned.
- Query for Structure, any compound attribute, and any assay or measurement, and query over an expanded set of comparison operators.
- Include multiple chemistry search criteria to more precisely find the subset of compounds of interest. Control system performance directly by choosing estimated vs. precise query result counts at different levels of precision.
- Save queries for easy re-use. Saved searches can be public or private.

Global Search uses the Batches, Compounds and Assay Endpoint Results tables from Signals Data Factory to provide the search capabilities.

9.1 Accessing the Global Search App

The Global Search App is available in the Signals Apps store which is accessed through the main Spotfire Interface. You will be required to login to the Signals Data Factory using your SSO credentials before you can access Global Search if you have not been authenticated or if your session has expired.

Note: If the SDF ApiKey Spotfire preference has been set, you will not be required to logon. Refer to Setting the SDF ApiKey section for further information.

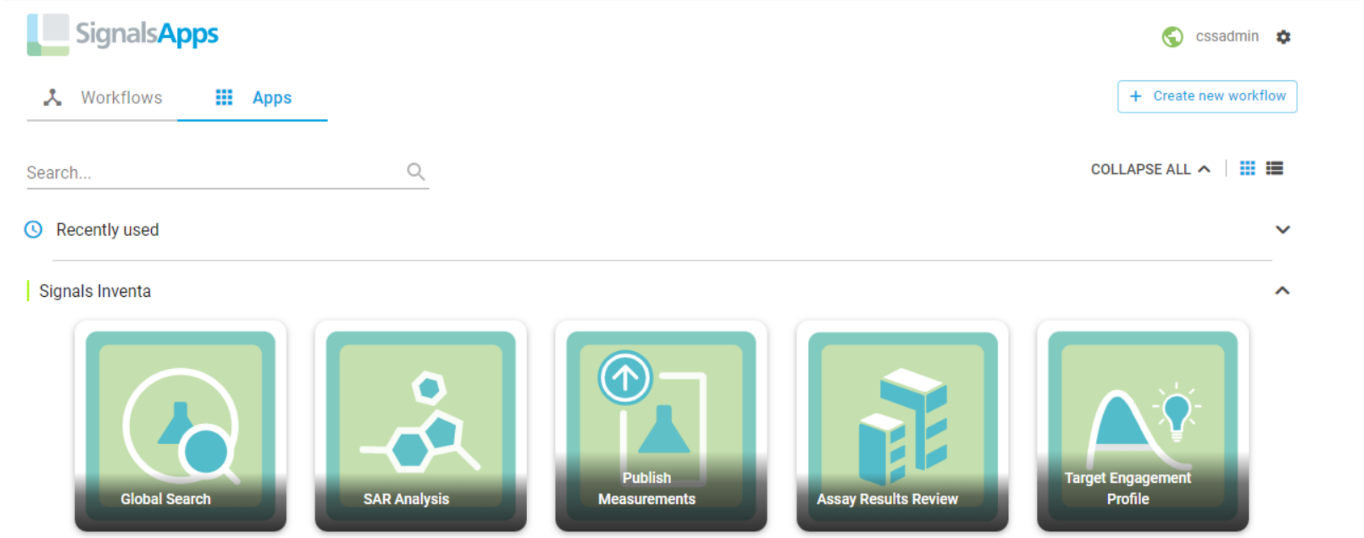
Note: If you are using Safari web browser, please make sure that it won't block the pop-up dialog from Signals Data Factory domain. To enable the pop-up dialog from Signals Data Factory:

1. In Safari, select **Preferences** menu.
2. In the **Preferences** dialog, choose **Websites** tab.
3. In the **Configured Websites** list, make sure that Signals Data Factory web page has been set to **Allow.**

To access the Global Search App:

In Spotfire Analyst Client:

1. Select **Tools > Signals Apps**.



2. To launch the app, click anywhere on the **Global Search App** card and it will be added to the document using the default app settings.

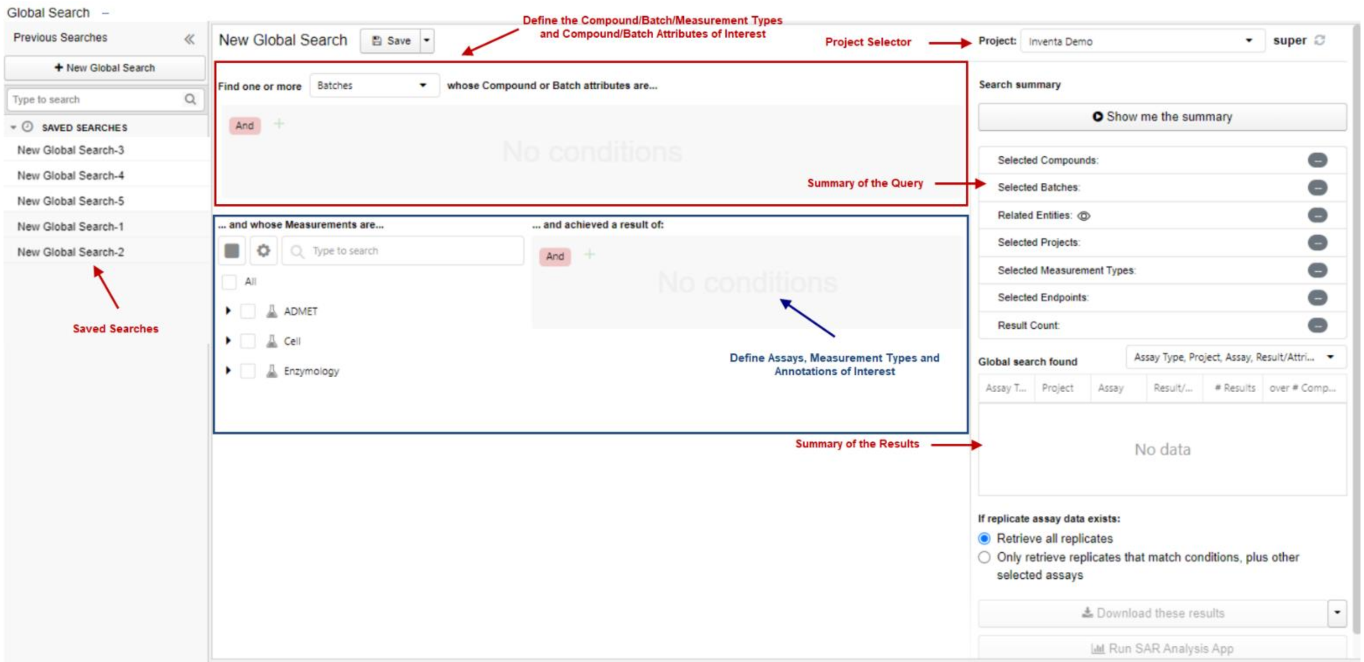
In Spotfire Web Player:

1. Open data in Spotfire.

2. Select **Tools > Signals Apps**.

3. To launch the app, click anywhere on the **Global Search App** card and it will be added to the document using the default app settings.

A Global Search page is displayed, similar to the example shown below.



Please refer to the Global Search section of the main Signals Inventa User Guide for information on using Global Search.

Note: You can change the name of the app by modifying the default settings. Click on the **Configure** button that will appear when you hover the mouse over the app card. The name of the added app page can be changed in the ‘Page Name’ field. It is recommended that you assign a unique name to the app page for clarity while working with the resulting Spotfire dashboard. Alternatively, you can change the page title by right clicking on the Global Search page tab and selecting **Rename Page** from the pop-up menu.

10 SAR Analysis App

The SAR Analysis App greatly simplifies the process of assembling and interpreting the Structure - Activity Relationship data that has been pulled into Spotfire from the Global Search App. With the SAR Analysis App, it is easy for a regular drug discovery scientist to:

- Define how the Compound and Assay data should be organized (e.g. by Compound or Compound Batch) and summarized (by mean, median, count, standard deviation, etc.).
- Customize long assay names into more meaningful, human-readable abbreviations.
- Configure intuitive tabular and graphical representations of the data through a point-and-click interface.
- Toggle between saved views of the data to easily navigate SAR analyses including many assays.
- Generate and compare compound lists with an interactive Venn diagram.

The SAR Analysis App makes use of the Compound, Batch and Assay Endpoint Results tables that are loaded into Spotfire from the Global Search App.

10.1 Accessing the SAR Analysis App

The SAR Analysis App is available in the Signals Apps store which is accessed through the main Spotfire Interface. You will be required to login to the Signals Data Factory using your SSO credentials before you can access this app if you have not been authenticated or if your session has expired.

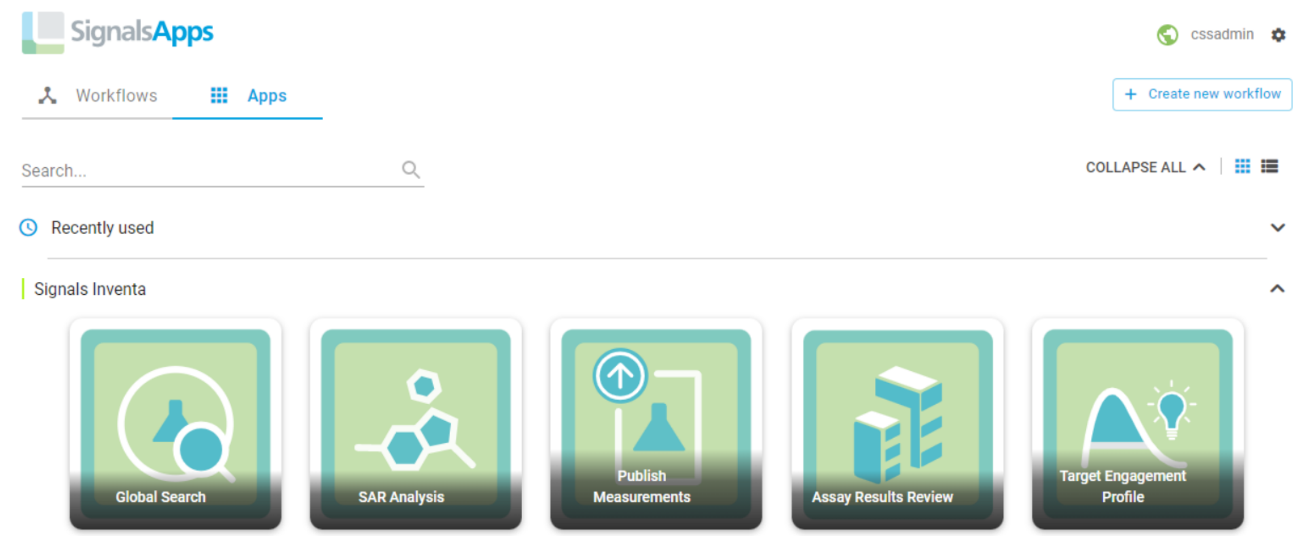
Note: If the SDF ApiKey Spotfire preference has been set, you will not be required to logon. Refer to Setting the SDF ApiKey section for further information.

The SAR Analysis App is available in the Signals Apps store which is accessed through the main Spotfire Interface.

To access the SAR Analysis App:

In Spotfire Analyst Client:

1. Select **Tools > Signals Apps**.

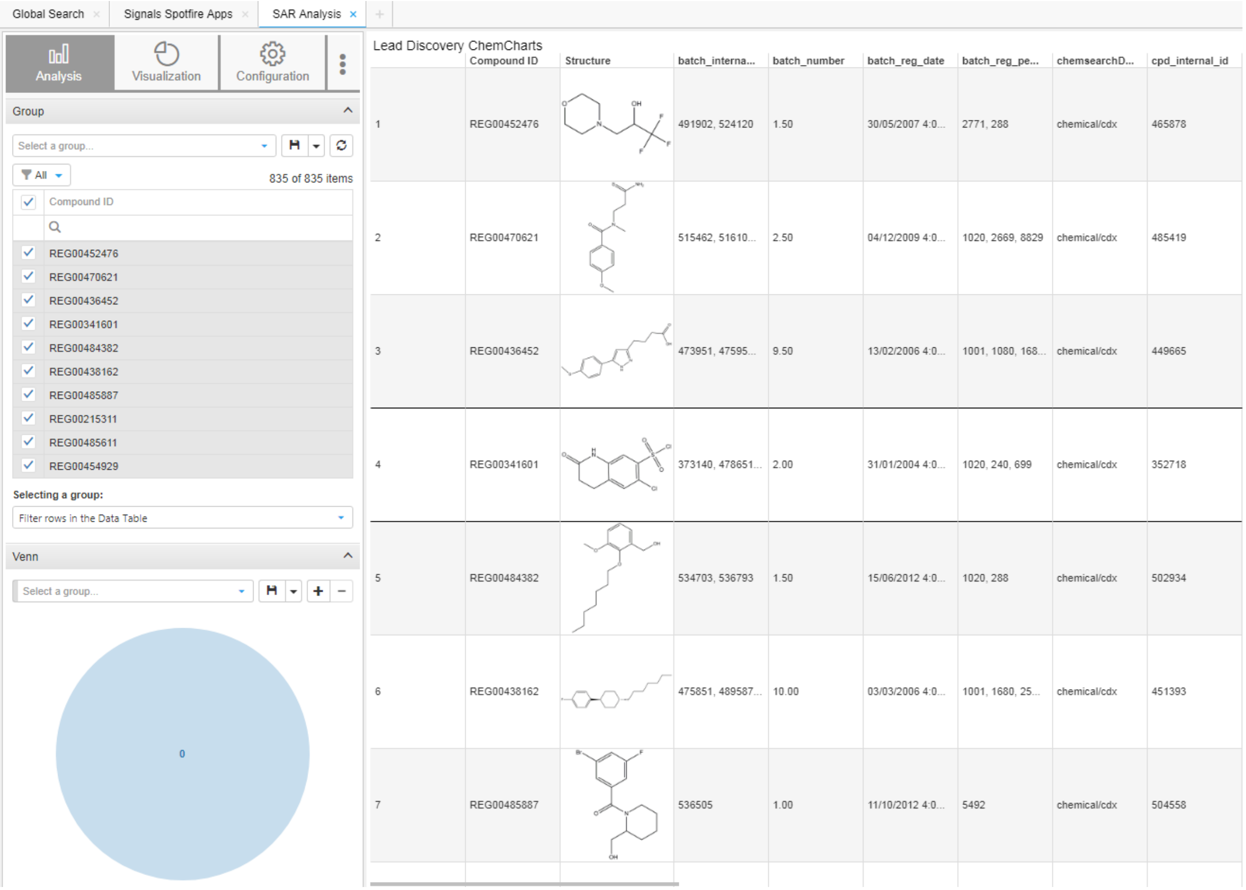


2. To launch the app, click anywhere on the **SAR Analysis App c**ard and it will be added to the document using the default app settings.

In Spotfire Web Player:

1. Open data in Spotfire.
2. Select **Tools > Signals Apps**.
3. To launch the app, click anywhere on the **SAR Analysis App** card and it will be added to the document using the default app settings.

A SAR Analysis page is displayed, similar to the example shown below.



Lead Discovery ChemCharts

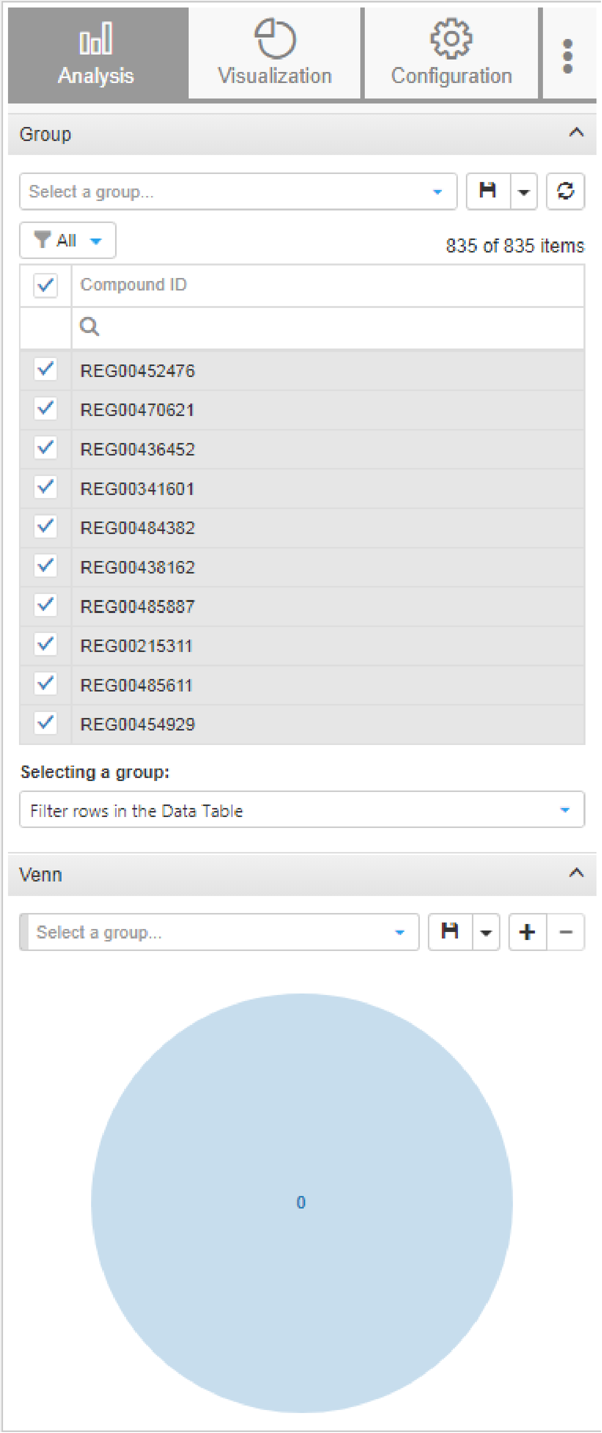
	Compound ID	Structure	batch_interna...	batch_number	batch_reg_date	batch_reg_pe...	chemsearchD...	cpd_internal_id
1	REG00452476		491902, 524120	1.50	30/05/2007 4:0...	2771, 288	chemical/cdx	465878
2	REG00470621		515462, 51610...	2.50	04/12/2009 4:0...	1020, 2669, 8829	chemical/cdx	485419
3	REG00436452		473951, 47595...	9.50	13/02/2006 4:0...	1001, 1080, 168...	chemical/cdx	449665
4	REG00341601		373140, 478651...	2.00	31/01/2004 4:0...	1020, 240, 699	chemical/cdx	352718
5	REG00484382		534703, 536793	1.50	15/06/2012 4:0...	1020, 288	chemical/cdx	502934
6	REG00438162		475851, 489587...	10.00	03/03/2006 4:0...	1001, 1680, 25...	chemical/cdx	451393
7	REG00485887		536505	1.00	11/10/2012 4:0...	5492	chemical/cdx	504558

Note: You can change the name of the app by modifying the default settings. Click on the **Configure** button that will appear when you hover the mouse over the app card. The name of the added app page can be changed in the 'Page Name' field. It is recommended that you assign a unique name to the app page for clarity while working with the resulting Spotfire dashboard. Alternatively, you can change the page title by right clicking on the SAR Analysis page tab and selecting **Rename Page** from the pop-up menu.

After defining the search criteria and clicking the **Download these results** button in Global Search, data from Signals Data Factory is downloaded, and two Spotfire data tables are generated; a 'Compounds' table and an 'Assay Endpoint Results' table. As the SAR Analysis app is loading, it is generating the SAR table for this data. When the app is first opened, the Analysis tab displays, by default, the generated SAR table in the Lead Discovery ChemCharts table in Spotfire.

10.2 Analysis tab

Here you can filter for compounds of interest by Compound ID or Compound Batch ID. The option available to you in the Analysis tab is based on the SAR table configuration. Refer to the Configuration section for more information.



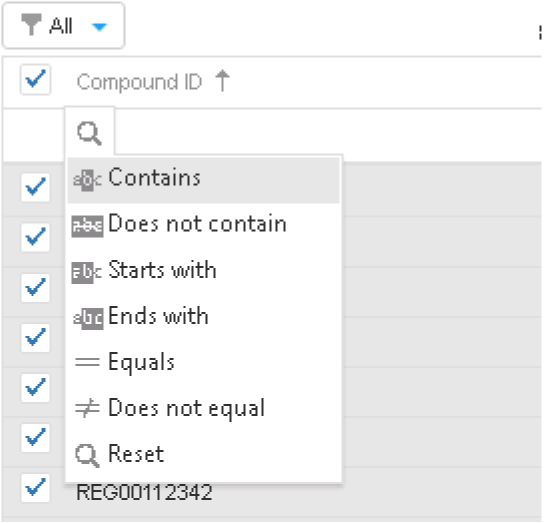
☑	Compound ID
☑	REG00452476
☑	REG00470621
☑	REG00436452
☑	REG00341601
☑	REG00484382
☑	REG00438162
☑	REG00485887
☑	REG00215311
☑	REG00485611
☑	REG00454929

Selecting a group: Filter rows in the Data Table

The visualization displayed in the right panel is determined by the selected visualization in the Visualizations tab. Refer to the Visualizations section for more information.

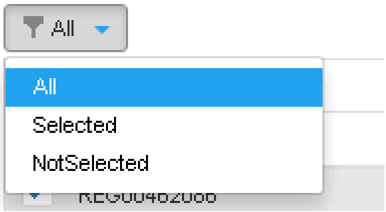
The Compound IDs (or Batch Compound IDs) can be sorted in ascending or descending order using the ↑ and ↓ buttons respectively.

Filter the rows to one or more compounds. This is a standard Spotfire filter – typing a compound identifier in the type-ahead box will bring that compound to the top of the list. Query operators are also available to help you find the compounds of interest.



Left-Click to select a compound from the list and Control-Click to single-select one or more individual compounds. To select a range of compounds, you will need to individually click the desired checkboxes, or use the Control-Click functionality. The Shift-Click operation does not work in this grid.

You can also choose to display All results, Selected results and Not Selected results based on the search criteria.



Changes made here are reflected in the visualization in the right panel.

10.2.1 Groups

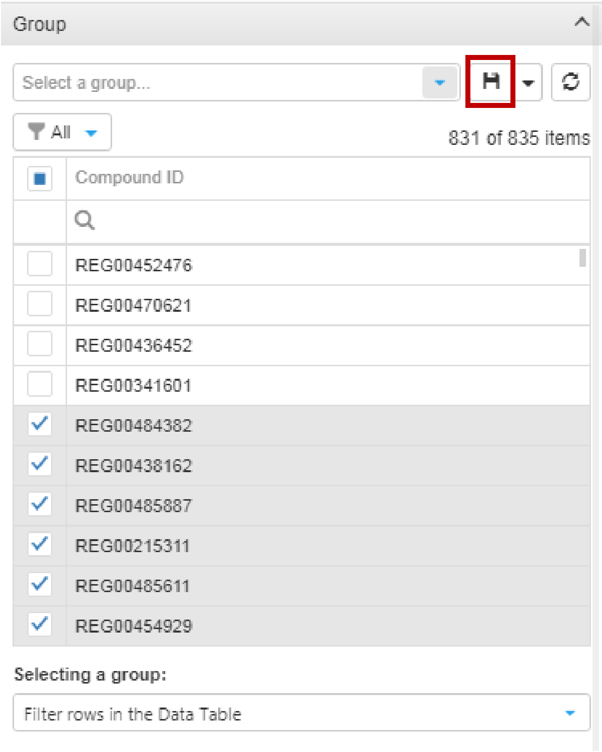
To make it easier to get an overview of the filters in the filter panel, you can create filter groups. Groups can be assigned a name and saved, and shared between multiple instances of the app.

Note: A default filter scheme “SAR Analysis Filter” is added to the document when the first SAR Analysis page is added. This default filter scheme is shared between all SAR Analysis pages in the document. This filter scheme cannot be renamed or deleted. The Group view only displays the values in the default “SAR Analysis Filter” and if you select a different filtering scheme in the SAR Analysis page, the selection binding between group and the visualization in the right panel will not work properly.

10.2.1.1 Working with Groups

To create a new group:

1. Filter the results to include in the group by checking/unchecking items in the list or by using the search filter.



Group

Select a group...

All

831 of 835 items

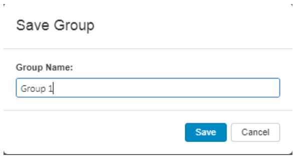
☑ Compound ID

☐ REG00452476
☐ REG00470621
☐ REG00436452
☐ REG00341601
☑ REG00484382
☑ REG00438162
☑ REG00485887
☑ REG00215311
☑ REG00485611
☑ REG00454929

Selecting a group:

Filter rows in the Data Table

2. Click on the Create new group based on current selection 💾 icon to save group. The Save Group dialog opens.

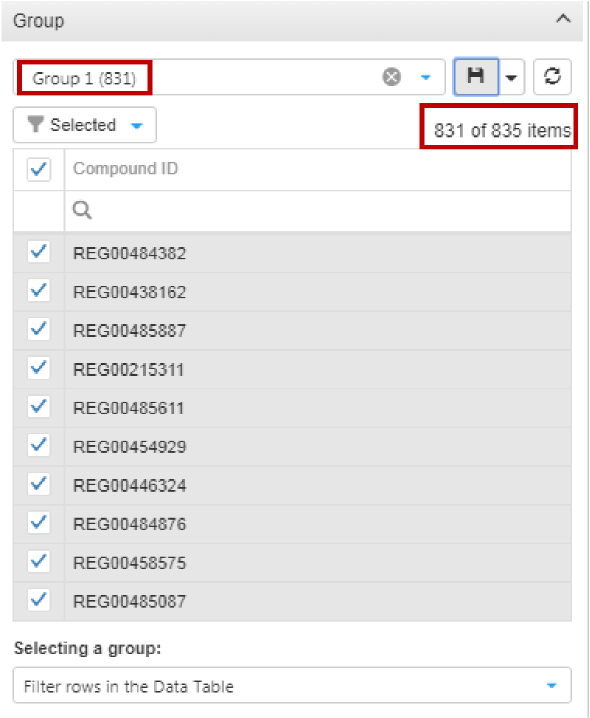


Save Group

Group Name: Group 1

3. Enter a unique Group Name.
4. Click **Save**.

The Group Name displays the number of Compound IDs (or Batch Compound IDs) (in parenthesis) in the group following the Group Name.



Using the Group drop-down list, you can switch between different groups. Changes made to the groups will be displayed in the visualization in the panel on the right.

To search and select a group:

1. From the Select a group drop-down list, input the group name in the Search or create edit box to search for the group. Alternatively, using the up and down arrow keys, you can search for the Group name in the list.
2. Select the Group name.

The newly selected group is reflected in the visualization in the right panel.

To search and create a new group:

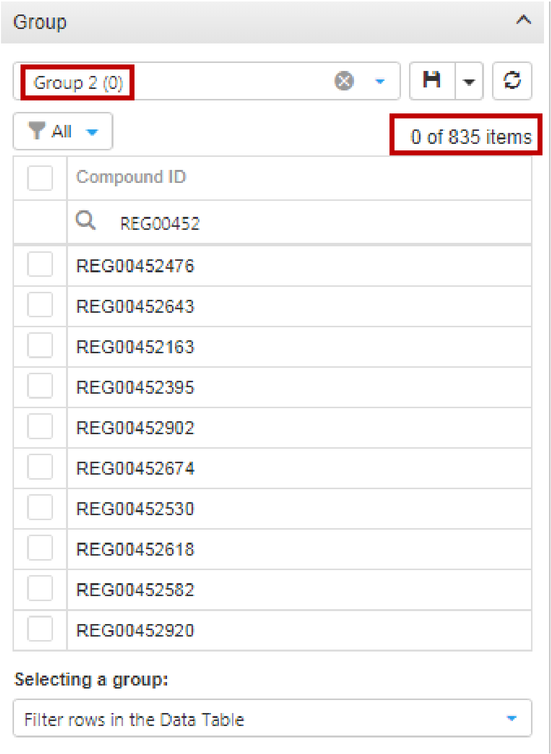
In the case where a search does not locate the group, you can create an empty group using this group name.

1. From the Select a group drop-down list, input the group name in the Search or create edit box to search for the group. There is no data to display for the specified Group name.
2. Click on the **+ Create Group: Group Name** button.

Group 2

No data to display

By default, all items will be shown as unchecked.

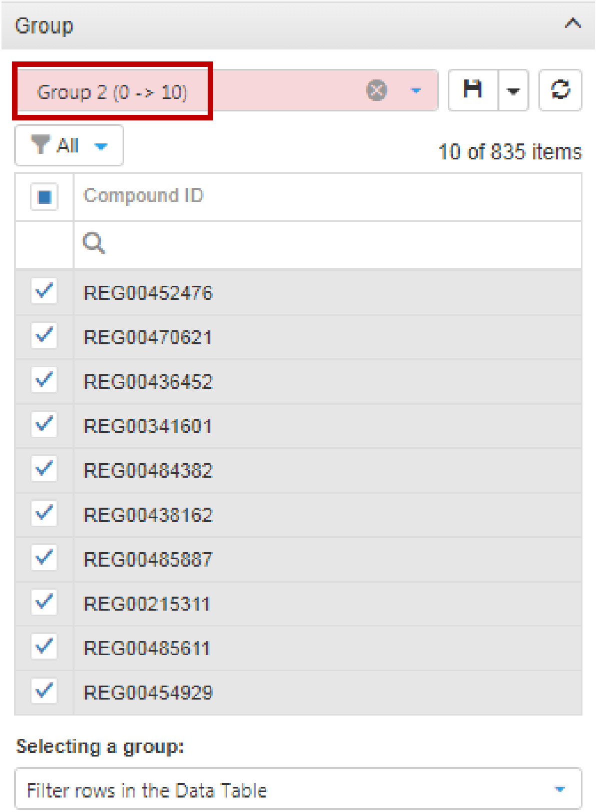


☐	Compound ID
	REG00452
☐	REG00452476
☐	REG00452643
☐	REG00452163
☐	REG00452395
☐	REG00452902
☐	REG00452674
☐	REG00452530
☐	REG00452618
☐	REG00452582
☐	REG00452920

Selecting a group:

Filter rows in the Data Table

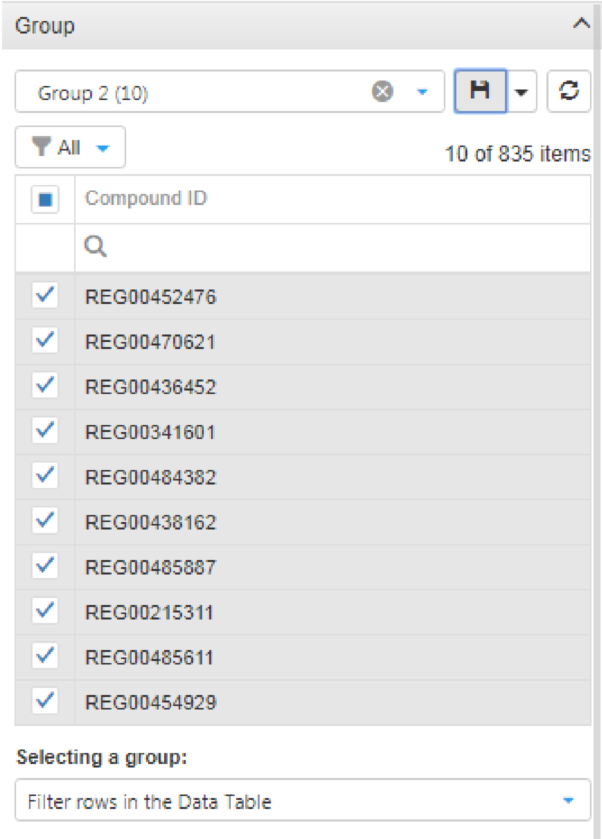
3. Check or filter the items to include in the new group.



- ☑ REG00452476
- ☑ REG00470621
- ☑ REG00436452
- ☑ REG00341601
- ☑ REG00484382
- ☑ REG00438162
- ☑ REG00485887
- ☑ REG00215311
- ☑ REG00485611
- ☑ REG00454929

Selecting a group: Filter rows in the Data Table

3. Click on the Save group to database 💾 icon to save the new group.



Alternatively, instead of clicking the **+ Create Group: Group Name** button to create a new group, you can also hit the Enter key directly in the Search or create edit box to create the new group.

Total Count and Dirty Flag

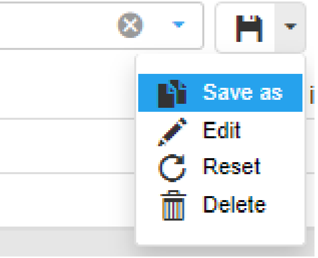
A group is flagged as dirty when changes are made to the group, and it has not yet been saved again. In the example below, Group 2 had 0 items when first created. Ten items were added to Group 2.
The Group is flagged as dirty (pink background) until the group is saved.

Also, as changes are made to the current group, the current total number of items in the group is displayed, as well as the original total number of items in the group with a “->” sign between the two counts. For example, (0 -> 10) indicates that initially the group has 0 items, however now it has changed, and the current number of items in the group is 10.

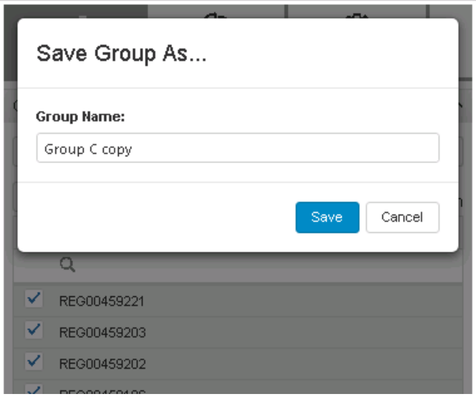
Once the Save group to database icon is clicked, the group is no longer flagged as dirty.

To save as a new group:

1. Filter the results to include in the group.
2. From the Save group to database drop-down menu select **Save As.**



The Save As Group dialog opens.

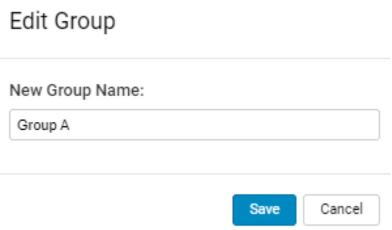


Group C copy

3. By default, the group name will be a copy of the selected group name. You can enter a new unique name for the group.
4. Click **Save**. The new group will be appended to the Group drop-down list.

To rename a group:

1. From the Save group to database drop-down menu, select **Edit** to open the Edit Group window**.**
2. Enter a new name for the group.



Group A

3. Click Save.

To reset a group:

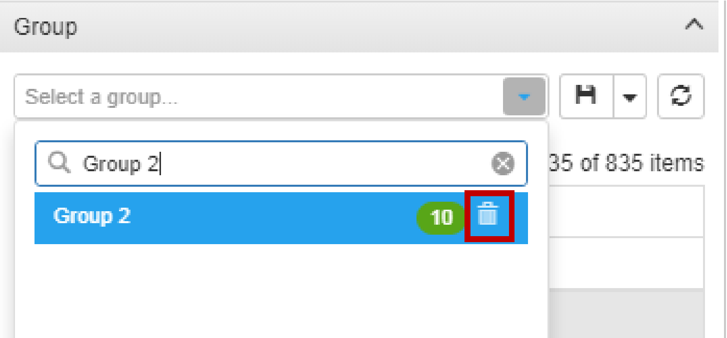
If a group is flagged as ‘’dirty”, you can reset the group to its original filter.

1. From the Save group to database drop-down menu, select **Reset**. You will be prompted to confirm the Reset operation.

To delete a group:

1. From the Save group to database drop-down menu, select **Delete**. You will be prompted to confirm the Delete operation.

You can also delete a group directly from the Select a group drop-down list, by selecting the 🗑 Delete icon next to the selected group name.



To refresh the list of results:

The Refresh ⟳ button will refresh the Group drop-down list. This is useful in the case where two users are working with the SAR app. For example, one user may have created a new group, however this new group will not be visible to the second user until the Refresh button is clicked.

Selecting a Group

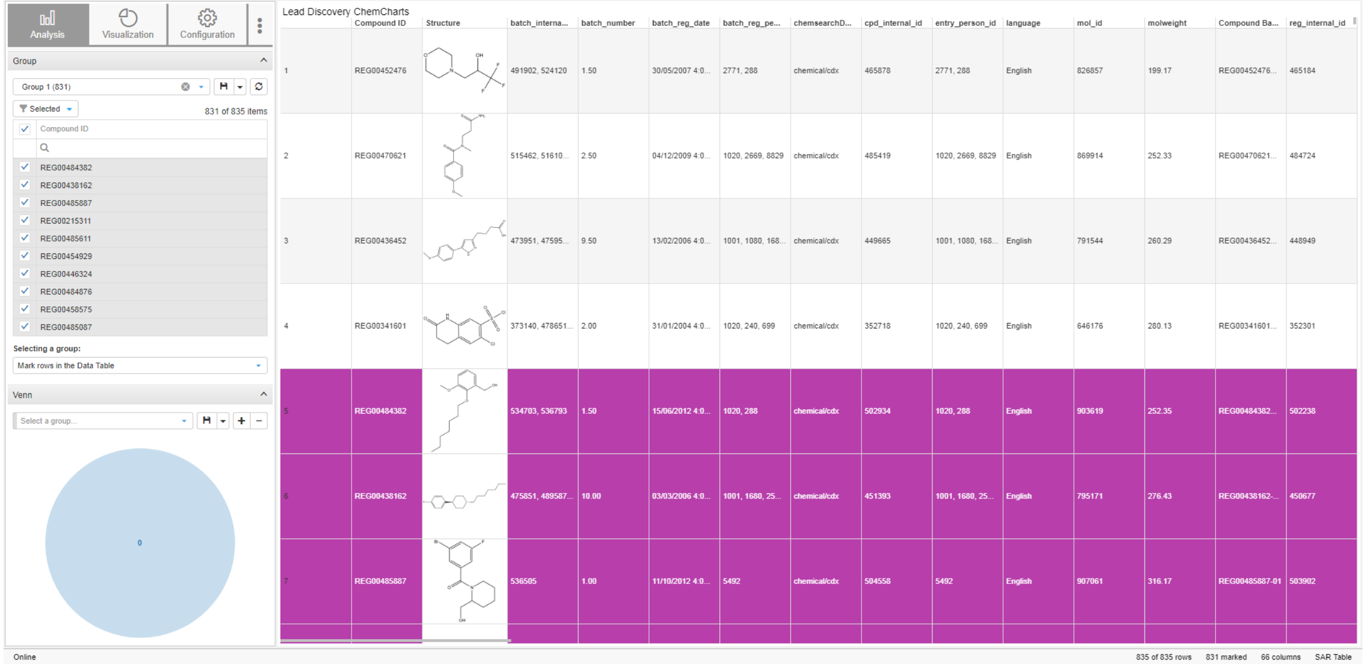
When selecting a group from the drop-down list, you have the option to filter rows in the data table or mark rows in the data table. From the Selecting a Group drop-down list, you can choose to ‘Filter Rows in the Data Table’ or “Mark Rows in the Data Table’.

i. Filter Rows in the Data Table

If you choose ‘Filter Rows in the Data Table’, the visualization displayed in the right panel will only displays the rows in the selected group.

ii. Mark Rows in the Data Table

If you choose ‘Mark Rows in the Data Table’, the visualization displayed in the right panel will display all rows in the data table and mark the rows that are in the selected group similar to the example shown below.



831 of 835 items

Compound ID

- ☑ REG00484382
- ☑ REG00438162
- ☑ REG00485887
- ☑ REG00215311
- ☑ REG00485611
- ☑ REG00454929
- ☑ REG00446324
- ☑ REG00484876
- ☑ REG00458575
- ☑ REG00485087

Selecting a group: Mark rows in the Data Table

Lead Discovery ChemCharts

	Compound ID	Structure	batch_interna...	batch_number	batch_reg_date	batch_reg_pe...	chemsearchD...	cpd_internal_id	entry_person_id	language	mol_id	molweight	Compound Ba...	reg_internal_id
1	REG00452476		491902, 524120	1.50	30/05/2007 4:0...	2771, 288	chemical/cdx	465878	2771, 288	English	826857	199.17	REG00452476...	465184
2	REG00470621		515462, 51610...	2.50	04/12/2009 4:0...	1020, 2669, 8829	chemical/cdx	485419	1020, 2669, 8829	English	869914	252.33	REG00470621...	484724
3	REG00436452		473951, 47595...	9.50	13/02/2006 4:0...	1001, 1080, 168...	chemical/cdx	449665	1001, 1080, 168...	English	791544	260.29	REG00436452...	448949
4	REG00341601		373140, 478651...	2.00	31/01/2004 4:0...	1020, 240, 699	chemical/cdx	352718	1020, 240, 699	English	646176	280.13	REG00341601...	352301
5	REG00484382		534703, 536793	1.50	15/06/2012 4:0...	1020, 288	chemical/cdx	502934	1020, 288	English	903619	252.35	REG00484382...	502238
6	REG00438162		475851, 489587...	10.00	03/03/2006 4:0...	1001, 1680, 25...	chemical/cdx	451393	1001, 1680, 25...	English	795171	276.43	REG00438162-...	450677
7	REG00485887		536505	1.00	11/10/2012 4:0...	5492	chemical/cdx	504558	5492	English	907061	316.17	REG00485887-01	503902

835 of 835 rows 831 marked 66 columns SAR Table

This option allows you to see what compounds are in the selected group, and then by viewing all the data in the data table, you can determine what compounds you want to add to the group.

In the example here, you may decide you want to include two additional compounds in Group 1. Once marked they will be added to Group 1 as shown below.

833 of 835 items

Compound ID

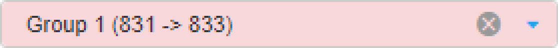
- ☑ REG00452476
- ☑ REG00470621
- ☑ REG00484382
- ☑ REG00438162
- ☑ REG00485887
- ☑ REG00215311
- ☑ REG00485611
- ☑ REG00454929
- ☑ REG00446324
- ☑ REG00484876

Selecting a group: Mark rows in the Data Table

Lead Discovery ChemCharts

	Compound ID	Structure	batch_interna...	batch_number	batch_reg_date	batch_reg_pe...	chemsearchD...	cpd_internal_id	entry_person_id	language	mol_id	molweight	Compound Ba...	reg_internal_id
1	REG00452476		491902, 524120	1.50	30/05/2007 4:0...	2771, 288	chemical/cdx	465878	2771, 288	English	826857	199.17	REG00452476...	465184
2	REG00470621		515462, 51610...	2.50	04/12/2009 4:0...	1020, 2669, 8829	chemical/cdx	485419	1020, 2669, 8829	English	869914	252.33	REG00470621...	484724
3	REG00436452		473951, 47595...	9.50	13/02/2006 4:0...	1001, 1080, 168...	chemical/cdx	449665	1001, 1080, 168...	English	791544	260.29	REG00436452...	448949
4	REG00341601		373140, 478651...	2.00	31/01/2004 4:0...	1020, 240, 699	chemical/cdx	352718	1020, 240, 699	English	646176	280.13	REG00341601...	352301
5	REG00484382		534703, 536793	1.50	15/06/2012 4:0...	1020, 288	chemical/cdx	502934	1020, 288	English	903619	252.35	REG00484382...	502238
6	REG00438162		475851, 489587...	10.00	03/03/2006 4:0...	1001, 1680, 25...	chemical/cdx	451393	1001, 1680, 25...	English	795171	276.43	REG00438162-...	450677
7	REG00485887		536505	1.00	11/10/2012 4:0...	5492	chemical/cdx	504558	5492	English	907061	316.17	REG00485887-01	503902

Group 1 will be tagged as dirty:



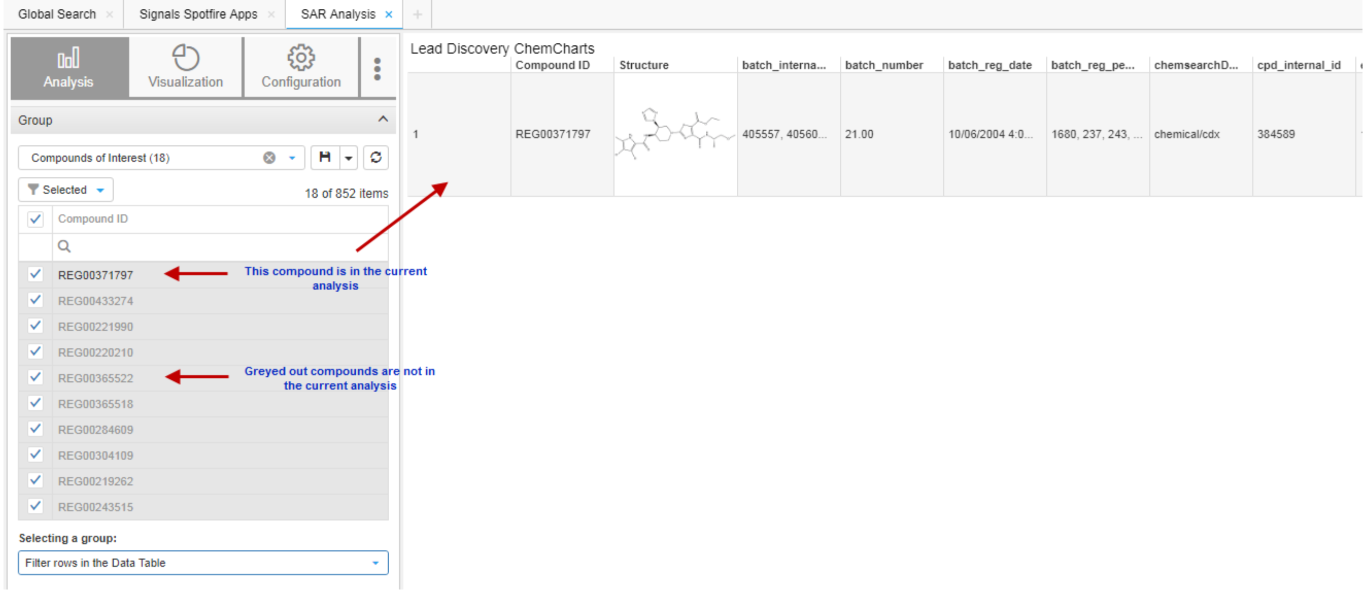
You can choose to reset the group to its original filter or click on the Save group to database icon to save Group 1 with the additional compounds.

Note: The Venn diagram in the lower section of the panel also has a similar drop-down list for Selecting a Venn diagram section. These two drop-down lists are synchronized, and changes to one are reflected in the other.

Groups in Current Analysis

There may be the case that a group is selected from the Select a group drop-down list, however not all the compounds in the group are in the current analysis.

In the example shown below, the Compounds of Interest group is selected. This group has 18 compounds. However, in the current analysis, there is only one compound in the group. In this case, the compounds in the group that are not in the current analysis are greyed out.



☑ Compound ID
☑ REG00371797
☑ REG00433274
☑ REG00221990
☑ REG00220210
☑ REG00365522
☑ REG00365518
☑ REG00284609
☑ REG00304109
☑ REG00219262
☑ REG00243515

This compound is in the current analysis

Greyed out compounds are not in the current analysis

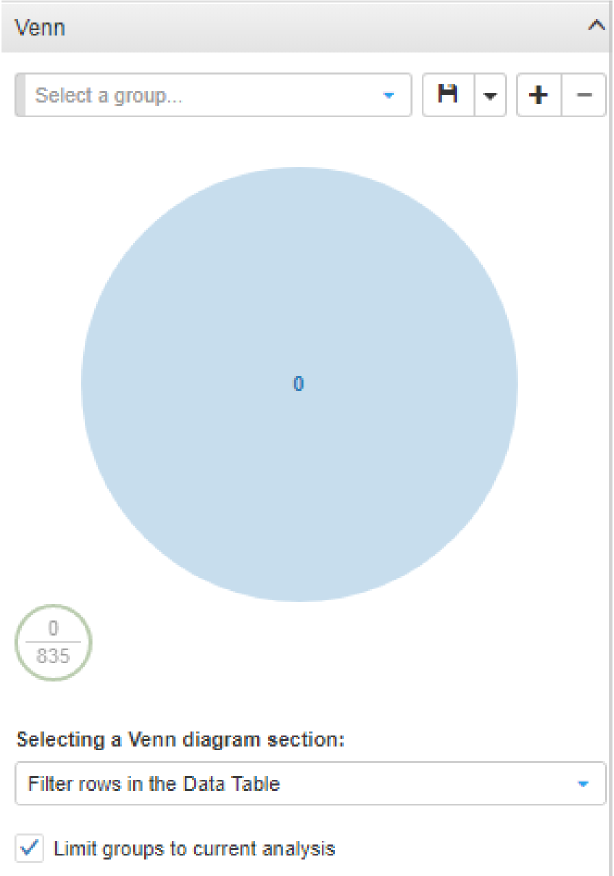
Selecting a group:
Filter rows in the Data Table

	Compound ID	Structure	batch_interna...	batch_number	batch_reg_date	batch_reg_pe...	chemsearchD...	cpd_internal_id
1	REG00371797		405557, 40560...	21.00	10/06/2004 4:0...	1680, 237, 243, ...	chemical/cdx	384589

Groups will always include the compound in the group even if it is not in the current analysis unless you manually uncheck a greyed-out compound (compound is not in the current analysis) and then save the group. In the example above, REG00365522 is not in the current analysis. If you manually uncheck this compound, the group will be flagged as dirty. Clicking on the Save group to database icon will save the group, and REG00365522 is deleted from the group.

10.2.2 Venn Diagram

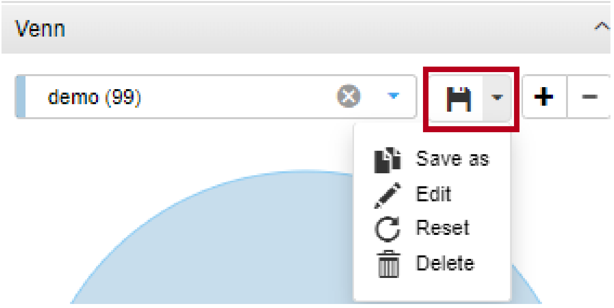
The Venn diagram allows you to graphically compare groups (of Compound IDs, Compound Batch IDs) such that you can arrive at a subset of compounds of value and interest more quickly.



Selecting a Venn diagram section: Filter rows in the Data Table

☑ Limit groups to current analysis

Working with groups in the Venn diagram is similar to working with groups in the Group panel. Using the Create new group based on current selection icon, and the Save group to database icon and drop-down menu, you can create a new group, save as a new group, rename, reset, and delete groups in the Venn diagram panel. Refer to Working with Groups section.



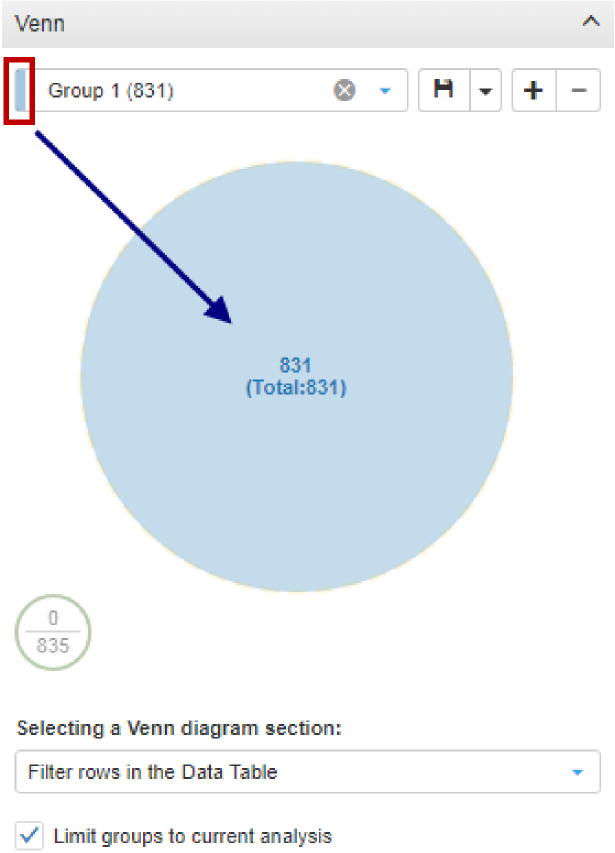
Any changes made to the groups in the Venn diagram panel will also update the corresponding groups in the Groups panel.

10.2.2.1 Working with the Venn Diagram

The first step in creating a Venn diagram is to define the groups to be included in the diagram.

To search and select a group to add to the Venn diagram:

1. From the Select a group drop-down list, input the group name in the Search or create edit box to search for the group. Alternatively, using the up and down arrow keys, you can search for the Group name in the list.



Selecting a Venn diagram section: Filter rows in the Data Table

☑ Limit groups to current analysis

The group is added to the Venn diagram, and the number of items in the group is labelled. The groups are color indicated making it easier for you to identify the groupings in the Venn diagram.

To search and create a new (empty) group to add to the Venn diagram:

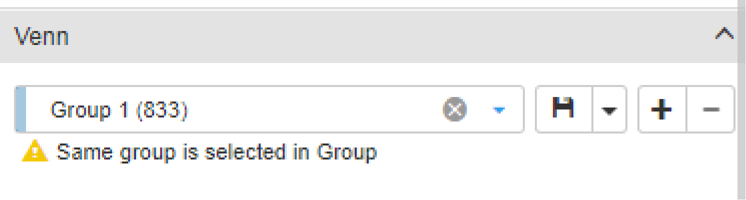
In the case where a search does not locate the group, you can create a new (empty) group for this group name.

1. From the Select a group drop-down list, input the group name in the Search or create edit box to search for the group. There is no data to display for the specified Group name.
2. Click on the **+ Create Group: Group Name** button.

An empty group will be created and added to the Venn diagram. Alternatively, instead of clicking the **+ Create Group: Group Name** button to create a new group, you can also hit the Enter key directly in the Search or create edit box to create the new (empty) group.

Once an empty group is created, you can mark rows in the visualization in the right-hand panel and using the drag-and-drop green ball, add compounds IDs to the group. Refer to the Drag and Drop Marked Rows into a Venn Diagram section.

Note: Before working with groups in the Venn Diagram, best practice is to clear any selected groups in the Groups section. A warning message, similar to the example shown below, will appear when you attempt to work with a group in the Venn Diagram that is currently selected in the Groups section above.



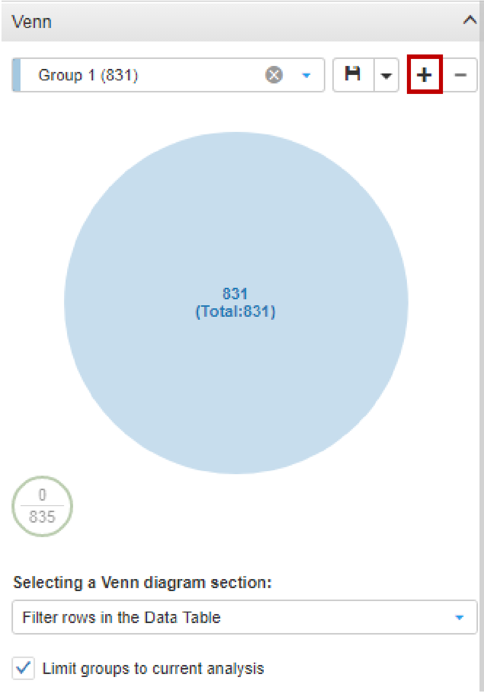
⚠ Same group is selected in Group

You may continue with the selected group however you may experience some unexpected behavior with the groups.

A similar message will appear when selecting a group from the Groups drop-down list if the group has already been selected for use in the Venn diagram.

Adding multiple groups to the Venn Diagram

1. Click on the + to add a new group select item.

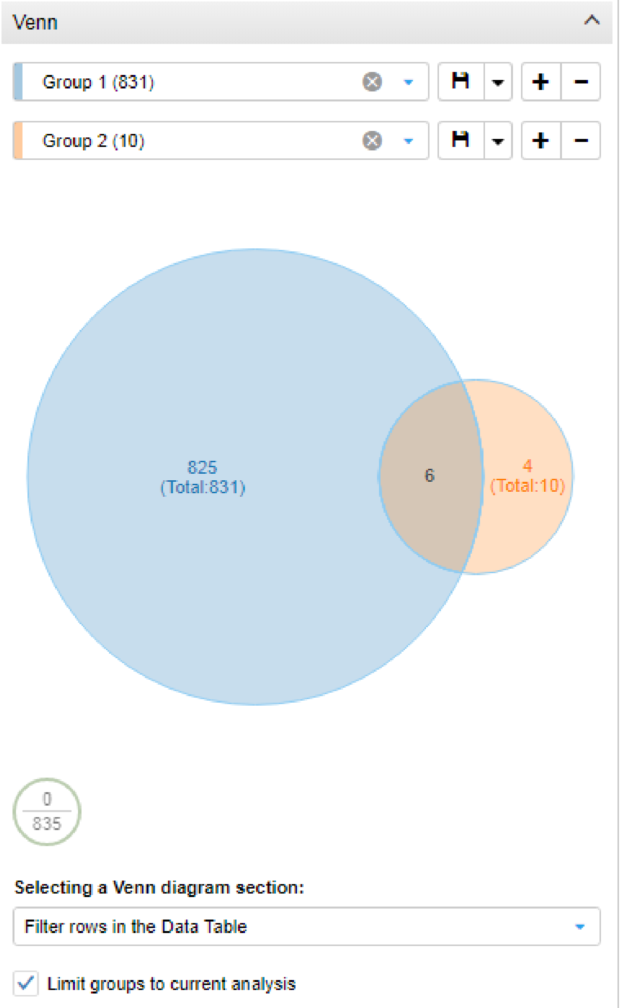


Selecting a Venn diagram section: Filter rows in the Data Table

☑ Limit groups to current analysis

2. From the Select a group drop-down list for the new group select item, search and select another group to include in the Venn diagram.

The Venn diagram will be updated with the new group. Note that the groups are proportionally represented in the Venn diagram.



Selecting a Venn diagram section:

Filter rows in the Data Table

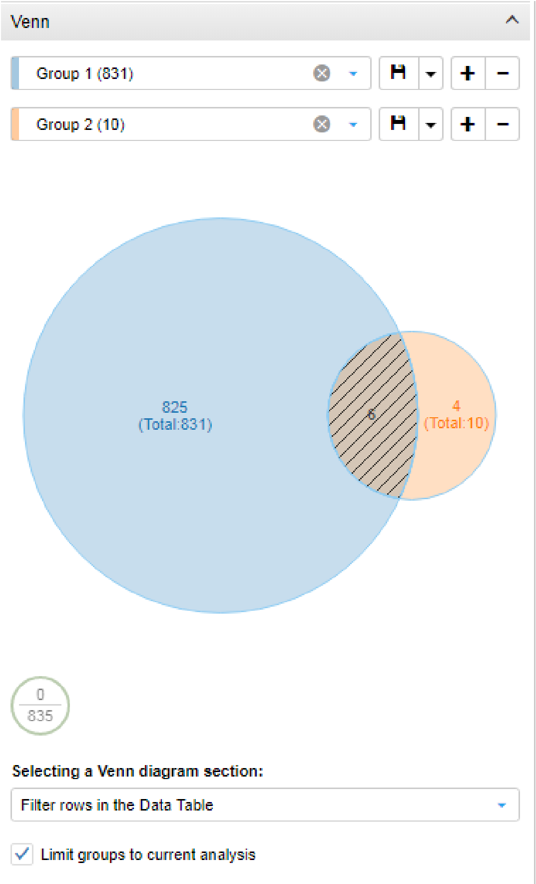
☑ Limit groups to current analysis

Note: A maximum of 5 groups can be added to the Venn diagram.

Understanding the Venn Diagram

The groups are color indicated making it easier for you to identify the groupings in the Venn diagram.

You can click different sections in the Venn diagram. The selected section will be indicated with slashes.



Group 1 (831)

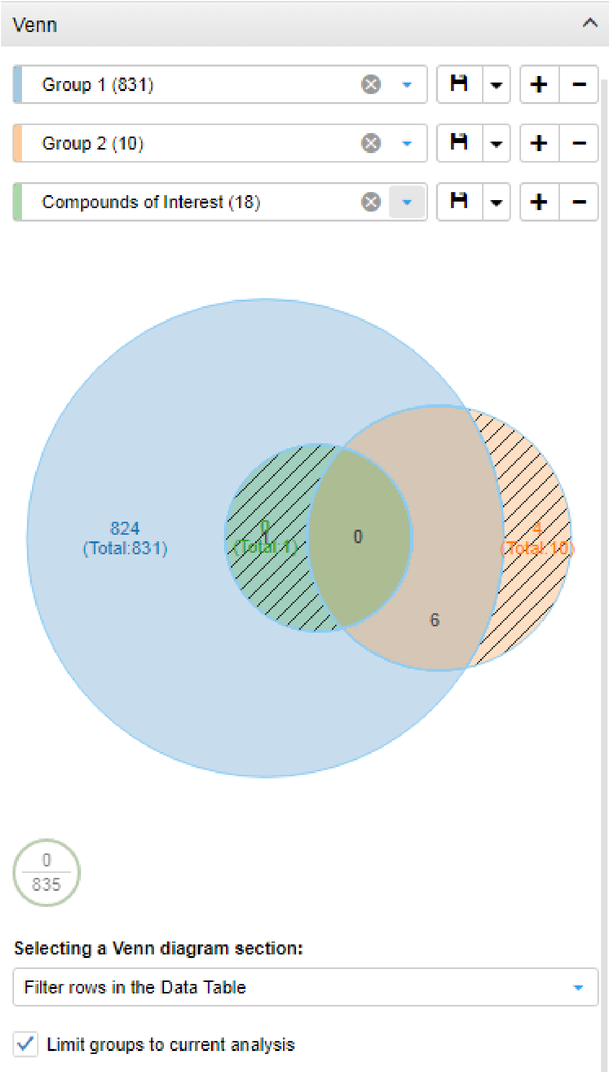
Group 2 (10)

Selecting a Venn diagram section:

Filter rows in the Data Table

☑ Limit groups to current analysis

If you select a section in the diagram, and holding the <Ctrl> key, you can select multiple sections in the diagram, similar to the example shown below.



Group 1 (831)

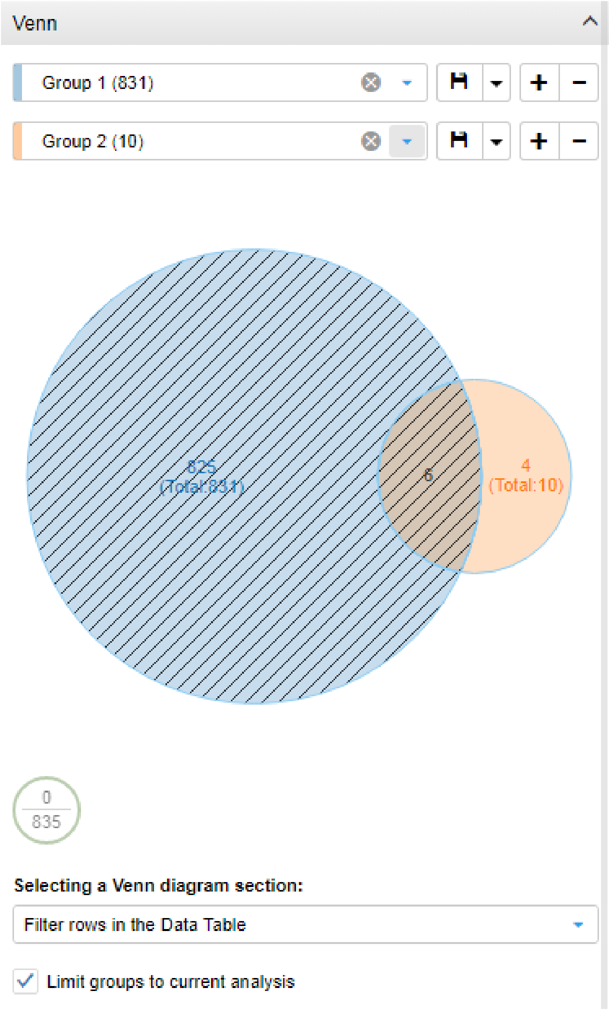
Group 2 (10)

Compounds of Interest (18)

Selecting a Venn diagram section: Filter rows in the Data Table

☑ Limit groups to current analysis

Clicking the label with the total count will select all the sections for the related group, similar to the example shown below. Clicking outside of any of the circles will clear all selections.



Group 1 (831)

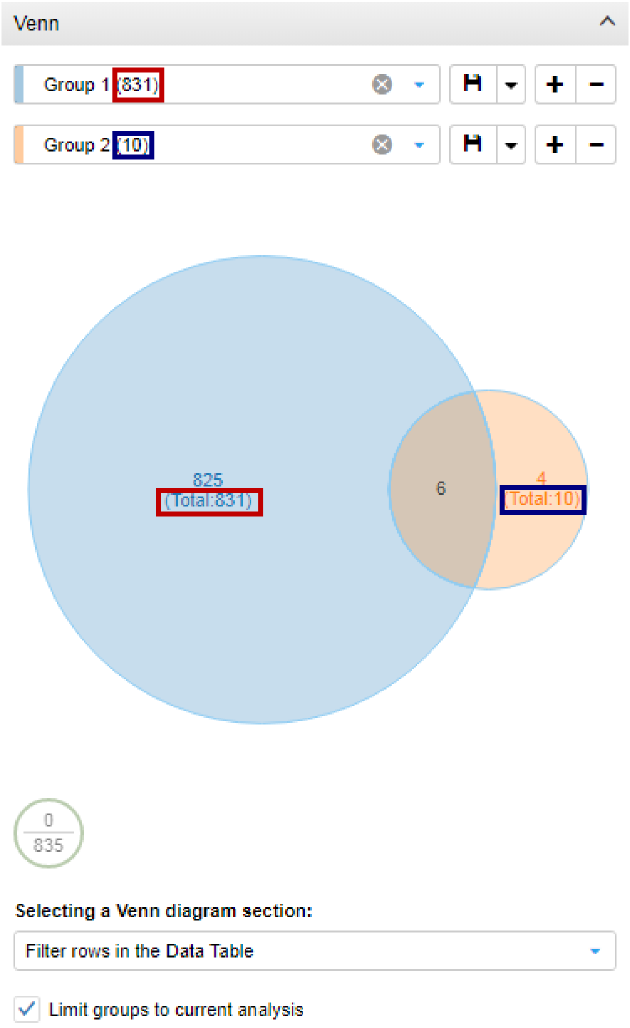
Group 2 (10)

Selecting a Venn diagram section:

Filter rows in the Data Table

☑ Limit groups to current analysis

Labelling of the Venn Diagram



Group 1 (831)

Group 2 (10)

Selecting a Venn diagram section:

Filter rows in the Data Table

☑ Limit groups to current analysis

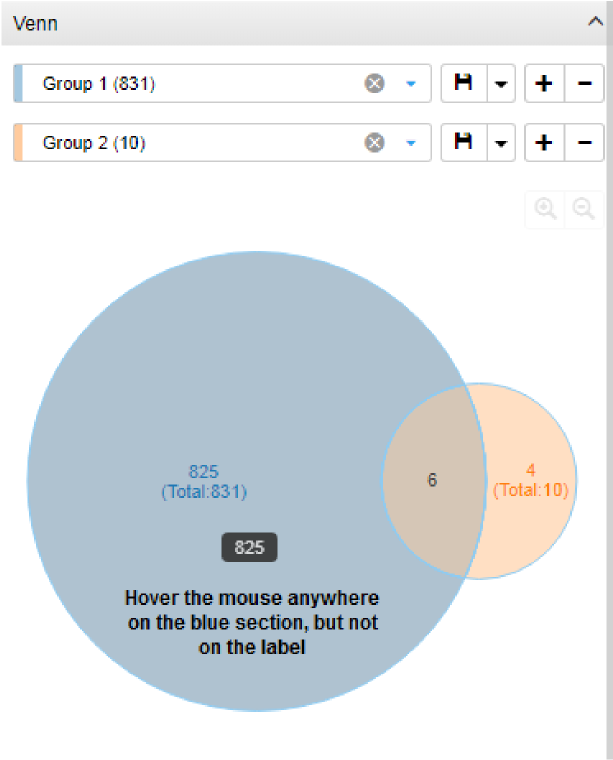
In the Venn diagram shown here, the Venn diagram labelling indicates the following:

- 831 indicates that there are 831 items in Group 1
- 825 indicates that there are 825 items which are **only** in Group 1
- 10 indicates that there are 10 items in Group 2
- 4 indicates that there are 4 items which are **only** in Group 2
- 6 indicates that there are 6 items which are in both Group 1 **and** Group 2

Tooltips

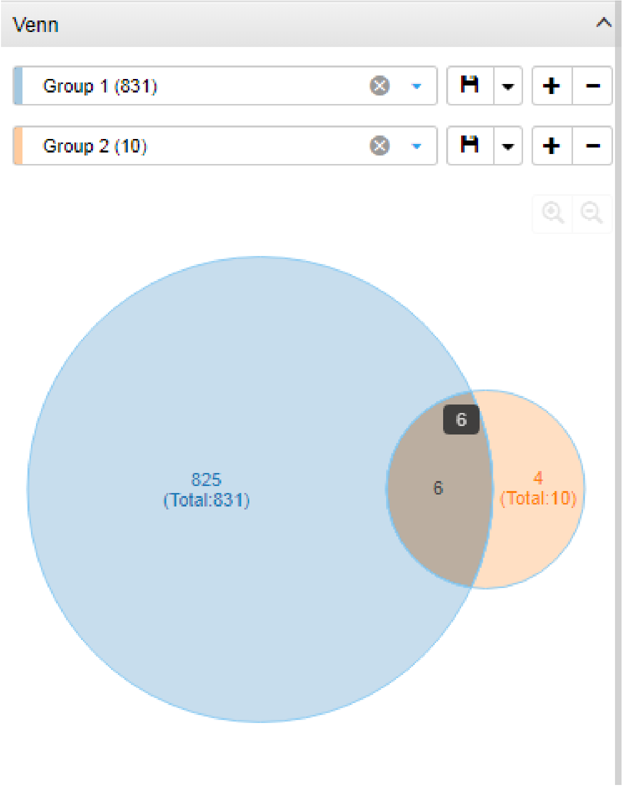
Hovering the mouse over different sections in the Venn diagram will display a tooltip indicating the count of items in the section.

In the example shown here, hover the mouse anywhere on the blue section except directly on the label. The selected section is items ONLY in Group 1. The count in the selected section is 825.

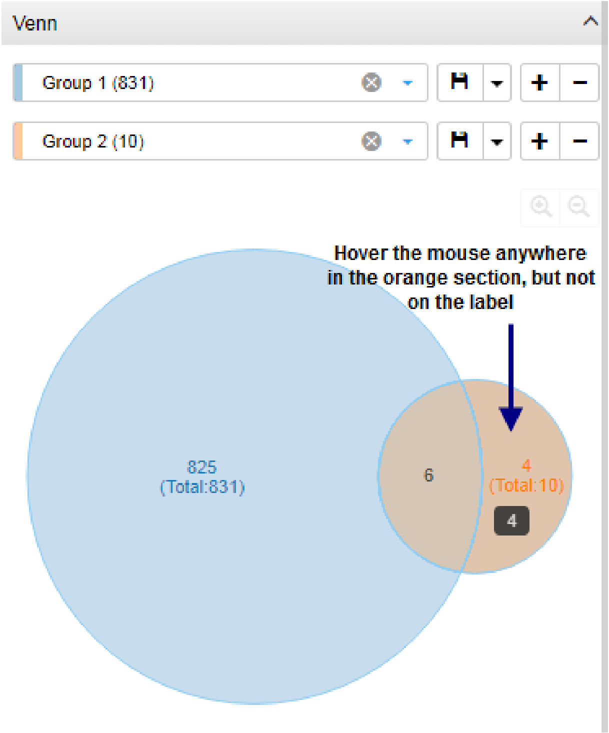


In the example shown here, hover directly over the blue label. The count in the selected section (Group 1) is 831 items.

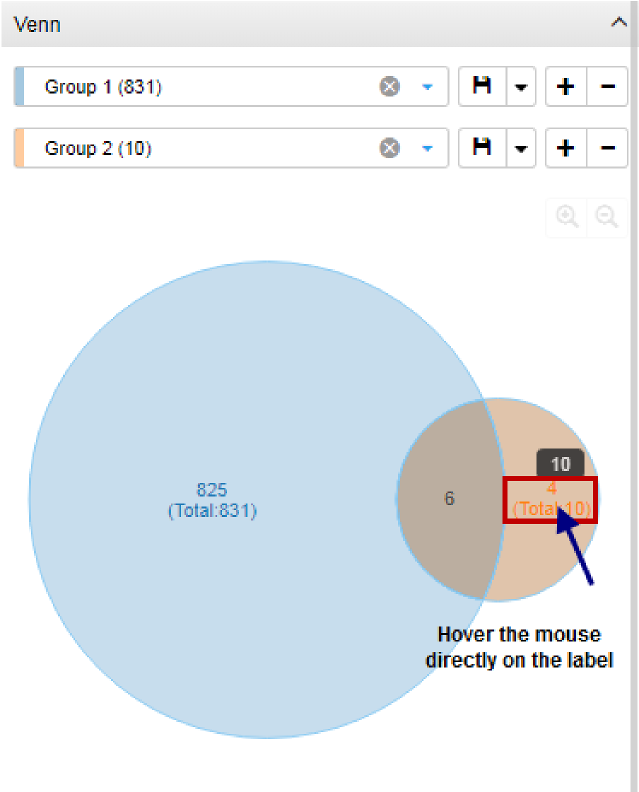
In the example shown here, hover the mouse over the intersection of the two groups. The selected section is the intersection of Group 1 and Group 2. The count in the selected section is 6 items.



Similarly, in the example shown here, hover the mouse anywhere on the orange section except directly on the label. The selected section is items ONLY in Group 2. The count in the selected section is 4.

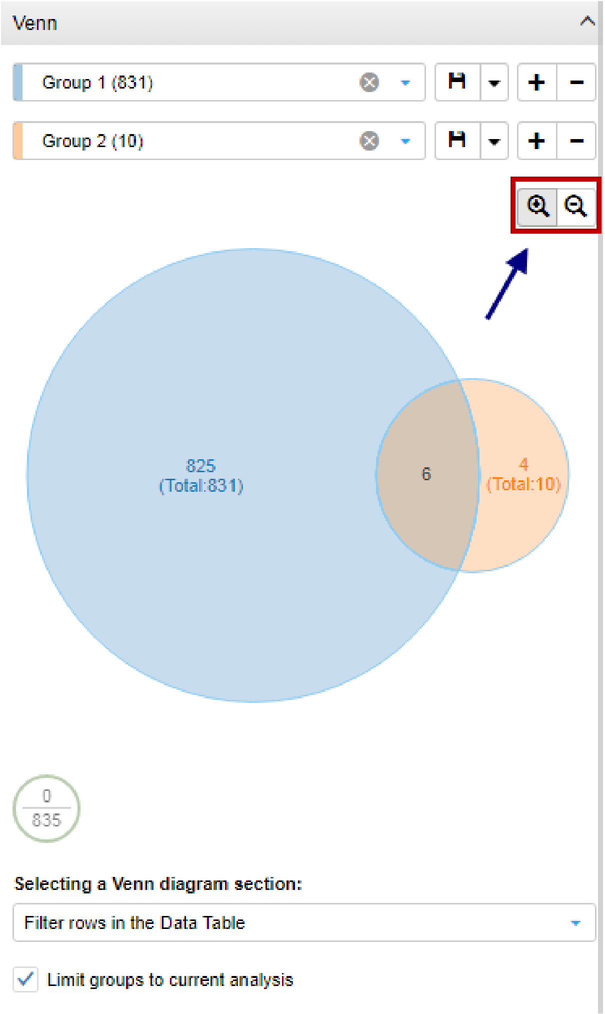


In the example shown here, hover directly over the orange label. The count in the selected section (Group 2) is 10 items.



Zoom In/Zoom Out

Hovering directly below the right corner of the last group select item will display the Zoom in and Zoom out buttons. Using these, you can zoom in to get a closer look at the groupings in the Venn diagram or zoom out to see more of the groupings in the Venn diagram at a reduced size.



Selecting a Venn diagram section:

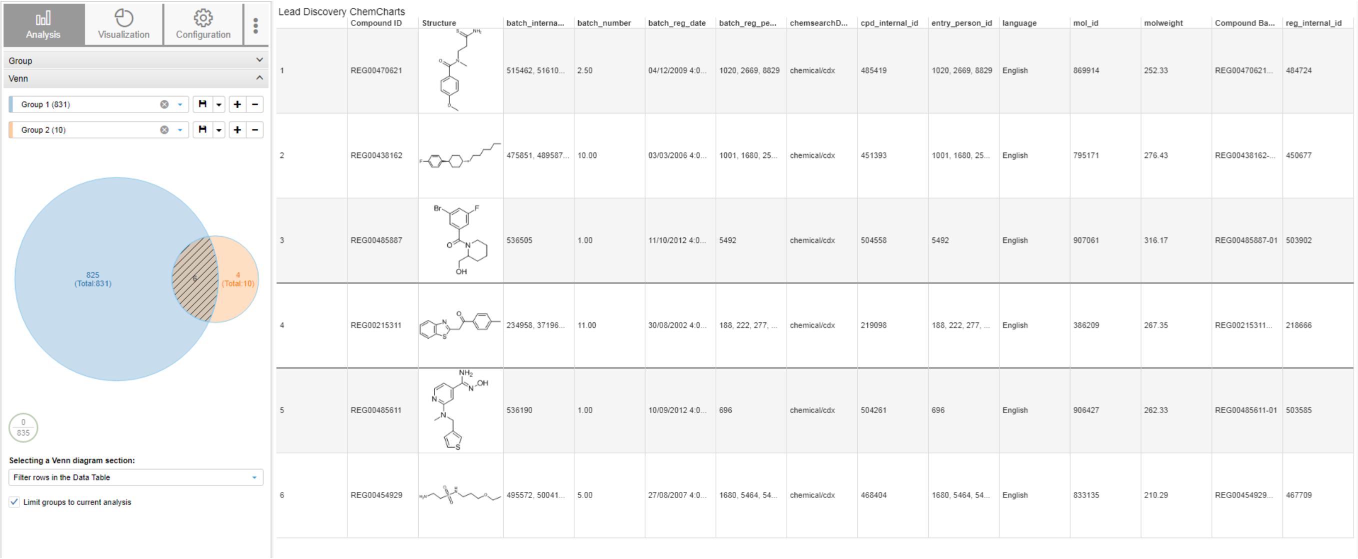
Filter rows in the Data Table

☑ Limit groups to current analysis

Selecting a Venn Diagram section

i. Filter Rows in the Data Table

If you choose ‘Filter Rows in the Data Table’, the visualization displayed in the right panel will only displays the rows in the selected section. In the example below, the user clicks on the intersection of Group 1 and 2 (6 Compounds IDs). In the visualization, the table is filtered to the 6 Compounds IDs in the selected section.



Selecting a Venn diagram section: Filter rows in the Data Table

☑ Limit groups to current analysis

Lead Discovery ChemCharts

	Compound ID	Structure	batch_interna...	batch_number	batch_reg_date	batch_reg_pe...	chemsearchD...	cpd_internal_id	entry_person_id	language	mol_id	molweight	Compound Ba...	reg_internal_id
1	REG00470621		515462, 51610...	2.50	04/12/2009 4:0...	1020, 2669, 8829	chemical/cdx	485419	1020, 2669, 8829	English	869914	252.33	REG00470621...	484724
2	REG00438162		475851, 489587...	10.00	03/03/2006 4:0...	1001, 1680, 25...	chemical/cdx	451393	1001, 1680, 25...	English	795171	276.43	REG00438162-...	450677
3	REG00485887		536505	1.00	11/10/2012 4:0...	5492	chemical/cdx	504558	5492	English	907061	316.17	REG00485887-01	503902
4	REG00215311		234958, 37196...	11.00	30/08/2002 4:0...	188, 222, 277, ...	chemical/cdx	219098	188, 222, 277, ...	English	386209	267.35	REG00215311...	218666
5	REG00485611		536190	1.00	10/09/2012 4:0...	696	chemical/cdx	504261	696	English	906427	262.33	REG00485611-01	503585
6	REG00454929		495572, 50041...	5.00	27/08/2007 4:0...	1680, 5464, 54...	chemical/cdx	468404	1680, 5464, 54...	English	833135	210.29	REG00454929...	467709

ii. Mark rows in the Data Table

Mark rows in the Data Table allow you to see all the data in the current data set and easily identify which compound(s) to add to a given group, and then mark the compound(s) and drag and drop it (or use the right click menu) into the group of interest. Refer to Drag and Drop Marked Rows into a Venn Diagram section and Right Click Menu sections.

Using the same example, if you choose "Mark rows in the data table" and select the intersection of Group 1 and 2 (6 Compound IDs), the visualization displays all data in the current data set and marks the 6 Compounds IDs in the selected section.

Selecting a Venn diagram section: Mark rows in the Data Table

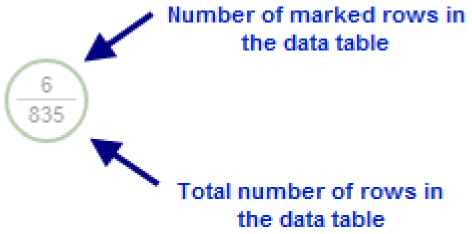
☑ Limit groups to current analysis

Lead Discovery ChemCharts

	Compound ID	Structure	batch_interna...	batch_number	batch_reg_date	batch_reg_pe...	chemsearchD...	cpd_internal_id	entry_person_id	language	mol_id	molweight	Compound Ba...	reg_internal_id
1	REG00452476		491902, 524120	1.50	30/05/2007 4:0...	2771, 288	chemical/cdx	465878	2771, 288	English	826857	199.17	REG00452476...	465184
2	REG00470621		515462, 51610...	2.50	04/12/2009 4:0...	1020, 2669, 8829	chemical/cdx	485419	1020, 2669, 8829	English	869914	252.33	REG00470621...	484724
3	REG00436452		473951, 47595...	9.50	13/02/2006 4:0...	1001, 1080, 168...	chemical/cdx	449665	1001, 1080, 168...	English	791544	260.29	REG00436452...	448949
4	REG00341601		373140, 478651...	2.00	31/01/2004 4:0...	1020, 240, 699	chemical/cdx	352718	1020, 240, 699	English	646176	280.13	REG00341601...	352301
5	REG00484382		534703, 536793	1.50	15/06/2012 4:0...	1020, 288	chemical/cdx	502934	1020, 288	English	903619	252.35	REG00484382...	502238
6	REG00438162		475851, 489587...	10.00	03/03/2006 4:0...	1001, 1680, 25...	chemical/cdx	451393	1001, 1680, 25...	English	795171	276.43	REG00438162-...	450677
7	REG00485887		536505	1.00	11/10/2012 4:0...	5492	chemical/cdx	504558	5492	English	907061	316.17	REG00485887-01	503902

Drag and Drop Marked Rows into a Venn Diagram section

The green circle displayed in the lower left corner of the Venn diagram panel indicates the number of marked rows in the data table and the total count of all rows in the data table.



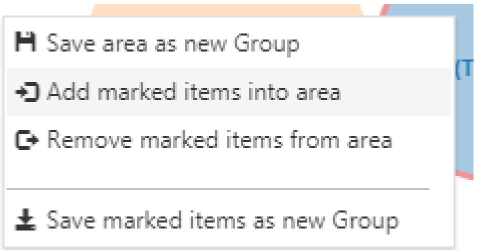
You can drag the green circle and drop it into a section in the Venn diagram. This will add the marked rows to the section.

If the drop is successful, a message will appear indicating that the # of marked rows has successfully been added to the section.

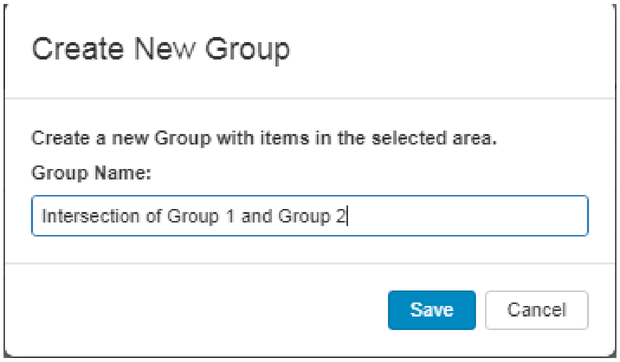
In the case that the selected section is an intersection of multiple groups, the marked rows will be added to each of the groups.

Right Click Menu

When working with sections in the Venn diagram, a right click menu is available for you to add marked items into a selected section, removed marked items from a selected section and save marked items as a new group. In addition, you can save a selected section in the Venn diagram as a new group.



When saving a selected section as a new group, you will be prompted to give the new group a unique name. Click **Save** to save this new group.



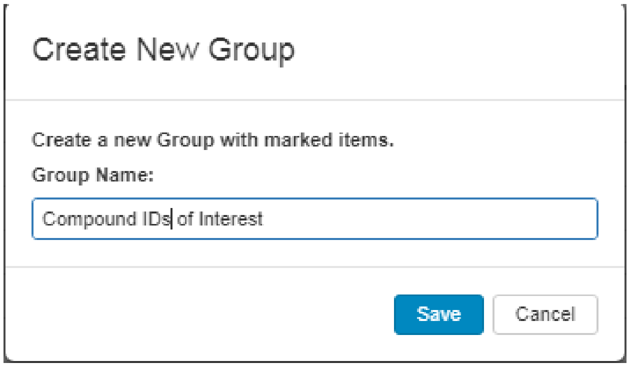
Create New Group

Create a new Group with items in the selected area.

Group Name: Intersection of Group 1 and Group 2

When marked items are added to a section, a message will appear indicating that the # of marked rows has successfully been added to the section. You will also be notified if the marked items already exist in the selected section.

When saving marked items as a new group, you will be prompted give the new group a unique name. Click **Save** to save this new group.



Create New Group

Create a new Group with marked items.

Group Name: Compound IDs of Interest

Limit Groups to current analysis

As noted in the Groups section, there may be the case that a group is selected from the Select a group drop-down list, however not all the compounds in the group are in the current analysis.

In this situation, you have the option to include all items in the group (not dependent on the current data set) in the Venn diagram or limit the group membership in the Venn diagram to only the items in the current data set.

☑ Limit groups to current analysis

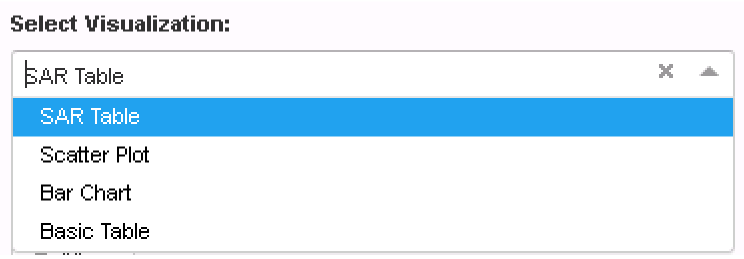
Using the Limit groups to current analysis checkbox, you can set the behavior to suit your requirements.

10.3 Visualizations

From the Select Visualization drop-down list, you can select the Spotfire visualization to view your results. Each visualization is configurable, so you can customize to suit your requirements.

To select a visualization:

1. From the Select Visualization drop-down box, select the visualization that you want to work with. The SAR Table visualization is selected by default.

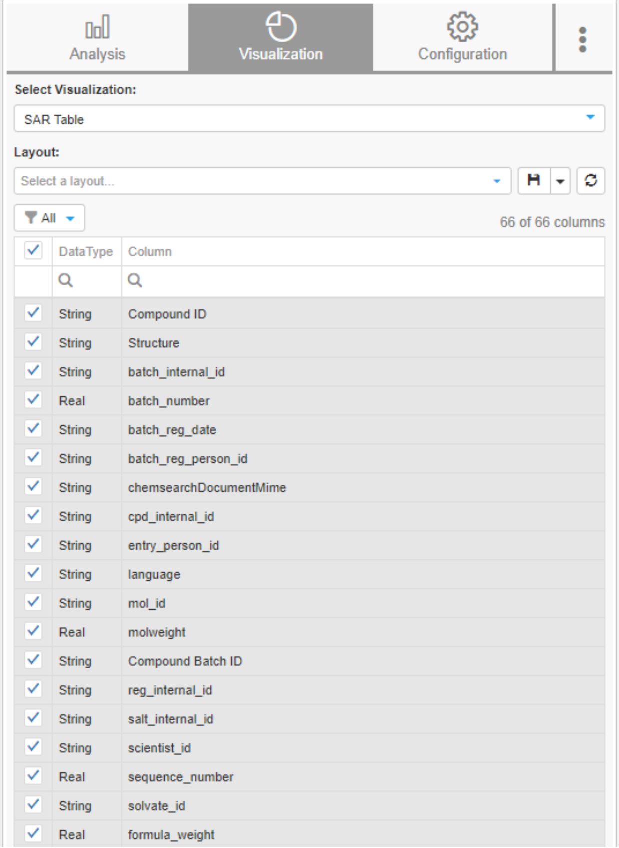


The configuration parameters for each visualization is described in detail below.

10.3.1 SAR Table

Here you can create the SAR table for the ChemCharts table developed in Lead Discovery ChemCharts (Lead Discovery Premium) by selecting the columns to add to the table.

The Column list contains all results (assays and annotations) that were selected in Global Search as well as some pre-defined compound attributes. You can select columns and they will appear in the SAR table in the order selected.



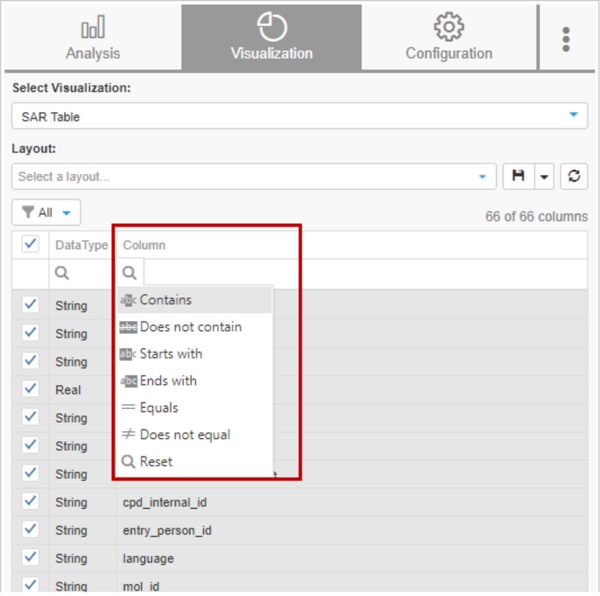
Select Visualization: SAR Table

Layout: Select a layout...

66 of 66 columns

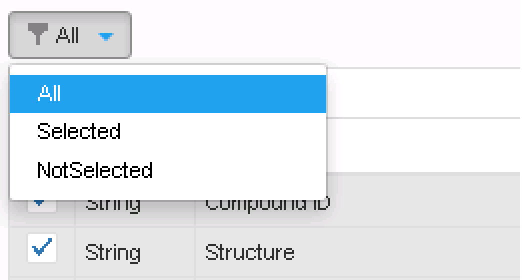
☑	DataType	Column
☑	String	Compound ID
☑	String	Structure
☑	String	batch_internal_id
☑	Real	batch_number
☑	String	batch_reg_date
☑	String	batch_reg_person_id
☑	String	chemsearchDocumentMime
☑	String	cpd_internal_id
☑	String	entry_person_id
☑	String	language
☑	String	mol_id
☑	Real	molweight
☑	String	Compound Batch ID
☑	String	reg_internal_id
☑	String	salt_internal_id
☑	String	scientist_id
☑	Real	sequence_number
☑	String	solvate_id
☑	Real	formula_weight

You can filter the rows to one or more columns. Typing a data type or column in the type-ahead box will bring that data type/column to the top of the list. Query operators are also available to help you find the data types and/or columns of interest.



Left-Click to select a column from the list and Control-Click to single-select one or more individual columns. To select a range of columns, you will need to individually select the desired checkboxes, or use the Control-Click functionality. The Shift-Click operation does not work in this grid.

You can also choose to display All results, Selected results and Not Selected based on the search criteria.



The SAR Table in the panel on the right will be updated as columns are selected/deselected.

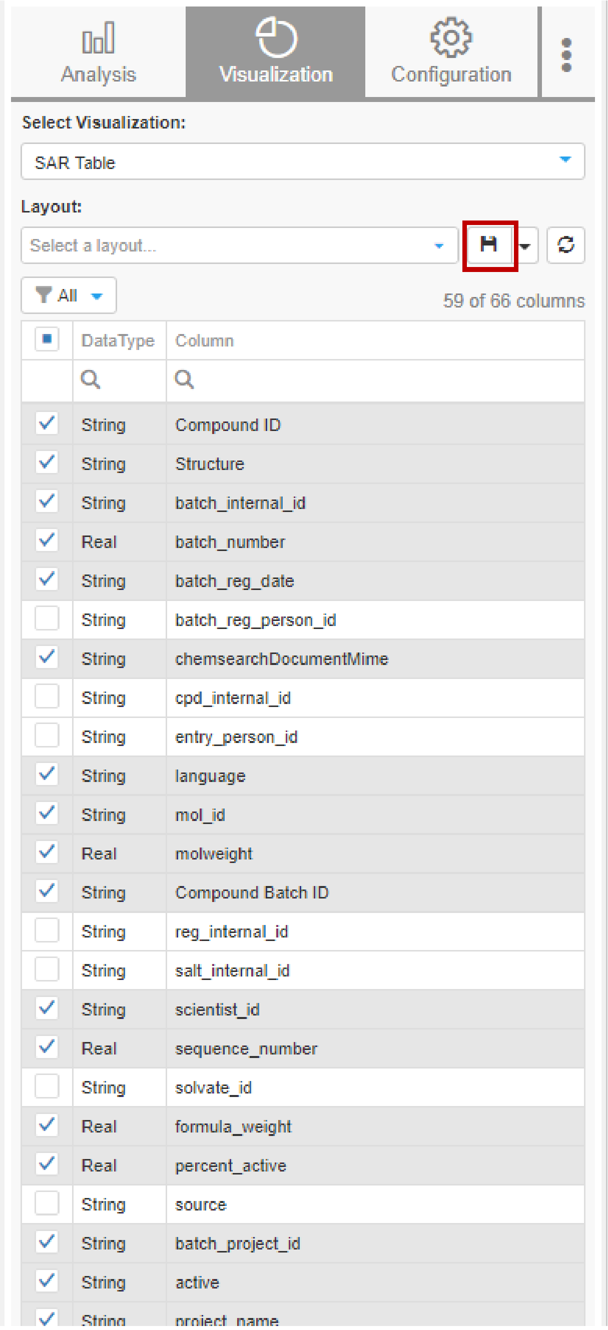
10.3.1.1 Layouts

To make it easier to get an overview of the column filters in the SAR table, you can create filter layouts. Layouts can be assigned a name and saved, and shared between multiple instances of the app.

Permissions can be assigned to a layout. They can be set to private or assigned to a group(s). Groups are retrieved from the Signals Data Factory.

To create a new layout:

1. Filter the columns to include in the layout by checking/unchecking columns in the list of by using a search filter.



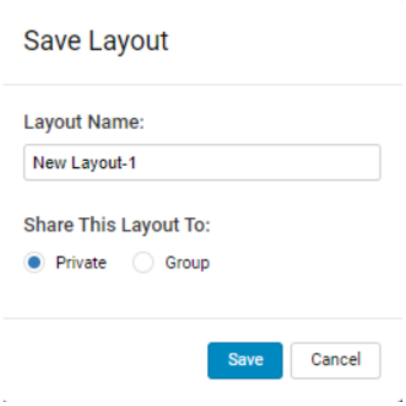
Select Visualization: SAR Table

Layout: Select a layout...

59 of 66 columns

■	DataType	Column
☑	String	Compound ID
☑	String	Structure
☑	String	batch_internal_id
☑	Real	batch_number
☑	String	batch_reg_date
☐	String	batch_reg_person_id
☑	String	chemsearchDocumentMime
☐	String	cpd_internal_id
☐	String	entry_person_id
☑	String	language
☑	String	mol_id
☑	Real	molweight
☑	String	Compound Batch ID
☐	String	reg_internal_id
☐	String	salt_internal_id
☑	String	scientist_id
☑	Real	sequence_number
☐	String	solvate_id
☑	Real	formula_weight
☑	Real	percent_active
☐	String	source
☑	String	batch_project_id
☑	String	active
☑	String	project_name

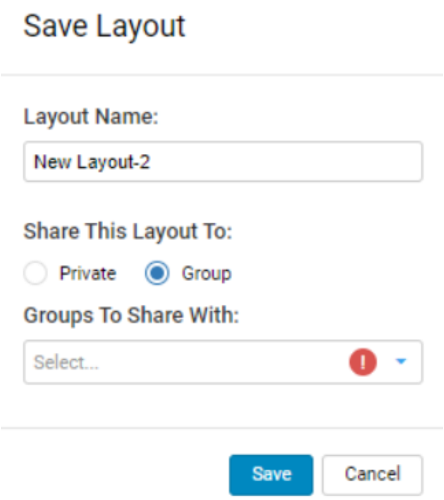
2. Click on the Create new layout based on current selection icon to save the layout. The Save Layout dialog opens.



Layout Name: New Layout-1

3. Enter a unique Layout Name.
4. Specify to Share This Layout to Private or Group. If Group is specified, you can select the group(s) to share with from the drop down list. The list of groups is retrieved from the Signals Data Factory.

Note: Admin users can see all groups. Other users can only see groups they are currently a member of.

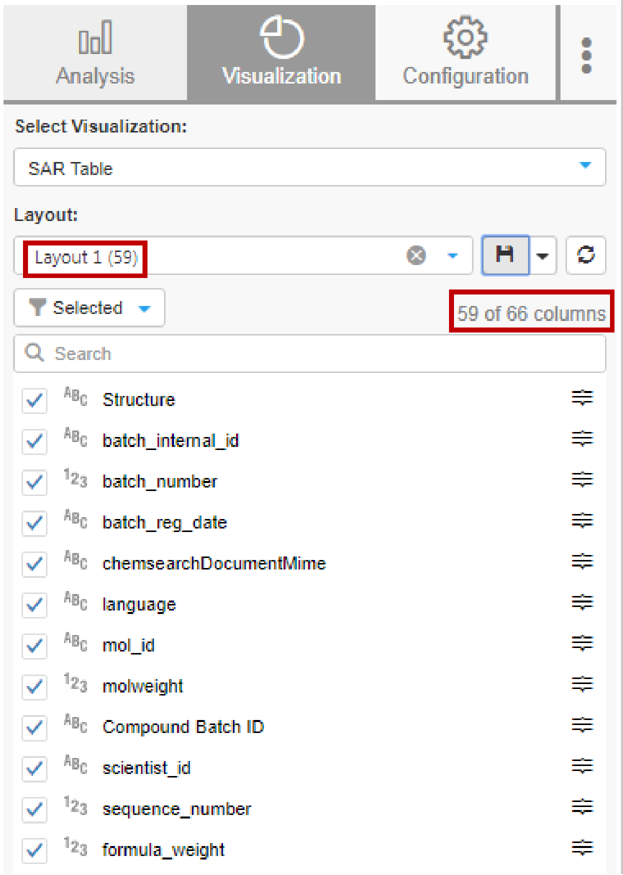


Layout Name: New Layout-2

You must select at least one group to share with.

5. Click **Save**.

The Layout Name displays the number of columns (in parenthesis) in the layout following the Layout Name.

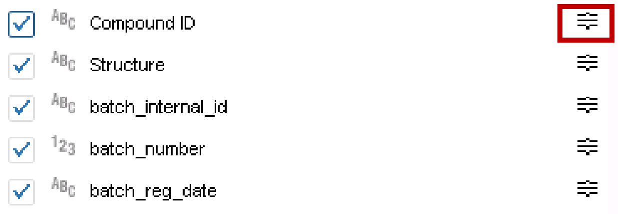


Select Visualization: SAR Table

Layout: Layout 1 (59)

59 of 66 columns

For each layout, you can move columns up and down in the list by dragging and dropping the column using the ≑ When columns are re-ordered, this will be reflected in the pivot SAR Table on the right.



Alternatively, you can access the **Properties > Columns** dialog, and move the columns using native Spotfire functionality. However, this will only affect the column order in the ‘Selected’ view. The ‘All’ and ‘NotSelected’ views will not be updated synchronously.

Using the Layout drop-down list, you can switch between different layouts. Changes made to the layouts will be displayed in the visualization in the panel on the right.

To search and select a layout:

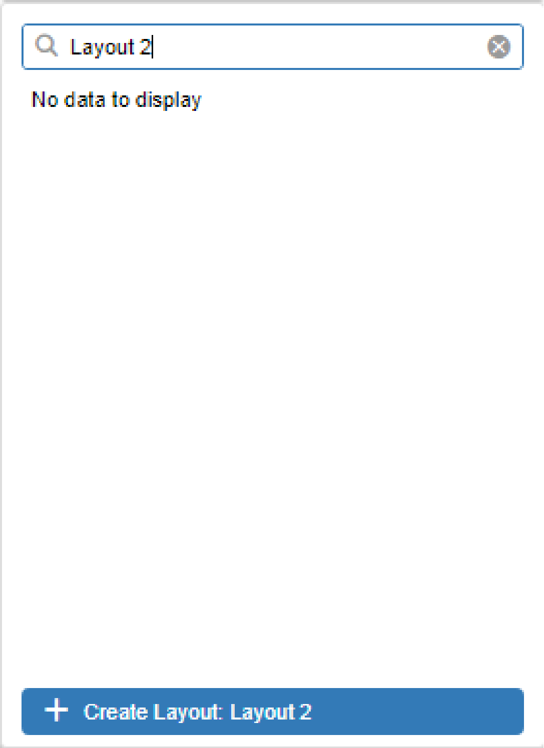
1. From the Select a layout drop-down list, input the layout name in the Search or create edit box to search for the layout. Alternatively, using the up and down arrow keys, you can search for the Layout name in the list.
2. Select the Layout name.

The newly selected layout is reflected in the visualization in the right panel.

To search and create a new layout:

In the case where a search does not locate the layout, you can create an empty layout for this layout name.

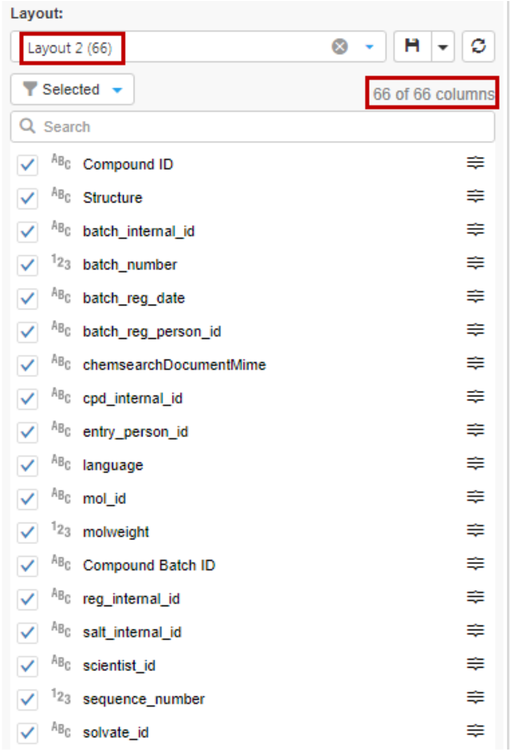
1. From the Select a layout drop-down list, input the layout name in the Search or create edit box to search for the layout. There is no data to display for the specified Layout name.
2. Click on the **+ Create Layout: Layout Name** button.



Layout 2

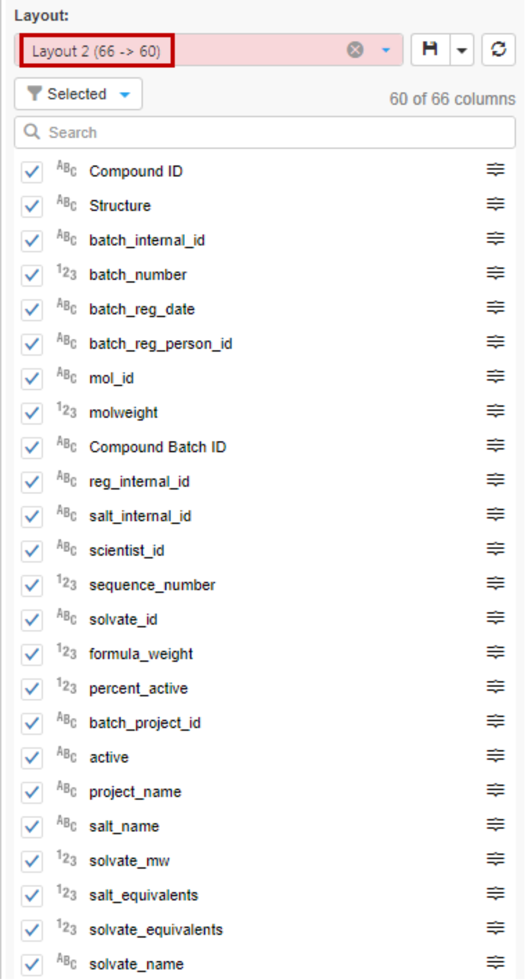
No data to display

By default, all columns will be selected.



☑ Compound ID
☑ Structure
☑ batch_internal_id
☑ batch_number
☑ batch_reg_date
☑ batch_reg_person_id
☑ chemsearchDocumentMime
☑ cpd_internal_id
☑ entry_person_id
☑ language
☑ mol_id
☑ molweight
☑ Compound Batch ID
☑ reg_internal_id
☑ salt_internal_id
☑ scientist_id
☑ sequence_number
☑ solvate_id

3. Uncheck or filter the columns to include in the new layout.



☑ Compound ID
☑ Structure
☑ batch_internal_id
☑ batch_number
☑ batch_reg_date
☑ batch_reg_person_id
☑ mol_id
☑ molweight
☑ Compound Batch ID
☑ reg_internal_id
☑ salt_internal_id
☑ scientist_id
☑ sequence_number
☑ solvate_id
☑ formula_weight
☑ percent_active
☑ batch_project_id
☑ active
☑ project_name
☑ salt_name
☑ solvate_mw
☑ salt_equivalents
☑ solvate_equivalents
☑ solvate_name

4. Click on the Save Layout to database icon to save the new layout.

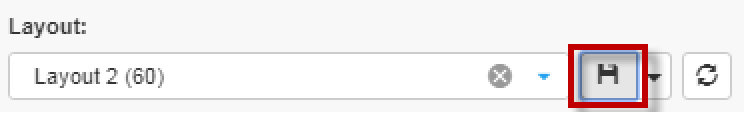
Alternatively, instead of clicking the **+ Create Layout: Layout Name** button to create a new group, you can also hit the Enter key directly in the Search or create edit box to create the new layout.

Total Count and Dirty Flag

A layout is flagged as dirty when changes are made to the layout, and it has not yet been saved again. In the example above, Group 2 had 66 columns when first created. Six columns were removed from Layout 2.
The layout is flagged as dirty (pink background) until the layout is saved.

Also, as changes are made to the current layout, the current total number of columns in the layout is displayed, as well as the original total number of columns in the layout with a "->" sign between the two counts. For example, (66 -> 60) indicates that initially the layout has 66 columns, however now it has changed, and the current number of columns in the layout is 60.

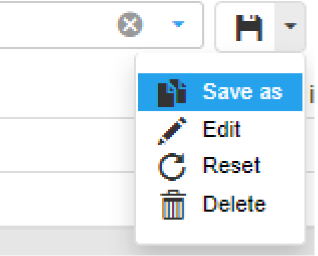
Once the Save layout to database 💾 icon is clicked, the layout is no longer flagged as dirty.



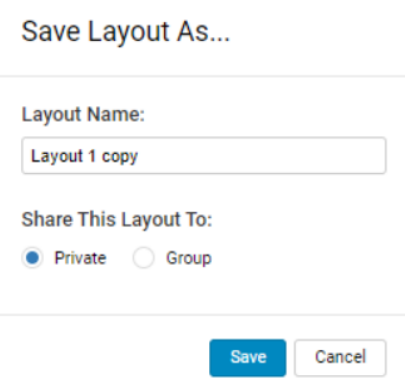
Layout: Layout 2 (60)

To save as a new layout:

1. Filter the columns to include in the layout.
2. From the Save Layout to database drop-down menu select **Save As.**



The Save Layout As dialog opens.



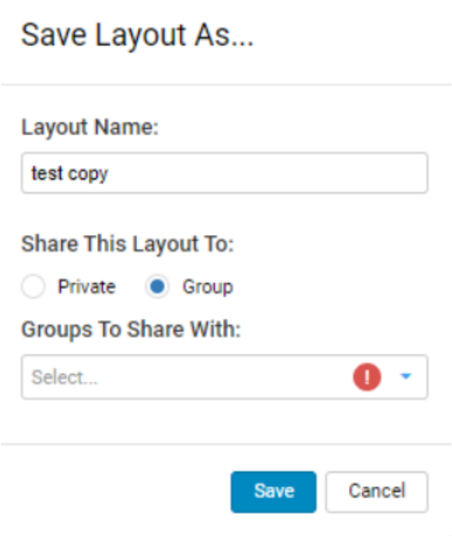
Save Layout As...

Layout Name: Layout 1 copy

Share This Layout To: ● Private ○ Group

3. By default, the layout name will a copy of the selected layout name. You can enter a new unique name for the layout.
4. Specify to Share This Layout to Private or Group. If Group is specified, you can select the group(s) to share with from the drop-down list. The list of groups is retrieved from the Signals Data Factory.

Note: Admin users can see all groups. Other users can only see groups they are currently a member of.



Save Layout As...

Layout Name: test copy

Share This Layout To: ○ Private ● Group

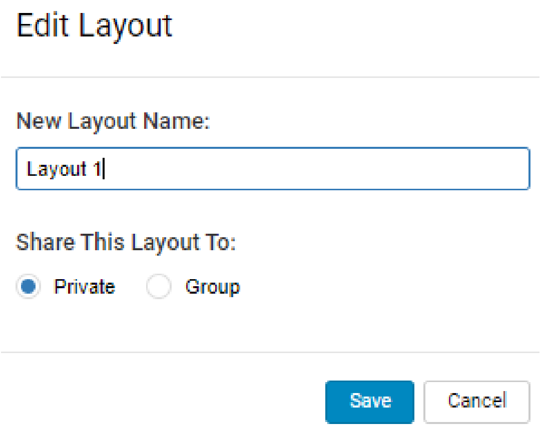
Groups To Share With: Select...

You must select at least one group to share with.

5. Click **Save**. The new layout will be appended to the Layout drop-down list.

To rename a layout:

1. From the Save Layout to database drop-down menu, select **Edit** to open the Edit Layout window**.**
2. Enter a new name for the layout.



Edit Layout

New Layout Name: Layout 1

Share This Layout To: ● Private ○ Group

3. Click **Save.**

Note: Only the administrator or the user who created the layout can rename the layout.

To reset a layout:

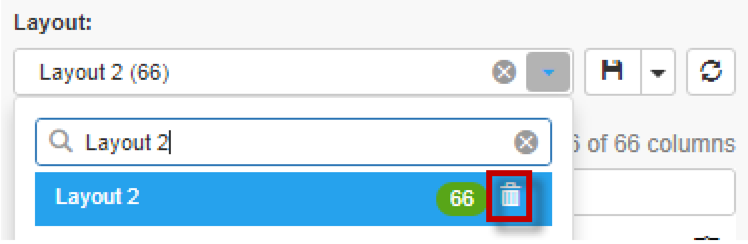
If a layout is flagged as ‘’dirty, you can reset the layout to its original filter.

1. From the Save Layout to database drop-down menu, select **Reset**. You will be prompted to confirm the Reset operation.

To delete a layout:

1. From the Save Layout to database drop-down menu, select **Delete**. You will be prompted to confirm the Delete operation.

You can also delete a layout directly from the Select a layout drop-down list, by selecting the 🗑 Delete icon next to the selected layout name.



Note: Only the administrator or the user who created the layout can delete the layout.

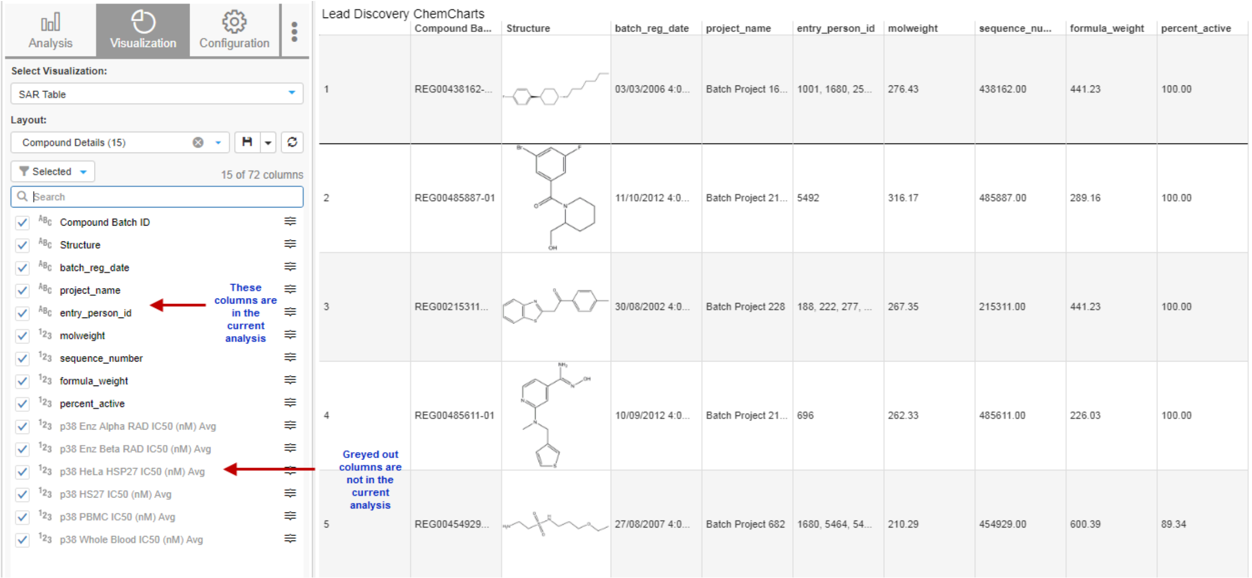
To refresh the list of layouts:

The Refresh ⟳ button will refresh the Layout drop-down list. This is useful in the case where two users are working with the SAR app. For example, one user may have created a new layout, however this new layout will not be visible to the second user until the Refresh button is clicked.

Layouts in Current Analysis

There may be the case that a layout is selected from the Select a layout drop-down list, however not all the columns in the layout are in the current analysis.

In the example shown below, the Compound Details layout is selected. This layout has 72 columns. However, of the 72 columns in the layout, there are only 15 columns in the current analysis. In this case, the columns in the layout that are not in the current analysis are greyed out.



Select Visualization: SAR Table

Layout: Compound Details (15)

Selected — 15 of 72 columns

Search

- ☑ Compound Batch ID
- ☑ Structure
- ☑ batch_reg_date
- ☑ project_name
- ☑ entry_person_id
- ☑ molweight
- ☑ sequence_number
- ☑ formula_weight
- ☑ percent_active
- ☑ p38 Enz Alpha RAD IC50 (nM) Avg
- ☑ p38 Enz Beta RAD IC50 (nM) Avg
- ☑ p38 HeLa HSP27 IC50 (nM) Avg
- ☑ p38 HS27 IC50 (nM) Avg
- ☑ p38 PBMC IC50 (nM) Avg
- ☑ p38 Whole Blood IC50 (nM) Avg

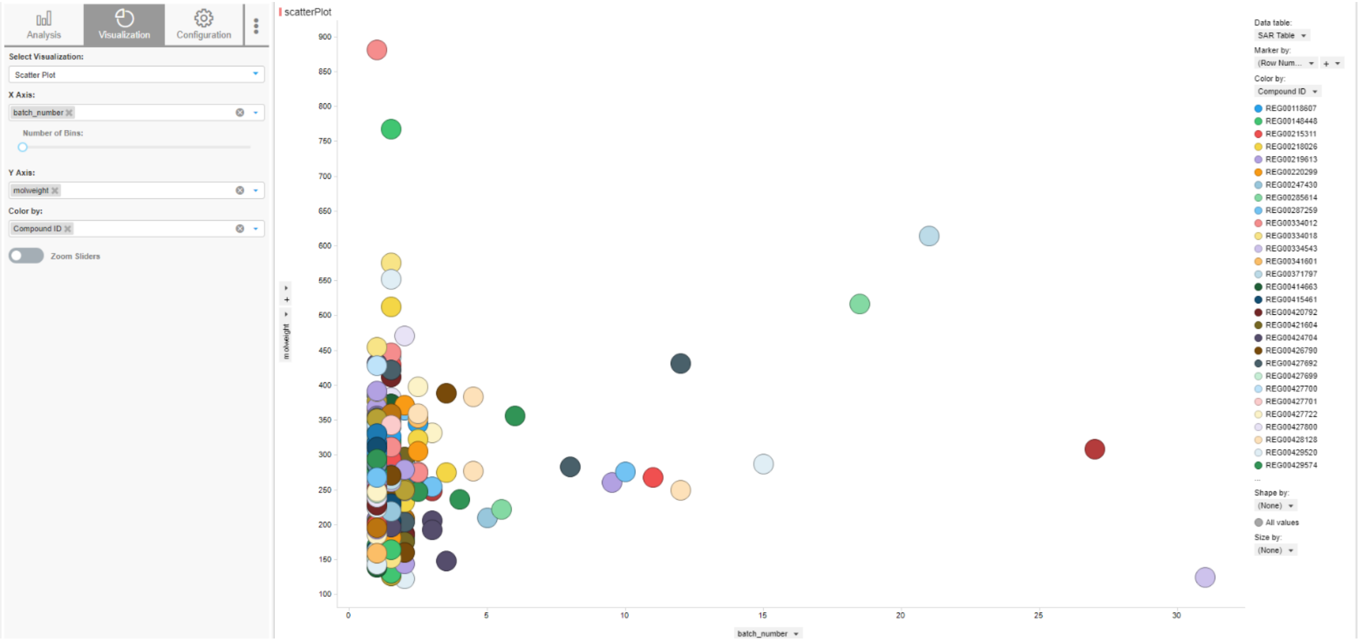
Lead Discovery ChemCharts

	Compound Ba...	Structure	batch_reg_date	project_name	entry_person_id	molweight	sequence_nu...	formula_weight	percent_active
1	REG00438162-...		03/03/2006 4:0...	Batch Project 16...	1001, 1680, 25...	276.43	438162.00	441.23	100.00
2	REG00485887-01		11/10/2012 4:0...	Batch Project 21...	5492	316.17	485887.00	289.16	100.00
3	REG00215311...		30/08/2002 4:0...	Batch Project 228	188, 222, 277, ...	267.35	215311.00	441.23	100.00
4	REG00485611-01		10/09/2012 4:0...	Batch Project 21...	696	262.33	485611.00	226.03	100.00
5	REG00454929...		27/08/2007 4:0...	Batch Project 682	1680, 5464, 54...	210.29	454929.00	600.39	89.34

Layouts will always include the column in the layout even if it is not in the current analysis unless you manually uncheck a greyed-out column (column that is not in the current analysis) and then save the layout.

10.3.2 Scatter Plot

Here you can configure an intuitive Scatter Plot used for correlating columns of data that have been downloaded.



Select Visualization: Scatter Plot

X Axis: batch_number

Number of Bins:

Y Axis: molweight

Color by: Compound ID

Zoom Sliders

Data table: SAR Table

Marker by: (Row Num...

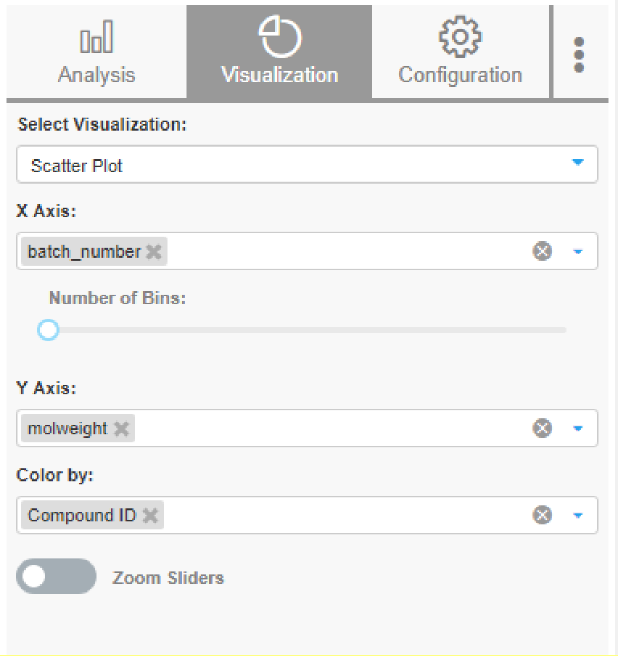
Color by: Compound ID

Shape by: (None)

Size by: (None)

All the results (assays and annotations) that were selected in the Global Search tab will appear in this SAR Table column list as well as a few pre-defined compound attributes. Key features include selectable X, and Y Axes and Color By option. Using the Number of Bins slider, the X axis can be configured to use binned data.

Zoom Sliders can be used to focus in on regions of interest within a plot. Turning on the Zoom Sliders toggle will add a zoom slider along both the X and Y axis. You can now grab the slider and drag it to the left of right to pan horizontally along the X axis, top to bottom to pan vertically along the Y axis.



Select Visualization: Scatter Plot

X Axis: batch_number

Number of Bins:

Y Axis: molweight

Color by: Compound ID

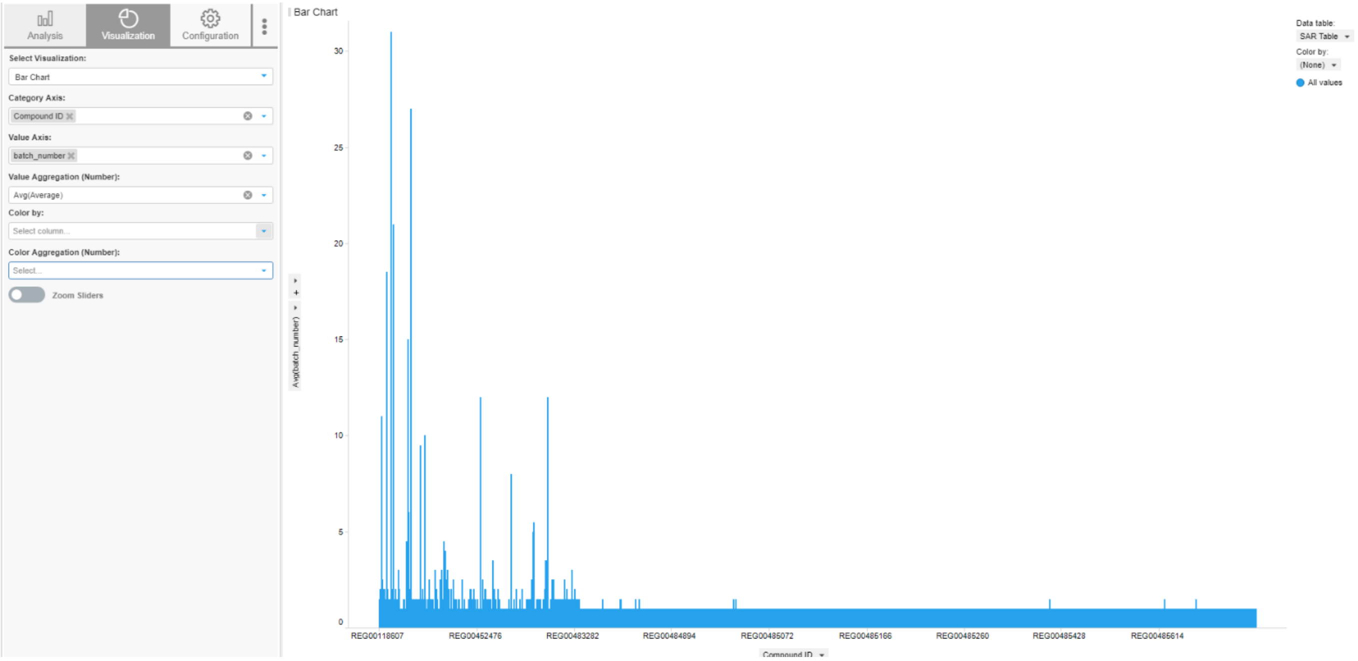
Zoom Sliders

Hovering the mouse cursor over a point in the scatter plot will display a tooltip showing the compound structure as well as any related data used to position that point in the plot. Left-clicking a point in the scatter plot will present a label with the image of that structure. Lassoing multiple points will display all the selected structures' images and allow you to drag the structure label to different positions in the display.

Note: Refer to the ***"Scatter Plot"*** topic of the Spotfire online help for additional information on this functionality.

10.3.3 Bar Chart

Here you can configure an intuitive Bar Chart (which acts as a histogram when numeric attributes are selected). This view is used for viewing the distribution of columns of data that have been downloaded.



Select Visualization: Bar Chart

Category Axis: Compound ID

Value Axis: batch_number

Value Aggregation (Number): Avg(Average)

Color by: Select column...

Color Aggregation (Number): Select...

Zoom Sliders

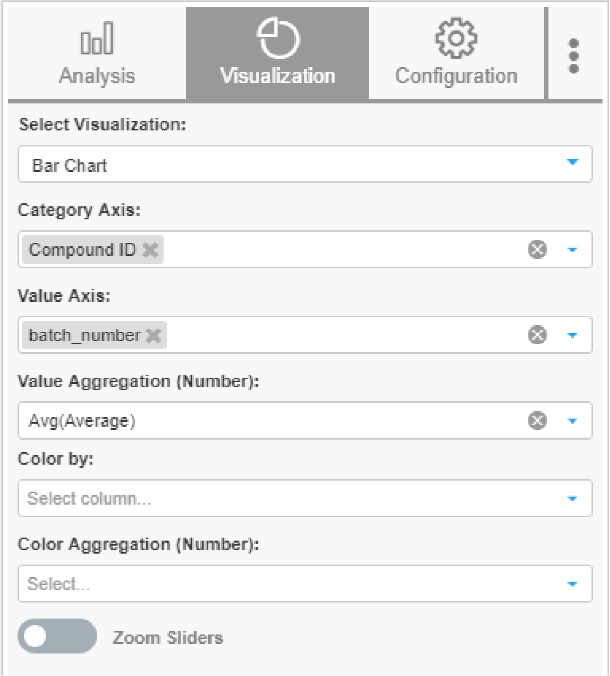
Data table: SAR Table

Color by: (None)

All the results (assays and annotations) that were selected in the Global Search tab will appear in this SAR Table column list as well as a few pre-defined compound attributes. Key features include selectable Category, Value and Color Axis as well as Value Aggregation and Color Aggregation.

Note: Refer to the ***"Bar Chart"*** topic of the Spotfire online help for additional information on this functionality.

Zoom Sliders can be used to get a closer look at details in the bar chart. Turning on the Zoom Sliders toggle will add a zoom slider along both the X and Y axis. You can now grab the slider and drag it to the left of right to pan horizontally along the X axis, top to bottom to pan vertically along the Y axis.



Select Visualization: Bar Chart

Category Axis: Compound ID

Value Axis: batch_number

Value Aggregation (Number): Avg(Average)

Color by: Select column...

Color Aggregation (Number): Select...

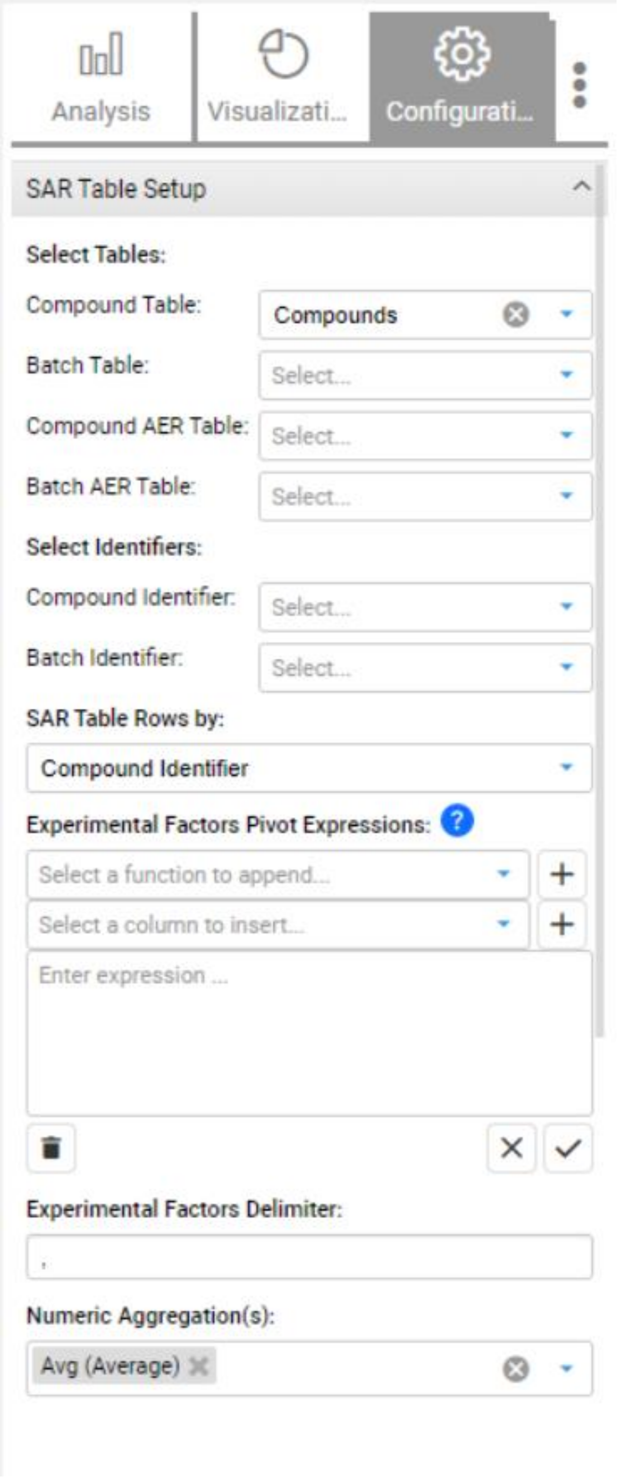
10.3.4 Basic Table

Here you can create the SAR table for the standard Spotfire data table by selecting the columns to add to the table.

Refer to the SAR Table section for information on creating or selecting a layout for the Basic Table.

10.4 Configuration

The Configuration tab allows you to configure the default SAR Table Setup as well as column aliases.



Select Tables:

Compound Table: Compounds

Batch Table: Select...

Compound AER Table: Select...

Batch AER Table: Select...

Select Identifiers:

Compound Identifier: Select...

Batch Identifier: Select...

SAR Table Rows by: Compound Identifier

Experimental Factors Pivot Expressions:

Select a function to append...

Select a column to insert...

Enter expression ...

Experimental Factors Delimiter: ,

Numeric Aggregation(s): Avg (Average)

10.4.1 SAR Table Setup

Select Tables:

The SAR table can be generated based on compound and batch results. Here you can define the Compound Table, Batch Table, Compound AER Table and Batch AER Table to be used to generate the SAR Table.

Select Identifiers:

Here you can specify which columns from Compound and Batch tables could be used as the identifiers (e.g. Compound ID, Compound Batch ID) to define the rows in the SAR table.

SAR Table Rows by:

The value of the "SAR Table Rows by" will identify the key column of the SAR Table. There are two selections available:

- Compound Identifier – the Compound ID column will be used to distinguish the SAR table rows.
- Batch Identifier – the Batch ID column will be used to distinguish the SAR table rows.

Validation errors are displayed to assist in proper selection of tables and identifiers.

Experiment Factor Pivot Expressions

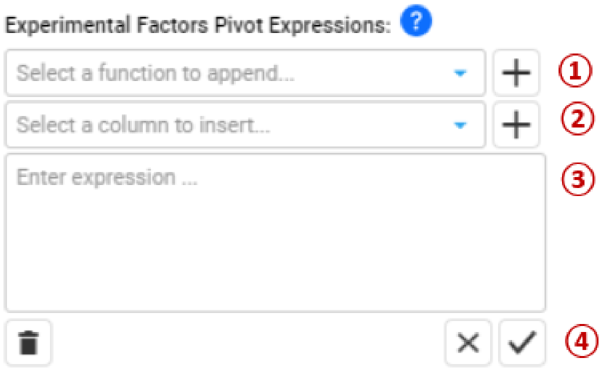
Here you can include one or more Experiment Factors in the pivot of data from the Batch/Compound Assay Endpoint Results.

In several cases, particularly in ADMET, one of the Experimental Factors will likely be a numeric value, most commonly Test Concentration, and because of experimental variability the determined Test Concentration will have experimental variability to it, resulting in small differences in the number from the target number (e.g. a concentration of 0.99nM when the target concentration is 1.0nM).

In defining the pivot to the SAR table, by default those will be pivoted into different SAR Table columns (e.g. "Result for 0.99nM", "Result for 1.0nM", etc., but the desired outcome is that they be pivoted into a single column (e.g. "Result for ~1.0nM")

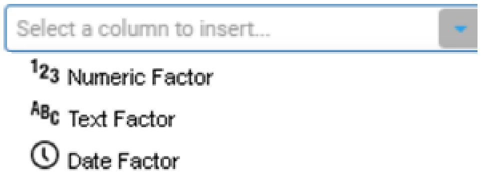
Using the Experiment Factor Pivot Expressions, you can define binned ranges on numeric Experimental Factors (e.g. Concentration) such that small difference in the Experimental Factors would be grouped together (e.g. 0.99 and 1.0 could be grouped into "1").

The expression editor has two modes: View and Edit. Click on the 'Enter expression' text area of the control to enter edit mode.



The ‘Select’ a function to append’ dropdown lists the Spotfire functions for [Binning] and [Logical]. Refer to the Binning functions and Logical functions sections respectively in the Spotfire User’s Guide for more information.

The ‘Select a column to insert’ drop-down lists the intersection columns of the Compound Assay Endpoint Results table and the Batch Assay Endpoint Results table. The internal reserved columns such as [Compound ID], [h1], [h2], [h3], [measurement type], [isnumeric] etc, have been removed.



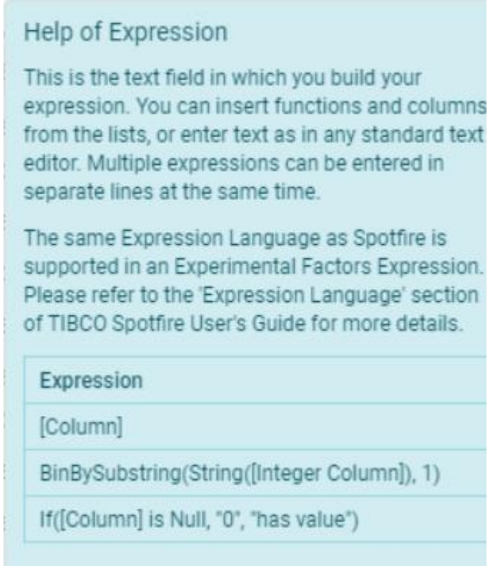
The ‘Enter Expression’ field allow you to edit an expression manually.

To build Experimental Factors Pivot Expressions:

1. Select a function and insert into the expression.
2. Select a column and insert into the expression.
3. Using the Expression editor, you can edit the expression manually.
4. Once the expression is built, you can click on the ✓ **Validate and apply expression** button.

After clicking the Validate and apply expression button, the SAR Analysis app will validate the expression. If there are errors, the expression will remain in edit mode, and the errors will be displayed.

The usage of the expression is described in a help page. You can open the Help dialog it by clicking the ? icon.



Help of Expression

This is the text field in which you build your expression. You can insert functions and columns from the lists, or enter text as in any standard text editor. Multiple expressions can be entered in separate lines at the same time.

The same Expression Language as Spotfire is supported in an Experimental Factors Expression. Please refer to the 'Expression Language' section of TIBCO Spotfire User's Guide for more details.

Expression
[Column]
BinBySubstring(String([Integer Column]), 1)
If([Column] is Null, "0", "has value")

To rename the experimental factors pivot:

The Experimental Factor name can be added to the new column headers.

By default, the name for the new column header is: [Endpoint name], Exp factor. Renaming the column to include the name of the experimental factor can be accomplished by using ‘concatenate’. For example,

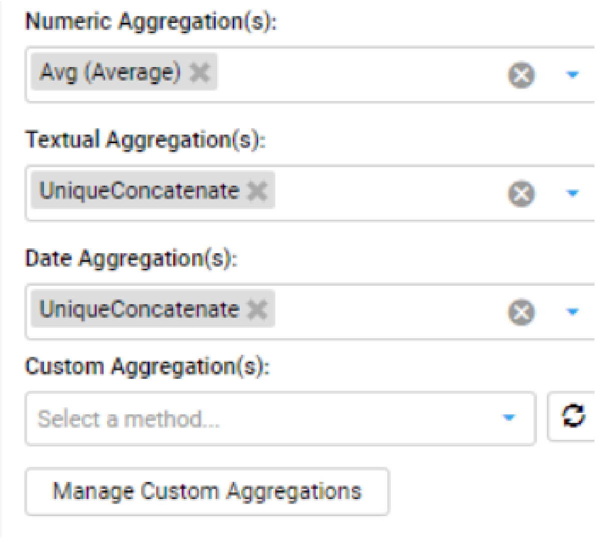
Concatenate('[Experimental Factor]: ', [Experimental Factor])

Experimental Factors Delimiter

Here you can specify the delimiter to separate the result name and the pivoted experimental factor values.

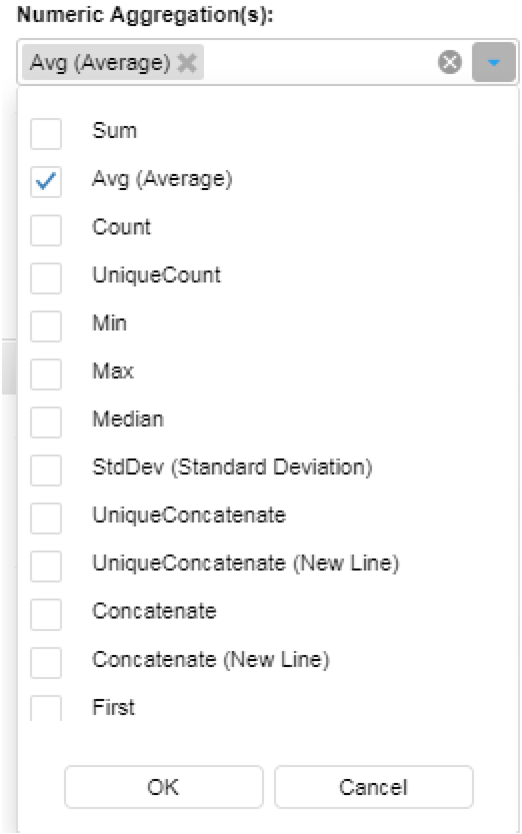
Aggregations

You can define how the assay endpoints should be pivoted and aggregated (e.g. Average, Min, Max, Median etc.). By default, one aggregation is assigned to each endpoint.



Note: The Concatenate and UniqueConcatenate aggregations will use the comma (,) as the separator when concatenating the values. If you prefer to use the New Line as the separator, you can choose the Concatenate (NewLine) and UniqueConcatenate(NewLine) aggregations. In certain cases, some performance degradation is to be expected.

Using the drop-down control for each aggregation, you can add multiple aggregations by enabling the checkbox and clicking **OK**.


Numeric Aggregation(s):
Avg (Average)

☐ Sum
☑ Avg (Average)
☐ Count
☐ UniqueCount
☐ Min
☐ Max
☐ Median
☐ StdDev (Standard Deviation)
☐ UniqueConcatenate
☐ UniqueConcatenate (New Line)
☐ Concatenate
☐ Concatenate (New Line)
☐ First

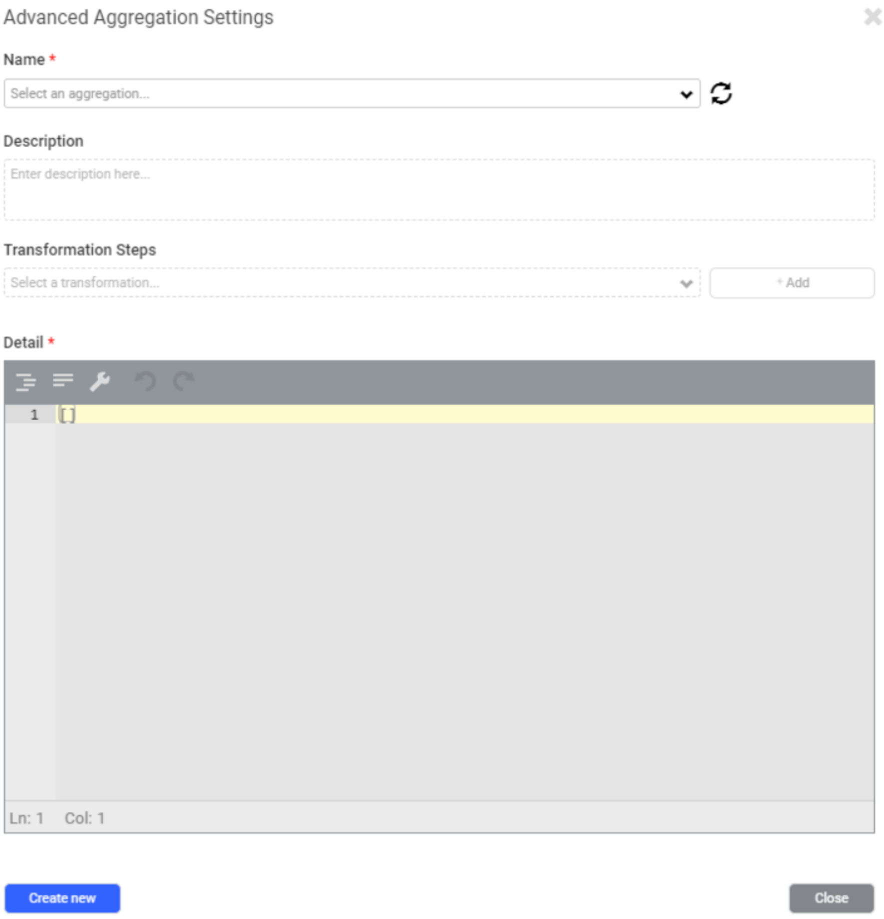
Custom Aggregations

Custom aggregations allows users to customize how data is transformed and the SAR table is formed by using the standard Spotfire transformation steps. This allows the user to have more control over the data transformation.

Each custom aggregation consists of one or more transformation steps. A transformation step is an operation applied on the SAR Table generated by the SAR Analysis App that performs a particular data transformation job. Some of these built-in transformation steps have the same name and functionality as those data transformations offered by Spotfire. Other transformation steps are actually pre-defined templates which by themselves consist of multiple transformation steps to perform more complex data transformation tasks.

Manage Custom Aggregations

Clicking on the **Manage Custom Aggregations** button will open the Advanced Aggregation Settings window similar to the example shown below. From here, you can edit previously defined custom aggregations or create new ones.



The Name drop-down list contains the names of all previously saved custom aggregation methods. A name can be entered in the Name field or you can use the type ahead to search for the name.

By default, the SAR Analysis app comes with four pre-defined templates to help you create your aggregations on the fly:

- **Avg +- StdDev**: Aggregate the result value by both Avg and StdDev methods and combine the aggregated result with +/- sign
- **Avg +- StdDev (Count)**: Aggregate the result value by both Avg and StdDev methods and combine the aggregated result with +/- sign, followed by the number of results being aggregated
- **Avg +- StdDev (Range, Count)**: Aggregate the result value by both Avg and StdDev methods and combine the aggregated result with +/- sign, followed by both the range and number of results being aggregated
- **All-In-One**: Concatenate the result value with the endpoint qualifier and aggregates the concatenated strings with the new-line separator

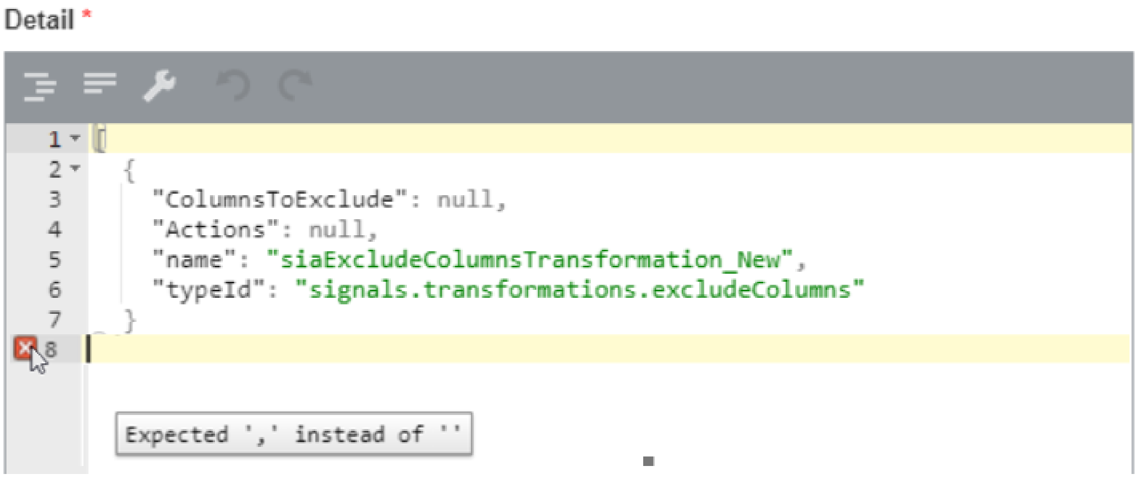
Creating a new custom aggregation:

1. From the Advanced Aggregrations Settings window, click on the **Create new** button. Clicking the **Create new** button clears all fields including the JSON text editor.
2. Enter a unique name for the aggregation. An optional description can be entered.
3. Select Transformation Steps.

The Transformation Steps drop-down list will list all the transformation steps that are implemented in Signals Inventa. Each corresponds to a data transformation in Spotfire but has the ability of being serialized to/deserialized from JSON strings.

Selecting a Transformation Step and clicking the **Add** button will add the JSON template of the selected Transformation Step into the JSON editor. Next, you can edit the JSON manually to update the definition or adjust the order of the transformation. Via the JSON editor, you can edit the JSON to define the custom aggregration method.

An error message will appear while you are typing if the content of the JSON editor is invalid. For example,



```
[
  {
    "ColumnsToExclude": null,
    "Actions": null,
    "name": "siaExcludeColumnsTransformation_New",
    "typeId": "signals.transformations.excludeColumns"
  }

```

Expected ',' instead of ''

In addition to creating a new custom aggregation method from scratch, you can edit or duplicate an existing aggregation method and modify as needed.

To edit an existing custom aggregation method:

1. From the Name dropdown list, select the aggregation method to rename.
2. Click on the Edit icon. This sets the dialog to editable mode.
3. Update the aggregation as required.
4. Click on the Update icon to save the changes.

To duplicate an existing custom aggregration method

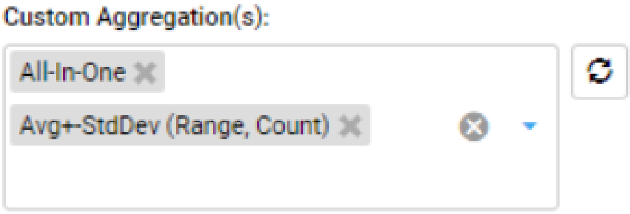
1. From the Name dropdown list, select the aggregation method to duplicate.
2. Click on the Duplicate icon. You will be prompted to confirm the duplication.
3. The suffix _Copy will be appended to the aggregation method name (e.g. All-in-One_Copy)
4. Click on the Edit icon to edit the aggregation method. This sets the dialog to editable mode.
5. Update the aggregation as required.
6. Click on the Update icon to save the changes.

The Name field becomes editable, enter a unique name for the aggregation method.

To delete an existing custom aggregration method:

1. From the Name dropdown list, select the aggregation method to delete.
2. Click on the Delete icon. You will be prompted to confirm the deletion.

After the custom aggregations are defined, users are able to apply the aggregations on the SAR table by using the drop-down control, after clicking **OK**, the selected aggregation(s) will be added to the box.



Using the Refresh icon, you can refresh the Custom Aggregation(s) list

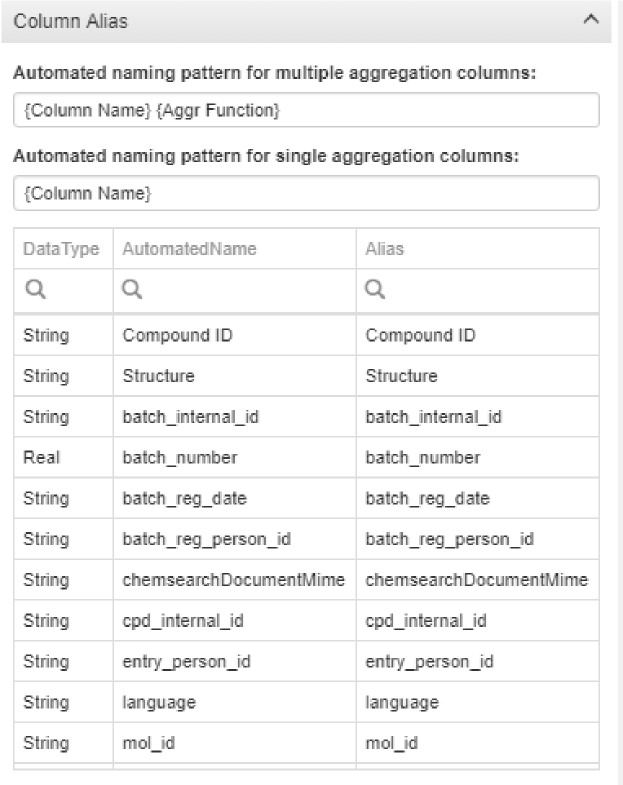
Note: For detailed explanation about each transformation step, please refer to Appendix C.

Exclude Empty Columns

Enabling the ‘Exclude Empty Columns’ checkbox will exclude any empty columns in the Compound/Batch tables from being generated in the SAR table.

10.2.1 Column Alias

Here you can change the column names in the SAR table by applying the column alias in a batch. You can define automated naming patterns for multiple aggregation columns and single aggregation columns.



Automated naming pattern for multiple aggregation columns: {Column Name} {Aggr Function}

Automated naming pattern for single aggregation columns: {Column Name}

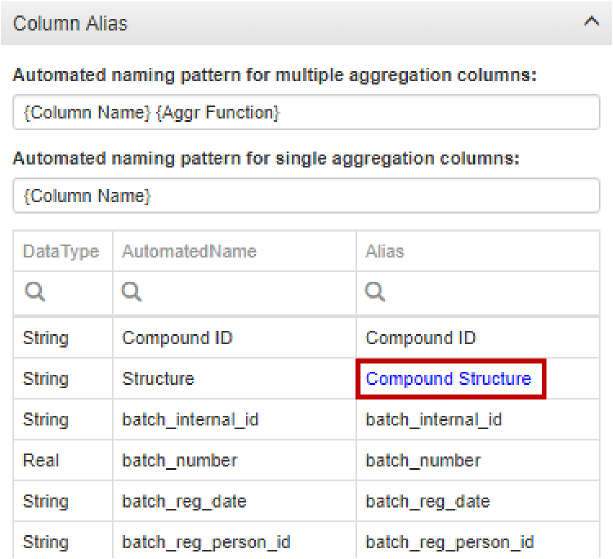
DataType	AutomatedName	Alias
String	Compound ID	Compound ID
String	Structure	Structure
String	batch_internal_id	batch_internal_id
Real	batch_number	batch_number
String	batch_reg_date	batch_reg_date
String	batch_reg_person_id	batch_reg_person_id
String	chemsearchDocumentMime	chemsearchDocumentMime
String	cpd_internal_id	cpd_internal_id
String	entry_person_id	entry_person_id
String	language	language
String	mol_id	mol_id

For example, a SAR table contains three columns (Text1, Number1, Date1). Two (or more) aggregation functions (e.g., Count and Max) are specified on Numeric columns. In this case, the ‘Multiple Aggregation’ rule will be applied to column ‘Number1’ when the SAR table is re-pivoted (e.g., Number1 Count, Number1 Max).

The column alias helps you to identify the aggregation functions used, and easily change the column names.

You can filter the columns in the grid based on data type, automated name or alias. Typing an identifier in the type-ahead box will bring the column matches to the top of the list. Query operators are also available.

If you change the alias, the font color changes to blue, similar to the example shown below.



Automated naming pattern for multiple aggregation columns:

{Column Name} {Aggr Function}

Automated naming pattern for single aggregation columns:

{Column Name}

DataType	AutomatedName	Alias
String	Compound ID	Compound ID
String	Structure	Compound Structure
String	batch_internal_id	batch_internal_id
Real	batch_number	batch_number
String	batch_reg_date	batch_reg_date
String	batch_reg_person_id	batch_reg_person_id

Note: Changing the column name from the Spotfire Column Properties dialog will not affect the column alias since the original column name is by design the key to identify the associated column alias. Changing the column name will affect the layout.

10.5 Multiple Apps

The SAR Analysis app can be added multiple times to the same document.

The app can be re-named through the Rename page menu item or directly on the tab.

Configuration is shared between multiples instances of the app.

Also, under the Analysis tab, filtering in the SAR Analysis panel is shared between app instances. However, Spotfire filter schemes are not shared between multiple instances of the app.

Under the Visualizations tab, the settings for visualizations will differ on a page by page basis, and therefore are not shared between multiple instances of the app. For example, even though two scatter plot visualizations are added to the same document, each plot may have its own look and feel. Layout settings are saved across multiple instances of the apps meaning each app captures the same layout list, however not necessarily the same.

11 Assay Results Review App

The Assay Results Review App loads historical assay results data and compares with the assay data in the current document.

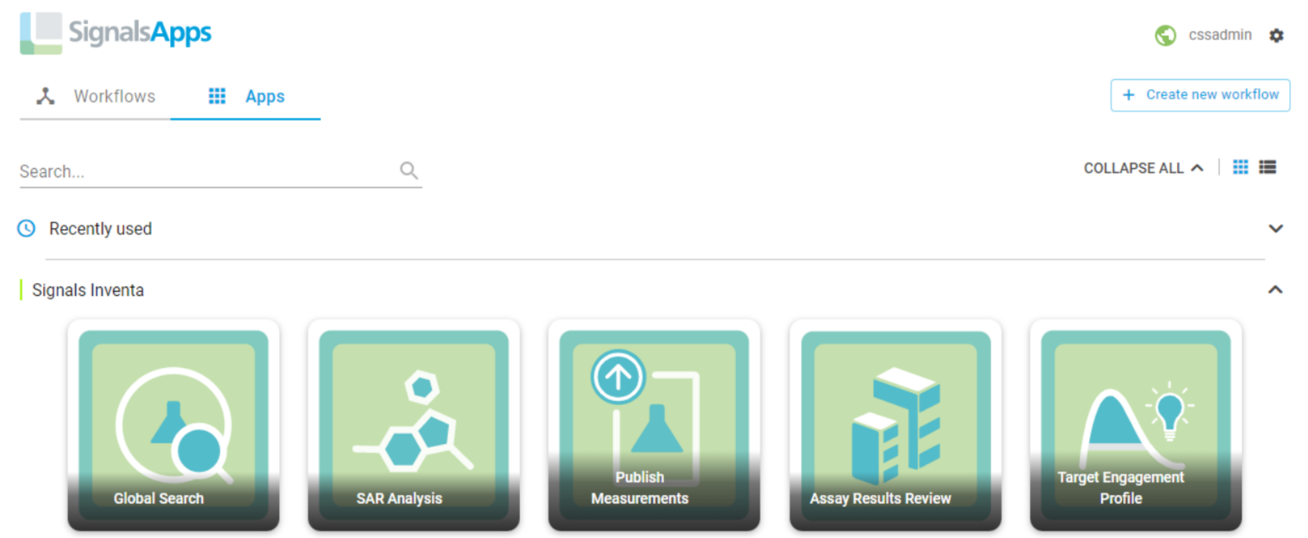
11.1 Accessing the Assay Results Review App

The Assay Results Review App is available in the Signals Apps store which is accessed through the main Spotfire Interface.

To access the Assay Results Review App:

In Spotfire Analyst Client:

1. Select **Tools > Signals Apps**.

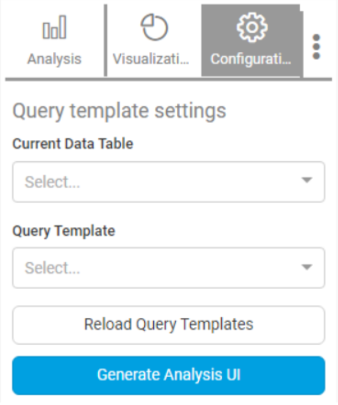


2. To launch the app, click anywhere on the **Assay Review Results App** card and it will be added to the document using the default app settings.

In Spotfire Web Player:

1. Open data in Spotfire.
2. Select **Tools > Signals Apps**.
3. To launch the app, click anywhere on the **Assay Review Results App** card and it will be added to the document using the default app settings.

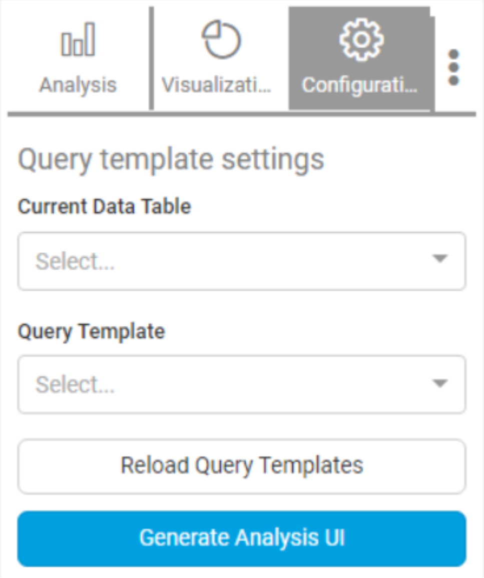
An Assay Review Results page is displayed, similar to the example shown below.



Note: When the app is opened within a workflow, the Analysis tab is the initial tab. However, when running outside of a workflow, the initial app is the Configuration tab.

11.2 Configuration tab

The Configuration tab allows you to select the query template and generate an Analysis UI (user interface).



Once the app has been configured properly as part of a workflow, these settings will be prepopulated, and the user of the workflow typically will not need to change the settings.

Current Data Table

Here you can select a Current Data Table. All data tables currently downloaded into Spotfire are available for selection.

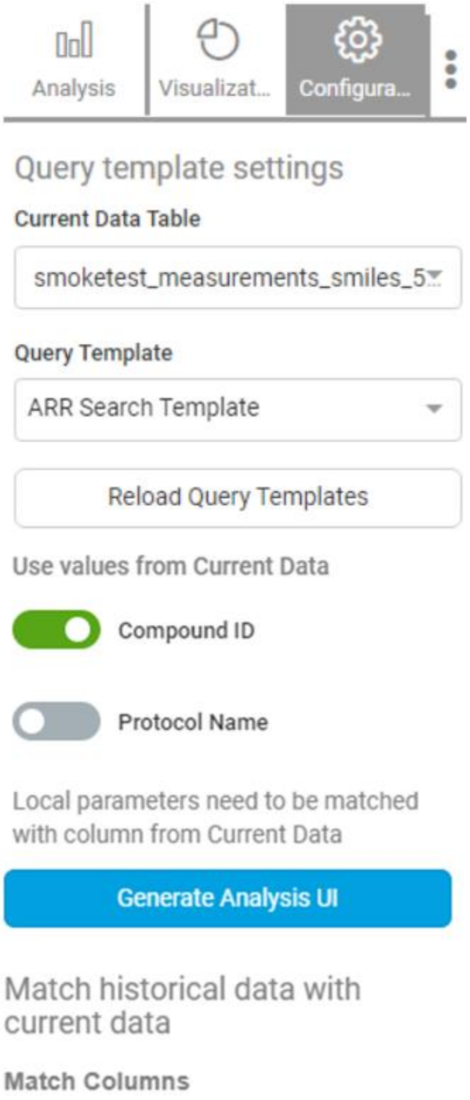
<u>Query template settings</u>

1. From the Query template settings drop-down list, select the Query template. The Assay Results Review app will retrieve all visible saved queries from the Signals Data Factory and only make available the query templates (saved searches with '@parameter' contained in the definition) in the app. Refer to the section

Creating a Query Template for use in Assay Results Review (ARR) App for more information on the query template.

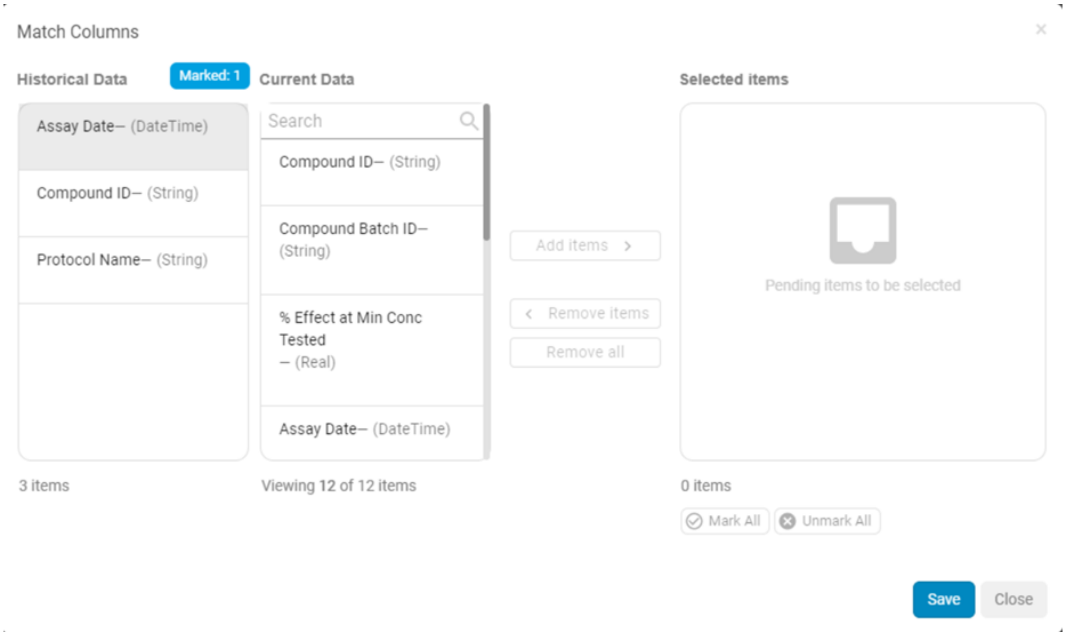
The query template is used to search the historical data of a measurement type.

2. Click **Generate Analysis UI** button.

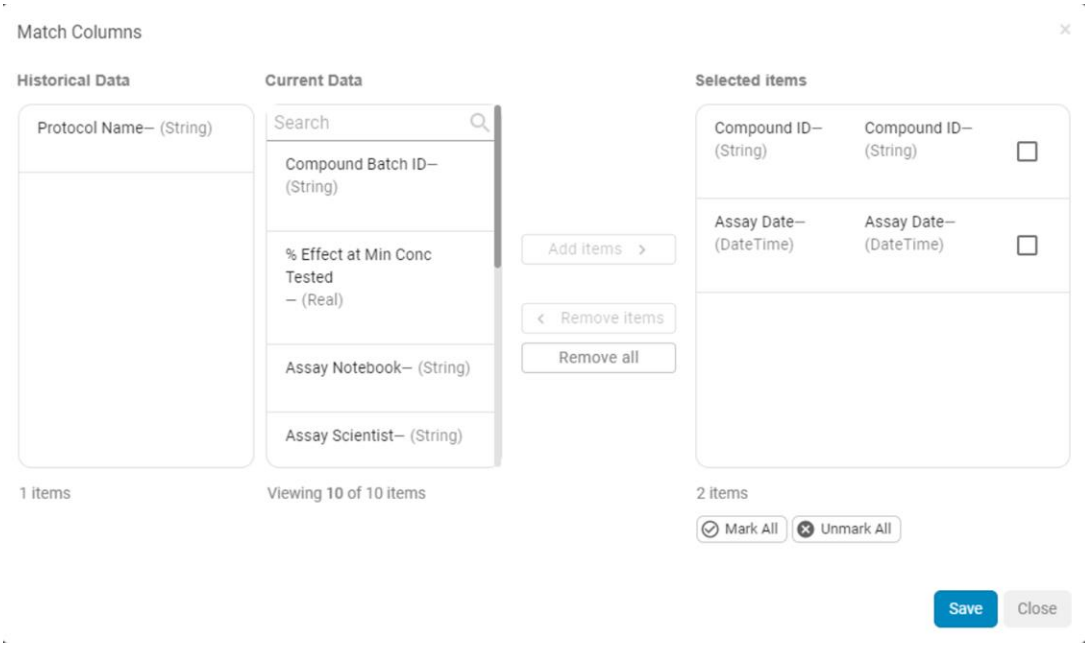


- **Use values from Current Data**: A toggle switch (default True) will appear per String type input parameter in the Query template. These toggles allow you to choose if the values from the current data should be used when provided the field values in the generated user interface. Based on the toggle statuses set here, UI controls for each of the query template parameters are generated (based on the parameter type) under the Analysis tab.
- **Match historical data with current data**. When you click on the plus-sign icon, a Match Columns window opens allowing you to match columns from historical and current data. This matching is required for values to

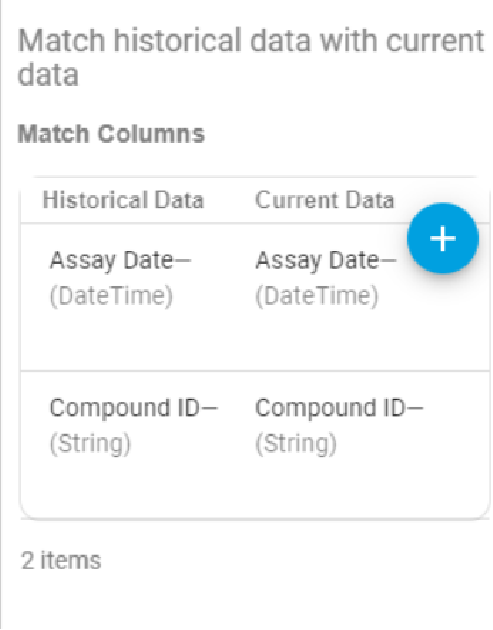
appear in the column value selectors under Analysis tab and for any columns used in the Current vs Historical visualization.



Any columns matched must have the same data type, otherwise a small warning triangle will appear in the overview after clicking the **Add Items** button.



After clicking the **Save** button, the Configuration tab is updated with the matched columns.


Match historical data with current data

Match Columns

Historical Data	Current Data
Assay Date–(DateTime)	Assay Date–(DateTime)
Compound ID–(String)	Compound ID–(String)

2 items

11.3 Analysis tab

The Assay Results Review app **Analysis** section contains a wizard like configuration panel where you can configure the settings for two different Analysis steps:

1. **Retrieval**: This step contains controls that allow you to specify the input parameter values for querying the historical data. The controls displayed here are dependent on the toggle statuses for 'Use values from Current Data' set in the Configuration tab.

There are three types of inputs:

- **String inputs**. These types of input parameters can be configured in the Configuration tab to use values from current data or free-entry data.

  Current data: If you want to use current data, the parameter must first be matched with a local column. After this is done, the unique values of the local column will be shown in a column value selector.
  Free entry: This mode allows you to specify any value (not just local values) as input to the query. You should specify one value per line.

- **Numeric inputs (optional)**: For this type of input parameter, you can specify a range (min/max):
  - Both empty => parameter is ignored
  - Min only => include values larger than min
  - Max only => include values less than max
  - Min and Max => include values larger than min and less than max

- **Date inputs:** Start and stop dates. Includes rows after start date and before stop date. You can select the dates in the calendar that pops up when clicking on either of the date fields.

Note: A toggle to 'Download details measurements' is also displayed if the measurement type identified in the selected query template has a details measurement type. Turning on this toggle will also download the data of the details measurement type and build the table relation between the current measurement data and its details

Once the input parameter values are defined, clicking the **Retrieve** button will download the historical data from the Signals Data Factory that match the specified parameter values. If applicable, data from the details measurement type will also be downloaded.

2. **Comparison**: This step allows you to create two sets of visualizations:

- **Current vs Historical**. To configure this visualization, you need to select an endpoint column and a MarkerBy column. Because this visualization compares two sets of data (current and historical), both selections need to be of columns that have been previously matched (in Configuration tab). If not, a warning message will be shown, prompting you to match the columns. Once configured, this visualization shows the current endpoint values on the X-axis and the historical endpoint values on the Y axis, showing one marker per value in the MarkerBy column.

  After clicking '**Compare**', the comparison is performed, and the scatter plot visualization is displayed.

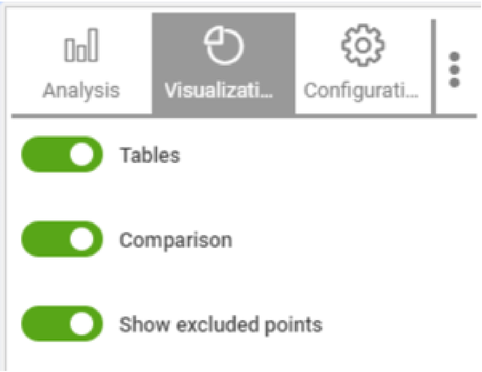
- **Identify trends**. To configure this visualization, you need to select the endpoint column, marker-by column and date column from the historical data. Those columns do not need to be mapped since this visualization involves only one set of data (historical). Once configured, this visualization shows the trend with the endpoint value on the Y axis and the date on the X axis, showing one marker per value in the MarkerBy column.

  After clicking '**Compare**', the comparison is performed, and an Identity Trend is plotted.

11.4 Visualizations tab

This section contains settings that affect what is displayed in the visualization area. Using the toggles, you can turn off and on groups of visualizations:

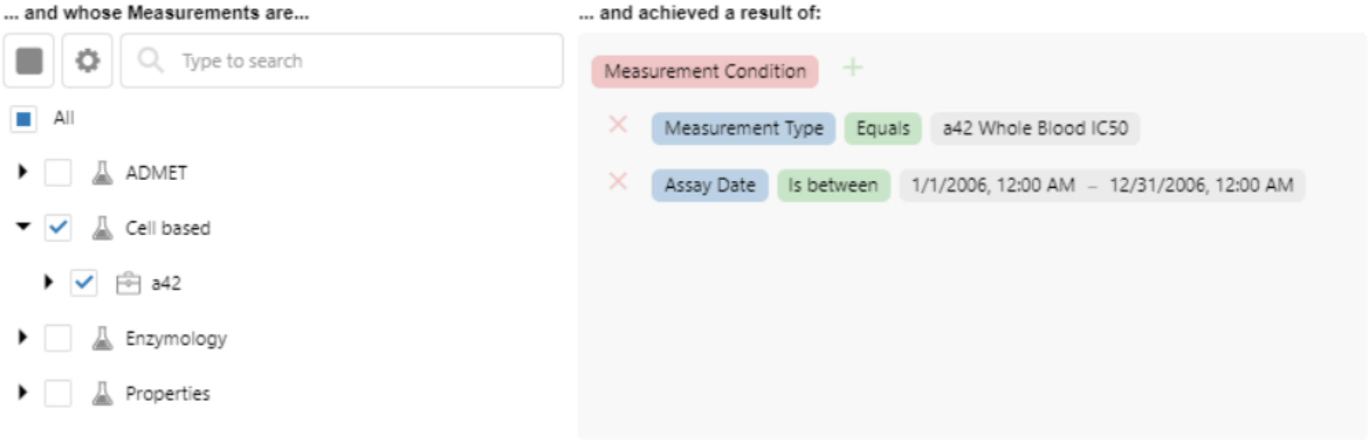
- **Tables**: This corresponds to the Historical Data and Current Data table plots.
- **Comparison**: This corresponds to the currently selected comparison plot in the second step of the wizard in the Analysis tab, i.e. Current vs Historical or Identify Trends.
- **Show excluded points -** This toggle allows the user to visualize where excluded points in the current analysis fall when compared to the historical data



11.5 Using the Assay Results Review App

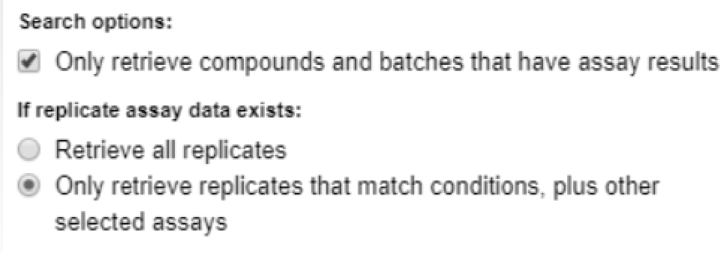
The following example outlines how the ARR app can be used to load historical assay results data and compare to the assay data in the current document.

1. Create a query template in Signals Data Factory. Refer to the section [Creating a Query Template for use in Assay Results Review App](). In this example, the query template (ARR Search Template) has been set up with the parameters, Assay Date, Compound ID and Protocol Name.
2. Using Global Search, create a search with measurements conditions similar to the following:



This search will retrieve for the a42 Whold Blood IC50 Measurement Type with an Assay Date between 1/1/2006 and 12/31/2006. This data will represent the 'Current Data' in the ARR app.

Ensure 'Only retrieve replicates that match conditions, plus other selected assays' is enabled under Search Options if replicate assay data exists.



Search options:

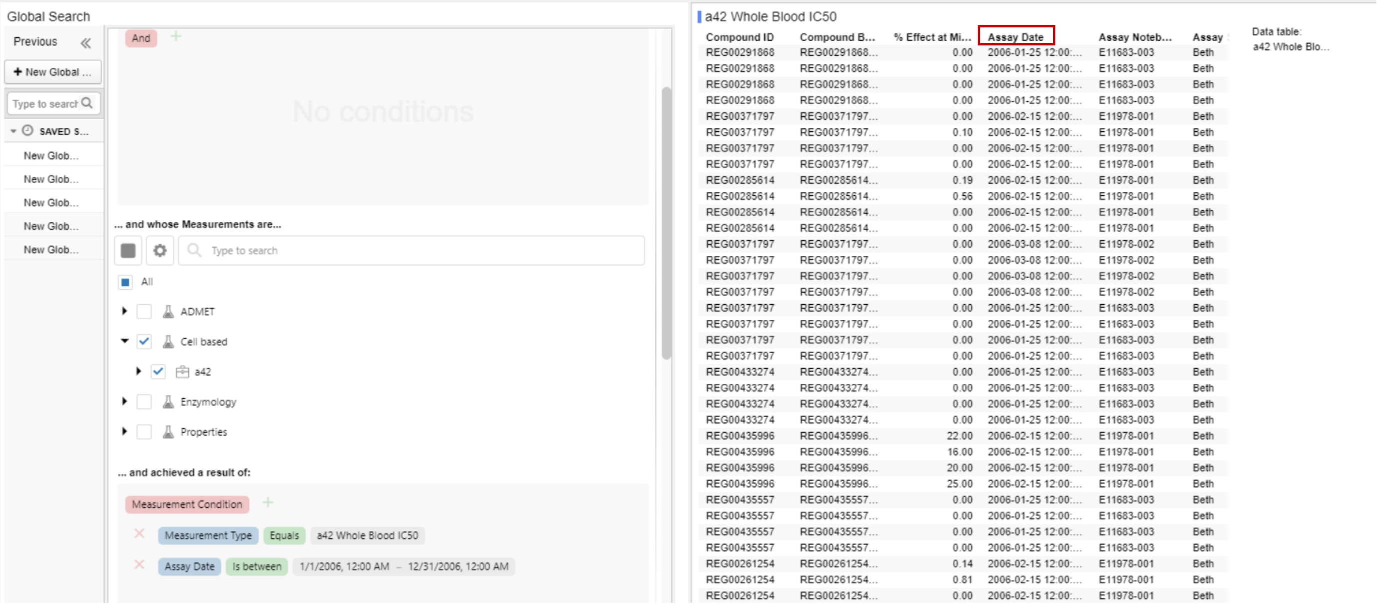
☑ Only retrieve compounds and batches that have assay results

If replicate assay data exists:

○ Retrieve all replicates

● Only retrieve replicates that match conditions, plus other selected assays

After downloading the data, all rows in the a42 Whole Blood IC50 table have assay data between 1/1/2006 and 12/31/2006.



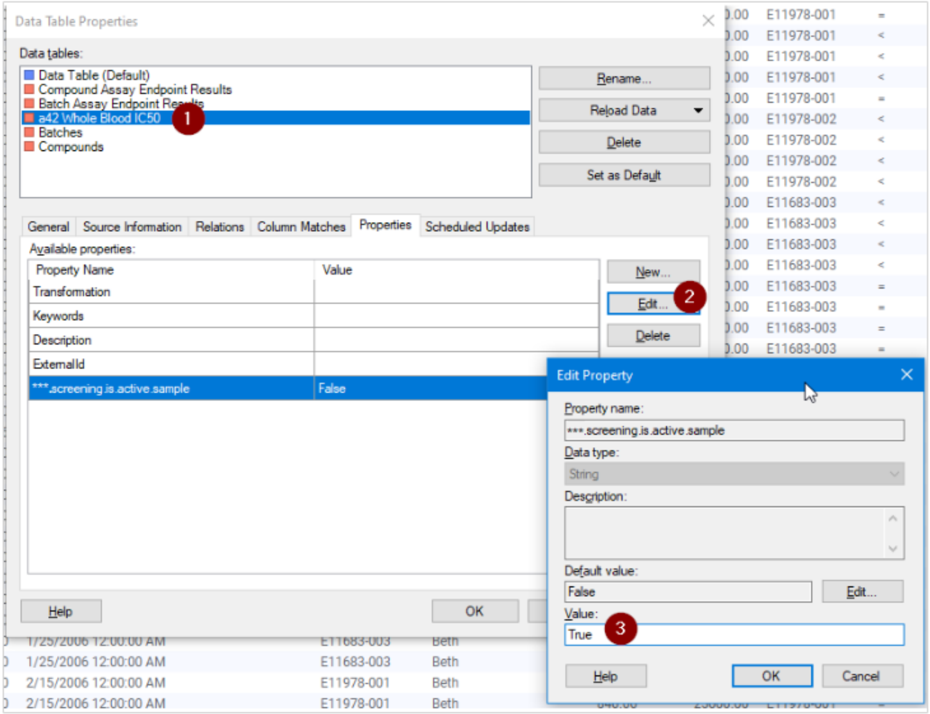
Measurement Type Equals a42 Whole Blood IC50

Assay Date Is between 1/1/2006, 12:00 AM – 12/31/2006, 12:00 AM

a42 Whole Blood IC50

Compound ID	Compound B...	% Effect at Mi...	Assay Date	Assay Noteb...	Assay
REG00291868	REG00291868...	0.00	2006-01-25 12:00:...	E11683-003	Beth
REG00291868	REG00291868...	0.00	2006-01-25 12:00:...	E11683-003	Beth
REG00291868	REG00291868...	0.00	2006-01-25 12:00:...	E11683-003	Beth
REG00291868	REG00291868...	0.00	2006-01-25 12:00:...	E11683-003	Beth
REG00371797	REG00371797...	0.00	2006-02-15 12:00:...	E11978-001	Beth
REG00371797	REG00371797...	0.10	2006-02-15 12:00:...	E11978-001	Beth
REG00371797	REG00371797...	0.00	2006-02-15 12:00:...	E11978-001	Beth
REG00371797	REG00371797...	0.00	2006-02-15 12:00:...	E11978-001	Beth
REG00285614	REG00285614...	0.19	2006-02-15 12:00:...	E11978-001	Beth
REG00285614	REG00285614...	0.56	2006-02-15 12:00:...	E11978-001	Beth
REG00285614	REG00285614...	0.00	2006-02-15 12:00:...	E11978-001	Beth
REG00285614	REG00285614...	0.00	2006-02-15 12:00:...	E11978-001	Beth
REG00371797	REG00371797...	0.00	2006-03-08 12:00:...	E11978-002	Beth
REG00371797	REG00371797...	0.00	2006-03-08 12:00:...	E11978-002	Beth
REG00371797	REG00371797...	0.00	2006-03-08 12:00:...	E11978-002	Beth
REG00371797	REG00371797...	0.00	2006-03-08 12:00:...	E11978-002	Beth
REG00371797	REG00371797...	0.00	2006-01-25 12:00:...	E11683-003	Beth
REG00371797	REG00371797...	0.00	2006-01-25 12:00:...	E11683-003	Beth
REG00371797	REG00371797...	0.00	2006-01-25 12:00:...	E11683-003	Beth
REG00371797	REG00371797...	0.00	2006-01-25 12:00:...	E11683-003	Beth
REG00433274	REG00433274...	0.00	2006-01-25 12:00:...	E11683-003	Beth
REG00433274	REG00433274...	0.00	2006-01-25 12:00:...	E11683-003	Beth
REG00433274	REG00433274...	0.00	2006-01-25 12:00:...	E11683-003	Beth
REG00433274	REG00433274...	0.00	2006-01-25 12:00:...	E11683-003	Beth
REG00435996	REG00435996...	22.00	2006-02-15 12:00:...	E11978-001	Beth
REG00435996	REG00435996...	16.00	2006-02-15 12:00:...	E11978-001	Beth
REG00435996	REG00435996...	20.00	2006-02-15 12:00:...	E11978-001	Beth
REG00435996	REG00435996...	25.00	2006-02-15 12:00:...	E11978-001	Beth
REG00435557	REG00435557...	0.00	2006-01-25 12:00:...	E11683-003	Beth
REG00435557	REG00435557...	0.00	2006-01-25 12:00:...	E11683-003	Beth
REG00435557	REG00435557...	0.00	2006-01-25 12:00:...	E11683-003	Beth
REG00435557	REG00435557...	0.00	2006-01-25 12:00:...	E11683-003	Beth
REG00261254	REG00261254...	0.14	2006-02-15 12:00:...	E11978-001	Beth
REG00261254	REG00261254...	0.81	2006-02-15 12:00:...	E11978-001	Beth
REG00261254	REG00261254...	0.00	2006-02-15 12:00:...	E11978-001	Beth

3. From the **Data** menu item in the Spotfire client, select the **Data table properties** sub-menu item open the Data Table Properties window. Make sure that for table **a42 Whole Blood IC50**, there is a table property *****.screening.is.active.sample** defined and its value is **True**. If this property is not defined, please define it manually.



Property Name	Value
Transformation	
Keywords	
Description	
ExternalId	
***.screening.is.active.sample	False

Property name: ***.screening.is.active.sample

Data type: String

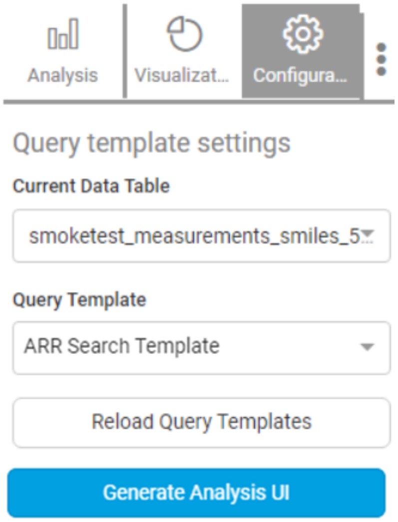
Description:

Default value: False

Value: True

The Assay Results Review app uses this property to identify which table contains the ‘Current Data’. This table is then used when creating the mapping workflow in the app. In this example, the ‘Current Data’ is prepared using Global Search, however you can also import existing CSV files to represent the current data.

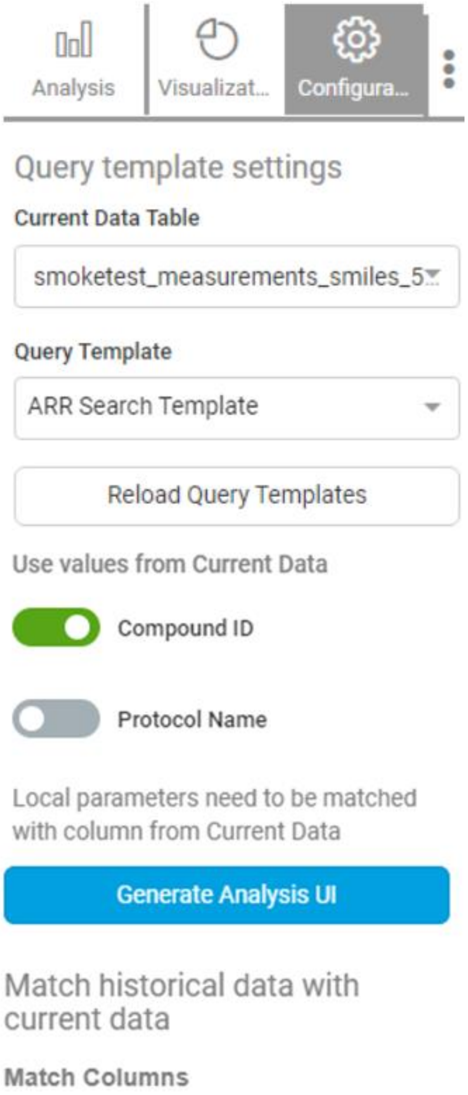
4. From the **Tools > Signals Apps** menu item, open the Assay Results Review app. From the Configuration tab, select the current data table and query template (e.g. ARR Search Template).



Current Data Table: smoketest_measurements_smiles_5

Query Template: ARR Search Template

5. Click on the **Generate Analysis UI** button. The app will infer the parameters from the selected query template and the panel will be updated similar to the example shown below.



Query template settings

Current Data Table: smoketest_measurements_smiles_5

Query Template: ARR Search Template

Use values from Current Data

Compound ID (on)

Protocol Name (off)

Local parameters need to be matched with column from Current Data

Match historical data with current data

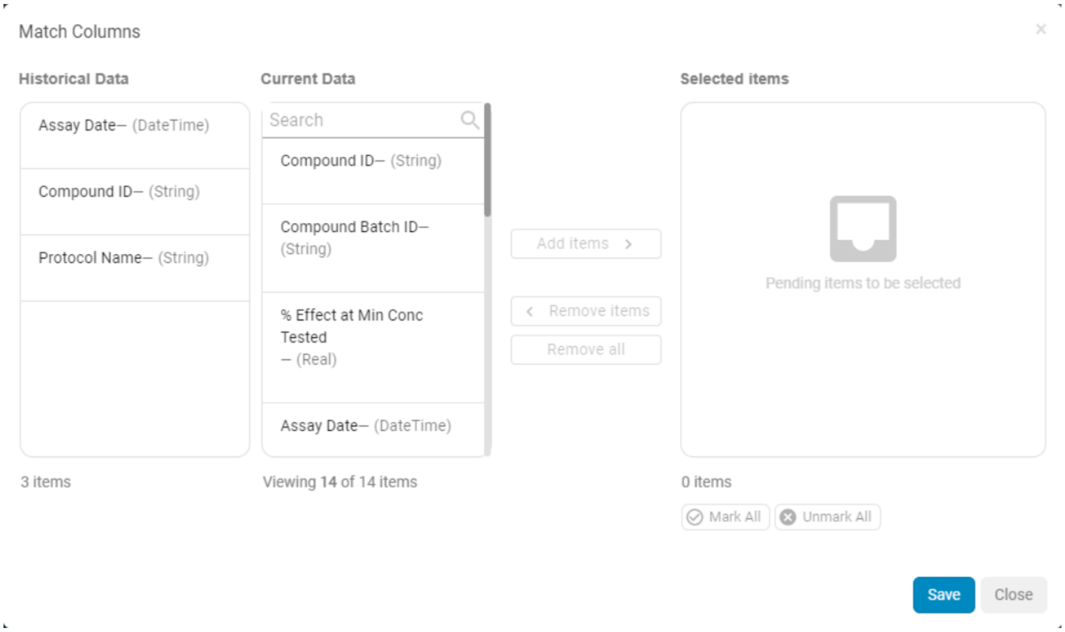
Match Columns

All text parameters (e.g, Compound ID, Protocol Name) are displayed with a toggle to indicate if the parameter values will be extracted from the ‘Current Data’ table, in this case, a42 Whole Blood IC50 data table.

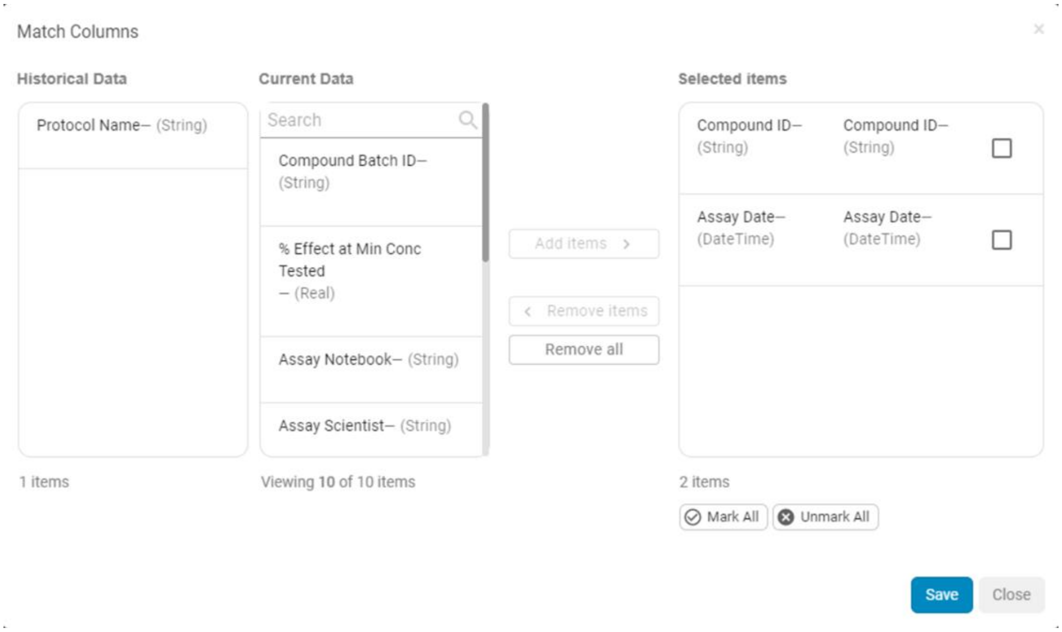
6. For this example, toggle off the Protocol Name parameter. Ensure the Compound ID toggle is turned on.

Next we need to define the mapping between the query parameter(s) and the columns in the ‘Current Data’ table (i.e. a42 Whole Blood IC50 data table).

7. Click on the plus icon to match historical data with current data. The Match Columns dialog is displayed, similar to the example shown below.

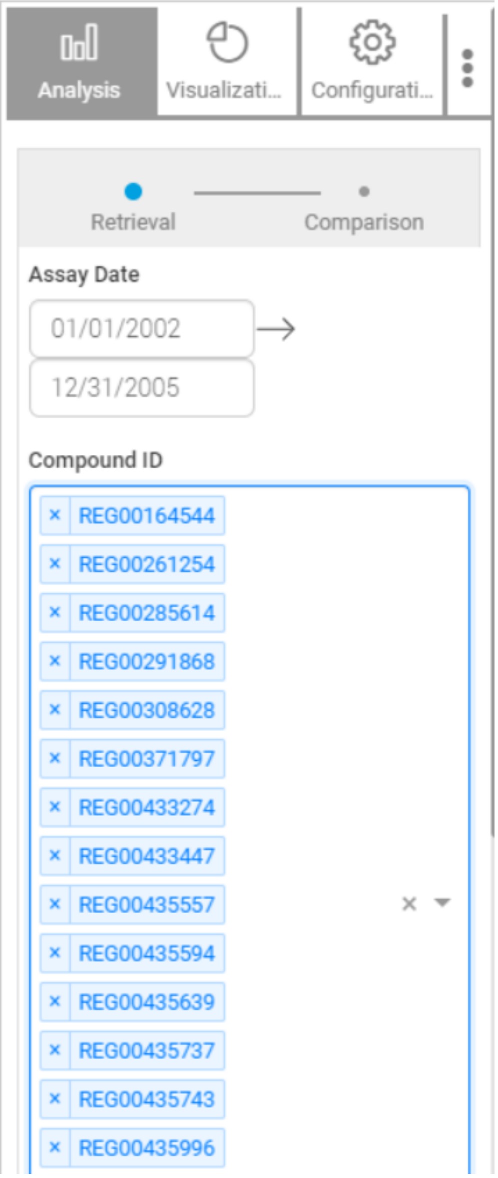


8. Match the columns from historical data to current data for Compound ID and Assay Date, similar to the example shown below. Click **Add Items** button. Click **Save**.



9. Navigate to the Analysis tab. As a result of the Compound ID toggle being enable in Step 6 above, the Compounds IDs are populated with the values from the ‘Current Data’ table (i.e. a42 Whole Blood IC50 data table).

10. Specify an assay data to compare the historical with the current data. In this example, we will compare the data from 1/1/2002 to 12/31/2005, similar to the example shown below.



Assay Date

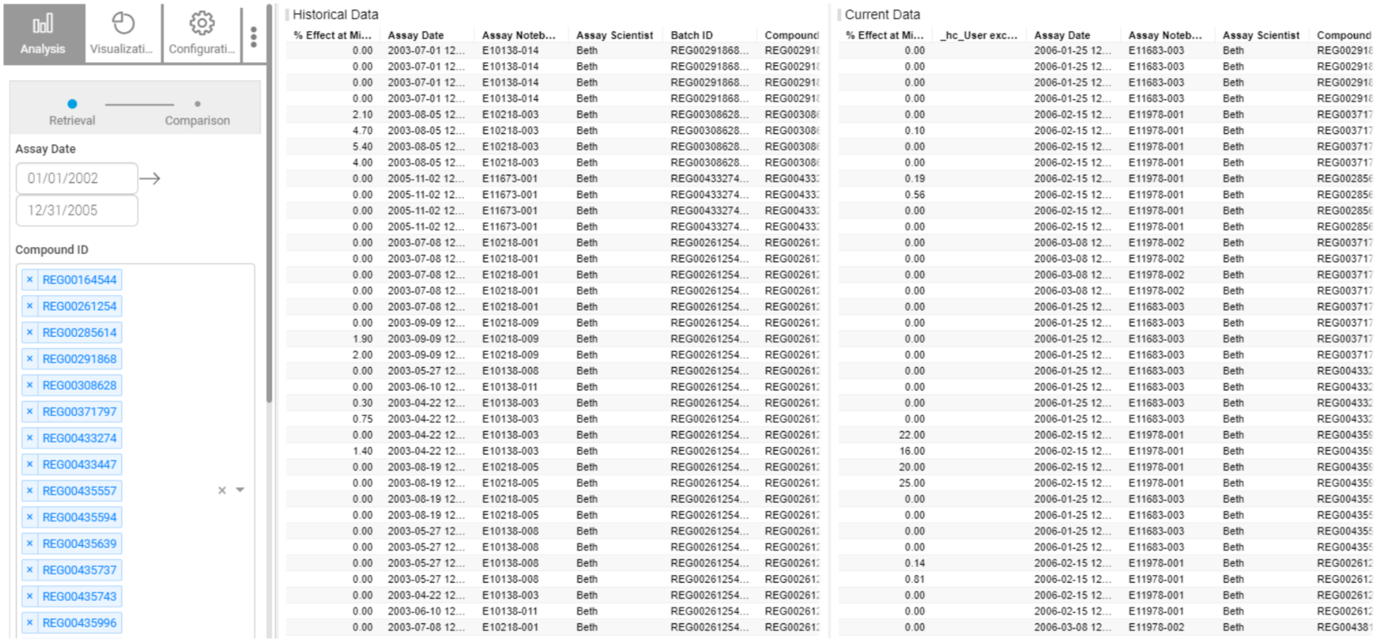
01/01/2002 →

12/31/2005

Compound ID

- REG00164544
- REG00261254
- REG00285614
- REG00291868
- REG00308628
- REG00371797
- REG00433274
- REG00433447
- REG00435557
- REG00435594
- REG00435639
- REG00435737
- REG00435743
- REG00435996

11. Click on the **Retrieve** button to download the historical data table.



Assay Date

01/01/2002 → 12/31/2005

Compound ID

- × REG00164544
- × REG00261254
- × REG00285614
- × REG00291868
- × REG00308628
- × REG00371797
- × REG00433274
- × REG00433447
- × REG00435557
- × REG00435594
- × REG00435639
- × REG00435737
- × REG00435743
- × REG00435996

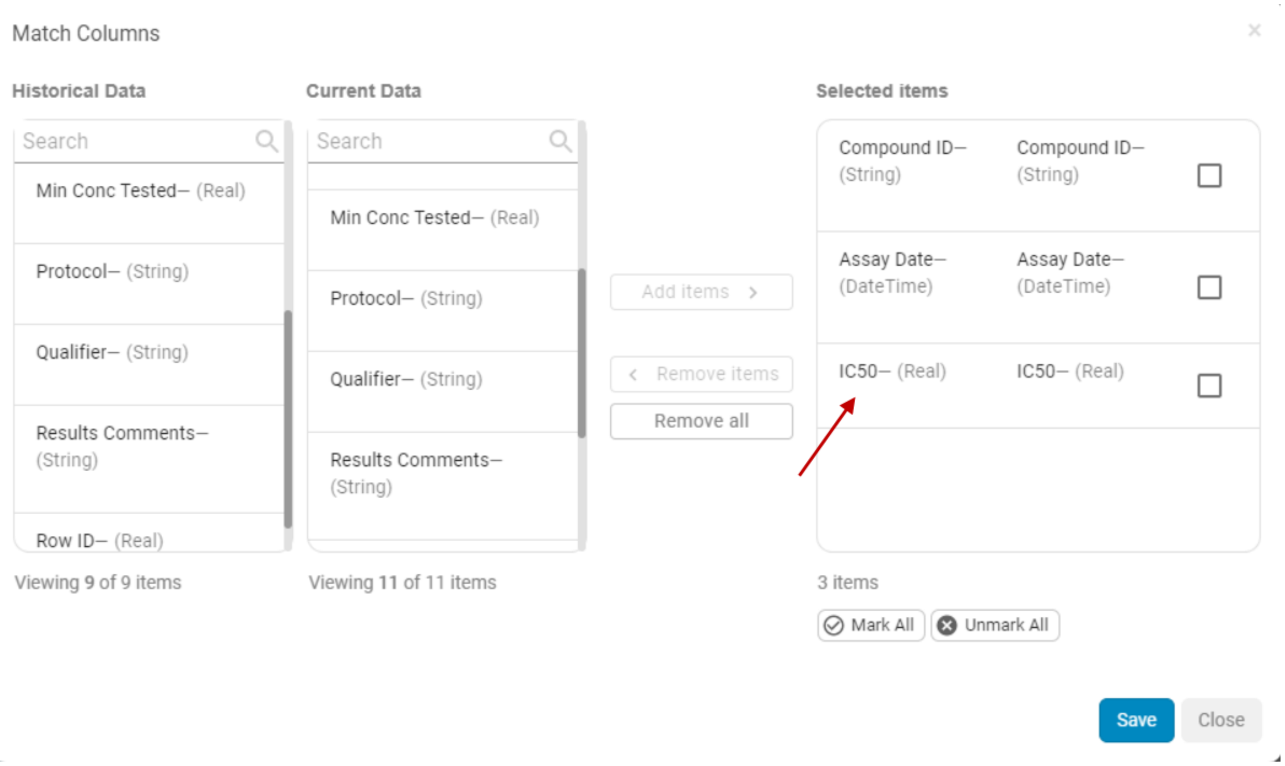
Historical Data

% Effect at Mi...	Assay Date	Assay Noteb...	Assay Scientist	Batch ID	Compound
0.00	2003-07-01 12...	E10138-014	Beth	REG00291868...	REG00291
0.00	2003-07-01 12...	E10138-014	Beth	REG00291868...	REG00291
0.00	2003-07-01 12...	E10138-014	Beth	REG00291868...	REG00291
0.00	2003-07-01 12...	E10138-014	Beth	REG00291868...	REG00291
2.10	2003-08-05 12...	E10218-003	Beth	REG00308628...	REG00308
4.70	2003-08-05 12...	E10218-003	Beth	REG00308628...	REG00308
5.40	2003-08-05 12...	E10218-003	Beth	REG00308628...	REG00308
4.00	2003-08-05 12...	E10218-003	Beth	REG00308628...	REG00308
0.00	2005-11-02 12...	E11673-001	Beth	REG00433274...	REG00433
0.00	2005-11-02 12...	E11673-001	Beth	REG00433274...	REG00433
0.00	2005-11-02 12...	E11673-001	Beth	REG00433274...	REG00433
0.00	2005-11-02 12...	E11673-001	Beth	REG00433274...	REG00433
0.00	2003-07-08 12...	E10218-001	Beth	REG00261254...	REG00261
0.00	2003-07-08 12...	E10218-001	Beth	REG00261254...	REG00261
0.00	2003-07-08 12...	E10218-001	Beth	REG00261254...	REG00261
0.00	2003-07-08 12...	E10218-001	Beth	REG00261254...	REG00261
0.00	2003-07-08 12...	E10218-001	Beth	REG00261254...	REG00261
0.00	2003-09-09 12...	E10218-009	Beth	REG00261254...	REG00261
1.90	2003-09-09 12...	E10218-009	Beth	REG00261254...	REG00261
2.00	2003-09-09 12...	E10218-009	Beth	REG00261254...	REG00261
0.00	2003-05-27 12...	E10138-008	Beth	REG00261254...	REG00261
0.00	2003-06-10 12...	E10138-011	Beth	REG00261254...	REG00261
0.30	2003-04-22 12...	E10138-003	Beth	REG00261254...	REG00261
0.75	2003-04-22 12...	E10138-003	Beth	REG00261254...	REG00261
0.00	2003-04-22 12...	E10138-003	Beth	REG00261254...	REG00261
1.40	2003-04-22 12...	E10138-003	Beth	REG00261254...	REG00261
0.00	2003-08-19 12...	E10218-005	Beth	REG00261254...	REG00261
0.00	2003-08-19 12...	E10218-005	Beth	REG00261254...	REG00261
0.00	2003-08-19 12...	E10218-005	Beth	REG00261254...	REG00261
0.00	2003-08-19 12...	E10218-005	Beth	REG00261254...	REG00261
0.00	2003-05-27 12...	E10138-008	Beth	REG00261254...	REG00261
0.00	2003-05-27 12...	E10138-008	Beth	REG00261254...	REG00261
0.00	2003-05-27 12...	E10138-008	Beth	REG00261254...	REG00261
0.00	2003-05-27 12...	E10138-008	Beth	REG00261254...	REG00261
0.00	2003-04-22 12...	E10138-003	Beth	REG00261254...	REG00261
0.00	2003-06-10 12...	E10138-011	Beth	REG00261254...	REG00261
0.00	2003-07-08 12...	E10218-001	Beth	REG00261254...	REG00261

Current Data

% Effect at Mi...	_hc_User exc...	Assay Date	Assay Noteb...	Assay Scientist	Compound
0.00		2006-01-25 12...	E11683-003	Beth	REG00291
0.00		2006-01-25 12...	E11683-003	Beth	REG00291
0.00		2006-01-25 12...	E11683-003	Beth	REG00291
0.00		2006-01-25 12...	E11683-003	Beth	REG00291
0.00		2006-02-15 12...	E11978-001	Beth	REG00371
0.10		2006-02-15 12...	E11978-001	Beth	REG00371
0.00		2006-02-15 12...	E11978-001	Beth	REG00371
0.00		2006-02-15 12...	E11978-001	Beth	REG00371
0.19		2006-02-15 12...	E11978-001	Beth	REG00285
0.56		2006-02-15 12...	E11978-001	Beth	REG00285
0.00		2006-02-15 12...	E11978-001	Beth	REG00285
0.00		2006-02-15 12...	E11978-001	Beth	REG00285
0.00		2006-03-08 12...	E11978-002	Beth	REG00371
0.00		2006-03-08 12...	E11978-002	Beth	REG00371
0.00		2006-03-08 12...	E11978-002	Beth	REG00371
0.00		2006-03-08 12...	E11978-002	Beth	REG00371
0.00		2006-01-25 12...	E11683-003	Beth	REG00371
0.00		2006-01-25 12...	E11683-003	Beth	REG00371
0.00		2006-01-25 12...	E11683-003	Beth	REG00371
0.00		2006-01-25 12...	E11683-003	Beth	REG00371
0.00		2006-01-25 12...	E11683-003	Beth	REG00433
0.00		2006-01-25 12...	E11683-003	Beth	REG00433
0.00		2006-01-25 12...	E11683-003	Beth	REG00433
0.00		2006-01-25 12...	E11683-003	Beth	REG00433
22.00		2006-02-15 12...	E11978-001	Beth	REG00435
16.00		2006-02-15 12...	E11978-001	Beth	REG00435
20.00		2006-02-15 12...	E11978-001	Beth	REG00435
25.00		2006-02-15 12...	E11978-001	Beth	REG00435
0.00		2006-01-25 12...	E11683-003	Beth	REG00435
0.00		2006-01-25 12...	E11683-003	Beth	REG00435
0.00		2006-01-25 12...	E11683-003	Beth	REG00435
0.00		2006-01-25 12...	E11683-003	Beth	REG00435
0.14		2006-02-15 12...	E11978-001	Beth	REG00261
0.81		2006-02-15 12...	E11978-001	Beth	REG00261
0.00		2006-02-15 12...	E11978-001	Beth	REG00261
0.00		2006-02-15 12...	E11978-001	Beth	REG00261
0.00		2006-03-08 12...	E11978-002	Beth	REG00438

12. Navigate to the Configuration tab. Click the plus icon on the Match Columns grid to open the Match Columns dialog. For this example, match the columns from historical data to current data for IC50. Click **Add Items** button. Click **Save**. This endpoint mapping will be used for data comparisons in the following steps.



Historical Data:

- Min Conc Tested– (Real)
- Protocol– (String)
- Qualifier– (String)
- Results Comments– (String)
- Row ID– (Real)

Viewing 9 of 9 items

Current Data:

- Min Conc Tested– (Real)
- Protocol– (String)
- Qualifier– (String)
- Results Comments– (String)

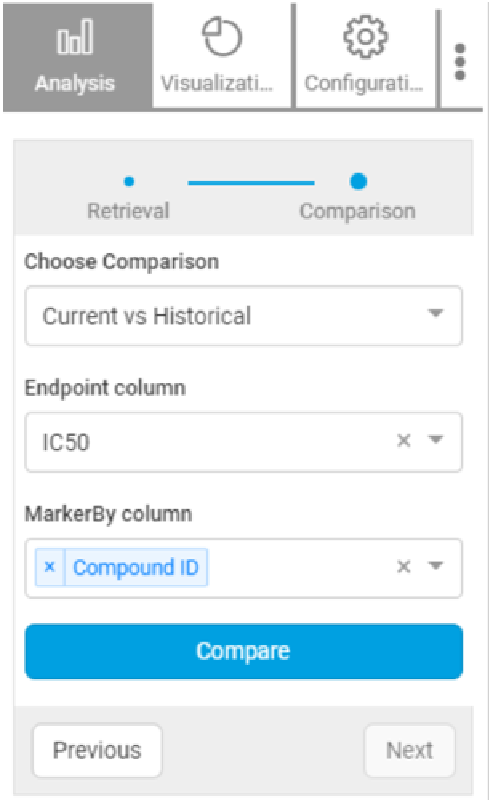
Viewing 11 of 11 items

Selected items:

Compound ID– (String)	Compound ID– (String)	☐
Assay Date– (DateTime)	Assay Date– (DateTime)	☐
IC50– (Real)	IC50– (Real)	☐

3 items

13. Navigate to the Analysis tab. Click **Next** at the bottom of the app panel to move to the Comparison step. For this example, from the drop-down lists, set the Choose Comparison to Current vs Historical, Endpoint column to IC50 and MarkerBy column to Compound ID.



Choose Comparison: Current vs Historical

Endpoint column: IC50

MarkerBy column: Compound ID

14. Click **Compare**. A scatter plot comparing IC50 (historical) vs IC50 (current), similar to the example shown below, is displayed for you to analyze.

Choose Comparison: Current vs Historical

Endpoint column: IC50

MarkerBy column: Compound ID

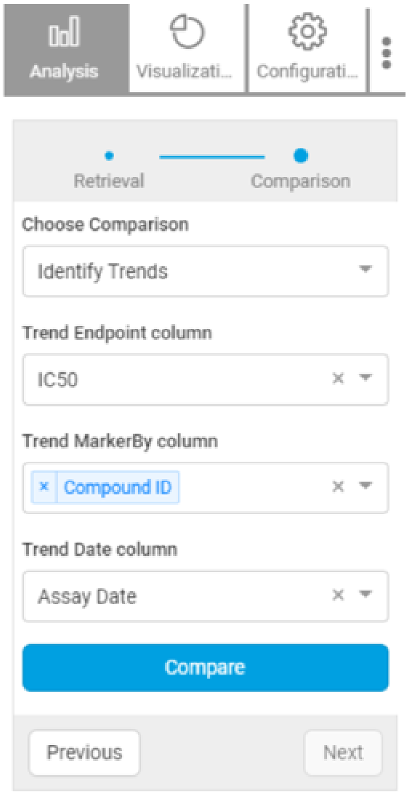
Historical Data

% Effect at Mi...	Assay Date	Assay Noteb...	Assay Scientist	Batch ID	Compound
0.00	2003-07-01 12...	E10138-014	Beth	REG00291868...	REG00291
0.00	2003-07-01 12...	E10138-014	Beth	REG00291868...	REG00291
0.00	2003-07-01 12...	E10138-014	Beth	REG00291868...	REG00291
0.00	2003-07-01 12...	E10138-014	Beth	REG00291868...	REG00291
0.00	2003-07-01 12...	E10138-014	Beth	REG00291868...	REG00291
0.00	2003-07-01 12...	E10138-014	Beth	REG00291868...	REG00291
0.00	2003-07-01 12...	E10138-014	Beth	REG00291868...	REG00291
0.00	2003-07-01 12...	E10138-014	Beth	REG00291868...	REG00291
0.00	2003-07-01 12...	E10138-014	Beth	REG00291868...	REG00291
0.00	2003-07-01 12...	E10138-014	Beth	REG00291868...	REG00291
0.00	2003-07-01 12...	E10138-014	Beth	REG00291868...	REG00291
0.00	2003-07-01 12...	E10138-014	Beth	REG00291868...	REG00291
0.00	2003-07-01 12...	E10138-014	Beth	REG00291868...	REG00291
0.00	2003-07-01 12...	E10138-014	Beth	REG00291868...	REG00291

Current Data

% Effect at Mi...	_hc_User exc...	Assay Date	Assay Noteb...	Assay Scientist	Compound
0.00		2006-01-25 12...	E11683-003	Beth	REG00291
0.00		2006-01-25 12...	E11683-003	Beth	REG00291
0.00		2006-01-25 12...	E11683-003	Beth	REG00291
0.00		2006-01-25 12...	E11683-003	Beth	REG00291
0.00		2006-02-15 12...	E11978-001	Beth	REG00371
0.10		2006-02-15 12...	E11978-001	Beth	REG00371
0.00		2006-02-15 12...	E11978-001	Beth	REG00371
0.00		2006-02-15 12...	E11978-001	Beth	REG00371
0.19		2006-02-15 12...	E11978-001	Beth	REG00285
0.56		2006-02-15 12...	E11978-001	Beth	REG00285
0.00		2006-02-15 12...	E11978-001	Beth	REG00285
0.00		2006-02-15 12...	E11978-001	Beth	REG00285
0.00		2006-03-08 12...	E11978-002	Beth	REG00371
0.00		2006-03-08 12...	E11978-002	Beth	REG00371

15. You can also view identity trends between the historical and current data. For this example, set the Choose Comparison to Identity Trends, Trend Endpoint column to IC50, Trend MarkerBy column to Compound ID and Trend Data column to Assay Date.



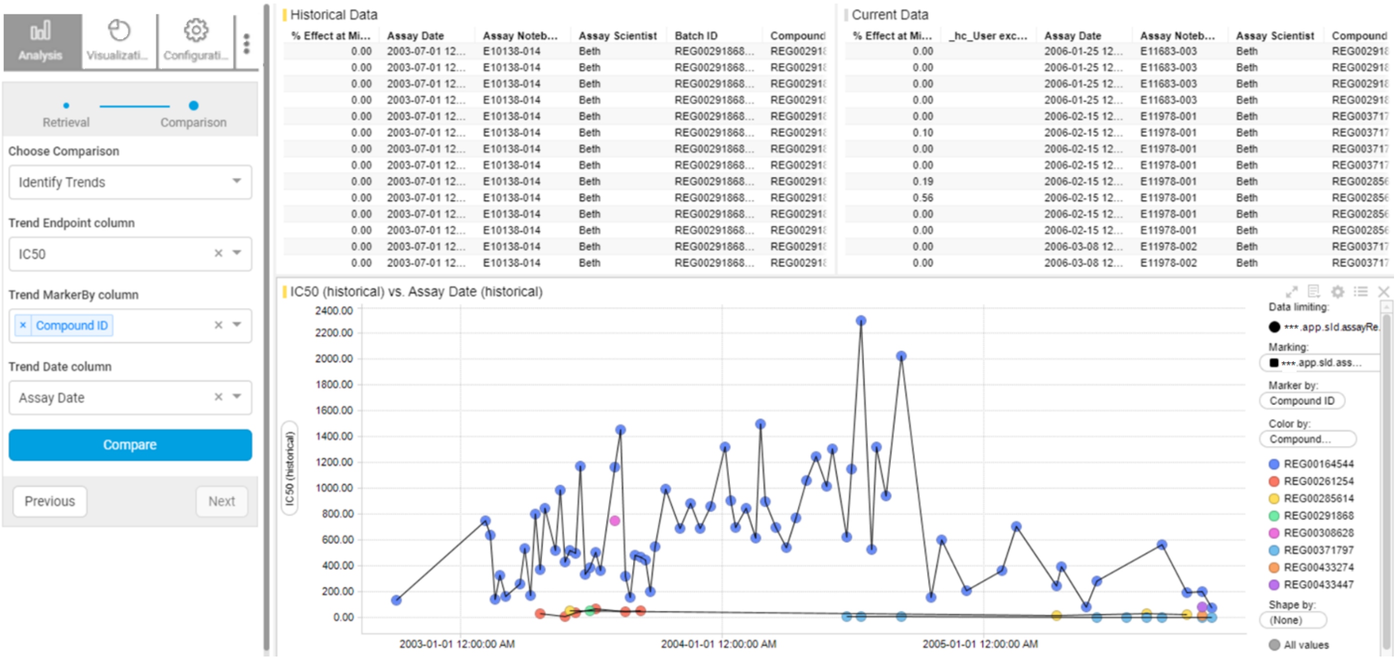
Choose Comparison: Identify Trends

Trend Endpoint column: IC50

Trend MarkerBy column: Compound ID

Trend Date column: Assay Date

16. Click **Compare**. A scatter plot comparing IC50 (historical) vs Assay Date, similar to the example shown below, is displayed for you to analyze.



Choose Comparison
Identify Trends

Trend Endpoint column
IC50

Trend MarkerBy column
Compound ID

Trend Date column
Assay Date

Historical Data

% Effect at Mi...	Assay Date	Assay Noteb...	Assay Scientist	Batch ID	Compound
0.00	2003-07-01 12...	E10138-014	Beth	REG00291868...	REG00291
0.00	2003-07-01 12...	E10138-014	Beth	REG00291868...	REG00291
0.00	2003-07-01 12...	E10138-014	Beth	REG00291868...	REG00291
0.00	2003-07-01 12...	E10138-014	Beth	REG00291868...	REG00291
0.00	2003-07-01 12...	E10138-014	Beth	REG00291868...	REG00291
0.00	2003-07-01 12...	E10138-014	Beth	REG00291868...	REG00291
0.00	2003-07-01 12...	E10138-014	Beth	REG00291868...	REG00291
0.00	2003-07-01 12...	E10138-014	Beth	REG00291868...	REG00291
0.00	2003-07-01 12...	E10138-014	Beth	REG00291868...	REG00291
0.00	2003-07-01 12...	E10138-014	Beth	REG00291868...	REG00291
0.00	2003-07-01 12...	E10138-014	Beth	REG00291868...	REG00291
0.00	2003-07-01 12...	E10138-014	Beth	REG00291868...	REG00291
0.00	2003-07-01 12...	E10138-014	Beth	REG00291868...	REG00291
0.00	2003-07-01 12...	E10138-014	Beth	REG00291868...	REG00291

Current Data

% Effect at Mi...	_hc_User exc...	Assay Date	Assay Noteb...	Assay Scientist	Compound
0.00		2006-01-25 12...	E11683-003	Beth	REG00291
0.00		2006-01-25 12...	E11683-003	Beth	REG00291
0.00		2006-01-25 12...	E11683-003	Beth	REG00291
0.00		2006-01-25 12...	E11683-003	Beth	REG00291
0.00		2006-02-15 12...	E11978-001	Beth	REG00371
0.10		2006-02-15 12...	E11978-001	Beth	REG00371
0.00		2006-02-15 12...	E11978-001	Beth	REG00371
0.00		2006-02-15 12...	E11978-001	Beth	REG00371
0.19		2006-02-15 12...	E11978-001	Beth	REG00285
0.56		2006-02-15 12...	E11978-001	Beth	REG00285
0.00		2006-02-15 12...	E11978-001	Beth	REG00285
0.00		2006-02-15 12...	E11978-001	Beth	REG00285
0.00		2006-03-08 12...	E11978-002	Beth	REG00371
0.00		2006-03-08 12...	E11978-002	Beth	REG00371

IC50 (historical) vs. Assay Date (historical)

12 Target Engagement Profile App

The **Target Engagement Profile (TEP)** app combines *in vivo* and *in vitro* data into a single, normalized graph corrected for plasma protein binding and calculates % inhibition over time.

Note that the critical *in vivo* PK assays and the *in vitro* assays must be annotated in the Signals Data Factory (SDF) system as the TEP app will load this data to perform the analysis. There are three **measurement type categories** which should be defined in SDF as a prerequisite to running the TEP App. Refer to the section Defining a New Measurement Type.

1. **PKStudy**: contains the *in vivo* PK parameters from the PK Parameters app, or another source
2. **PKDetail**: contains the *in vivo* raw data (i.e. mass spec data)
3. **pb**: contains the *in vivo* plasma protein binding data

The *in vitro* and *in vivo* assays should be published to Signals Inventa. The *in vitro* assay **Endpoint Unit** is especially important to include when publishing.

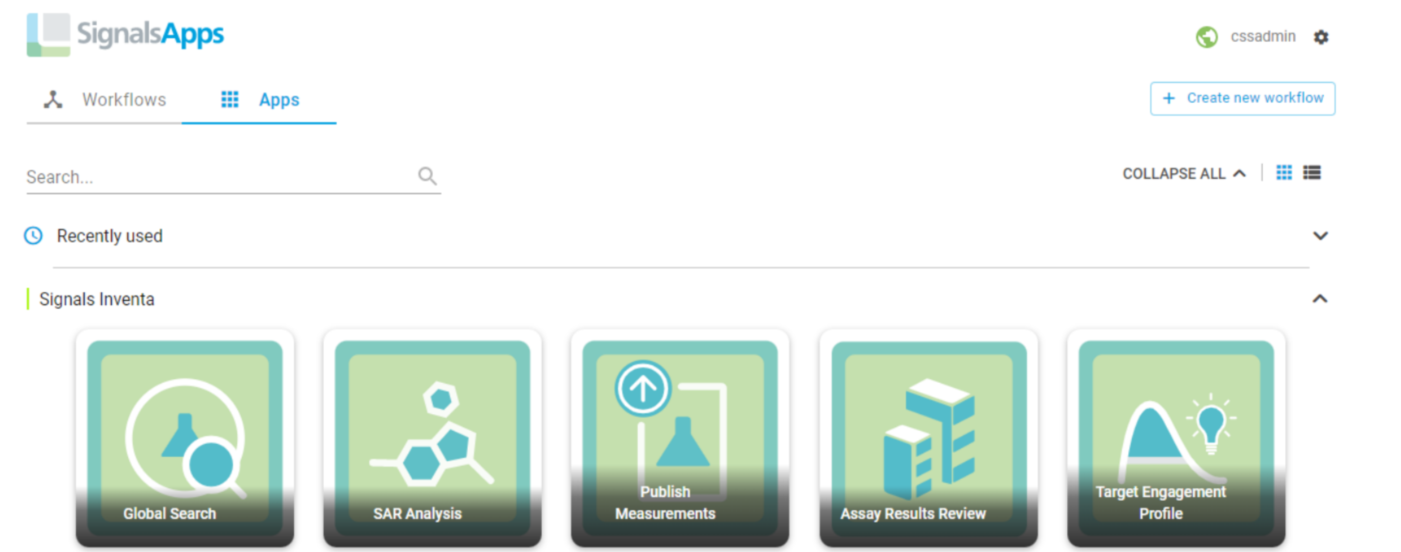
12.1 Accessing the Target Engagement Profile App

The **Target Engagement Profile** App is available in the Signals Apps store which is accessed through the main Spotfire® Interface.

To access the Target Engagement Profile App:

In Spotfire Analyst Client:

1. Select **Tools > Signals Apps**.
2. The **Workflows** tab opens by default. Select the **Apps** tab.

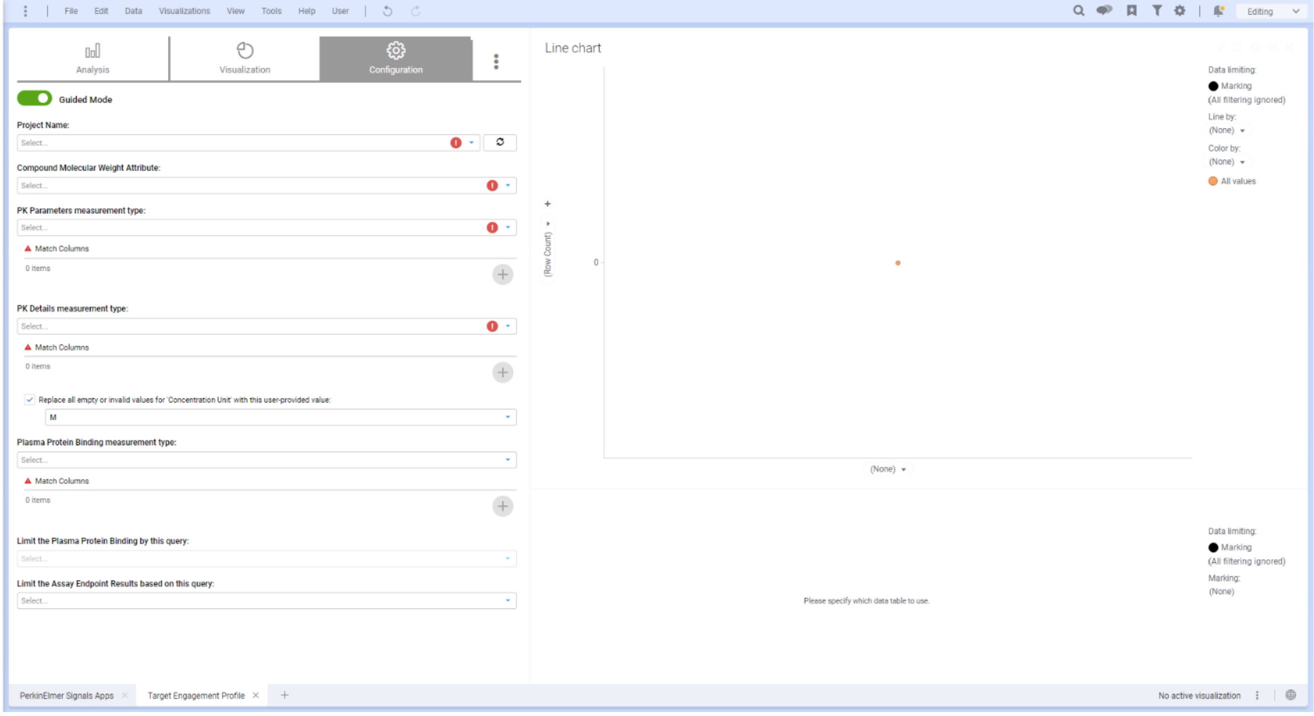


To launch the app, click anywhere on the **Target Engagement Profile** App card and it will be added to the document using the default app settings.

In Spotfire Web Player:

1. Open data in Spotfire.
2. Select **Tools > Signals Apps**.
3. The **Workflows** tab opens by default. Select the **Apps** tab.
4. To launch the app, click anywhere on the **Target Engagement Profile App** card and it will be added to the document using the default app settings.

A Target Engagement Profile page is displayed, similar to the example shown below. By default, the app opens to the **Configuration** tab.



12.2 Configuration Tab

In the **Configuration** tab the user can configure the source for the data types listed below. Mandatory fields contain an ❗ or ⚠ icon until an entry is selected or matched, respectively.

- **Guided Mode** – Enabled by default.
- **Project Name** – A dropdown to select the project to be used by the Target Engagement Profile app. By default, the app opens with the project defined in the Spotfire® preference (if applicable). Refer to Setting the Signals Data Factory Project Name preference for more information.
    - **Reload Data** – this icon refreshes the project data and will pull updates from SDF, if applicable.
- **Compound Molecular Weight Attribute** – A dropdown to select the compound/batch entity attribute that represents the molecular weight. This mapping is critical for unit conversion.

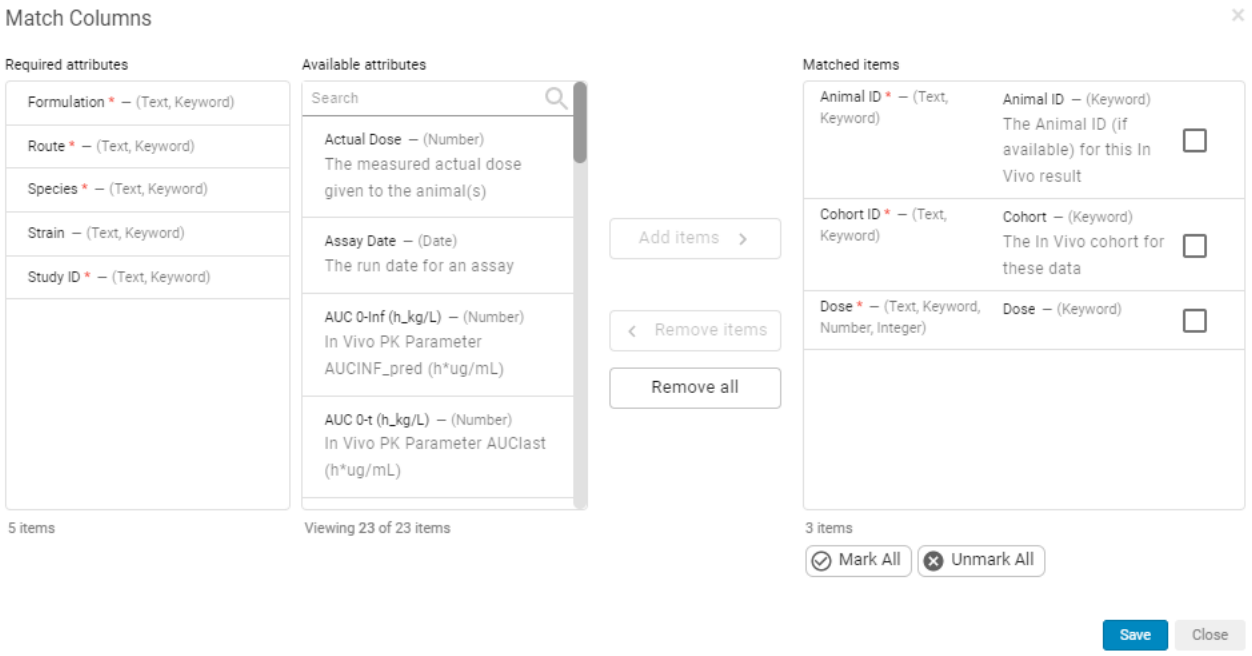
  Note: Both *in vitro* and *in vivo* measurement types must be associated with the same entity (either compound or batch, but not both compound and batches).
- **PK Parameters measurement type** – A dropdown to select the PK parameters measurement type. All measurement types (compound and batch) that have been tagged with the measurement type category **PKStudy** will be displayed. If none have been tagged, no entries will be listed.
    - Select the plus-sign **Add** icon to open the **Match Columns** UI. Match columns from the **Required attributes** and **Available attributes** lists then select **Add items** to match the two elements from both lists.

Note: The **Available attributes** displayed are the attributes associated with the selected PK Parameters measurement type. The **Required attributes** list contains the set of details that will be leveraged in the TEP App.

Matched items can be removed by selecting the entry in the **Matched items** list, then **Remove items.** The following elements must be matched prior to selecting **Save**:

- *Animal ID*
- *Cohort ID*
- *Dose*
- *Formulation*
- *Route*
- *Species*
- *Study ID*

Strain may be optionally mapped.



Required attributes

- Formulation * – (Text, Keyword)
- Route * – (Text, Keyword)
- Species * – (Text, Keyword)
- Strain – (Text, Keyword)
- Study ID * – (Text, Keyword)

5 items

Available attributes

- Actual Dose – (Number) The measured actual dose given to the animal(s)
- Assay Date – (Date) The run date for an assay
- AUC 0-Inf (h_kg/L) – (Number) In Vivo PK Parameter AUCINF_pred (h*ug/mL)
- AUC 0-t (h_kg/L) – (Number) In Vivo PK Parameter AUClast (h*ug/mL)

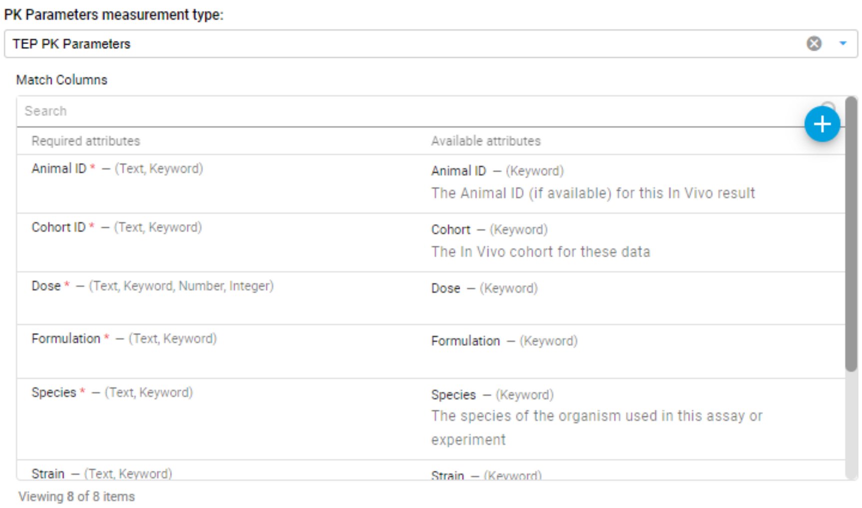
Viewing 23 of 23 items

Matched items

Animal ID * – (Text, Keyword)	Animal ID – (Keyword) The Animal ID (if available) for this In Vivo result	☐
Cohort ID * – (Text, Keyword)	Cohort – (Keyword) The In Vivo cohort for these data	☐
Dose * – (Text, Keyword, Number, Integer)	Dose – (Keyword)	☐

3 items

After selecting the **Save** button, the **Configuration** tab is updated with the matched columns.



PK Parameters measurement type:

TEP PK Parameters

Match Columns

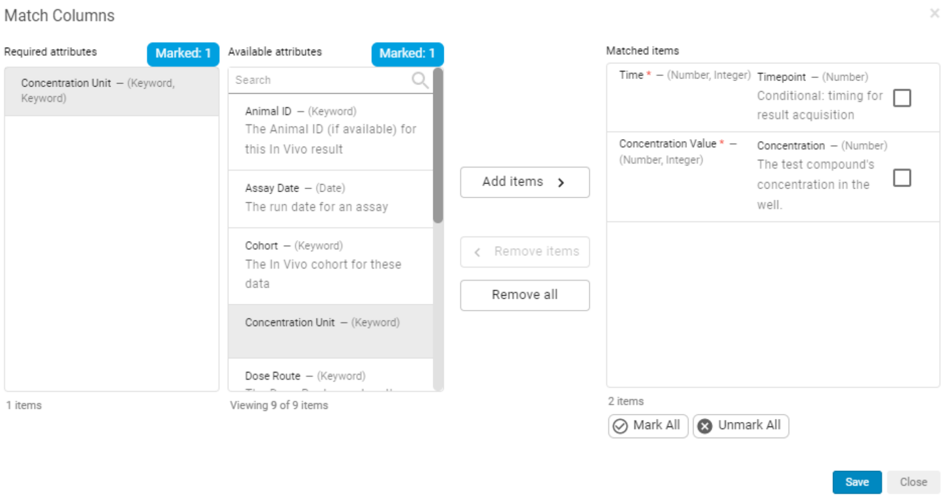
Search

Required attributes	Available attributes
Animal ID * – (Text, Keyword)	Animal ID – (Keyword) The Animal ID (if available) for this In Vivo result
Cohort ID * – (Text, Keyword)	Cohort – (Keyword) The In Vivo cohort for these data
Dose * – (Text, Keyword, Number, Integer)	Dose – (Keyword)
Formulation * – (Text, Keyword)	Formulation – (Keyword)
Species * – (Text, Keyword)	Species – (Keyword) The species of the organism used in this assay or experiment
Strain – (Text, Keyword)	Strain – (Keyword)

Viewing 8 of 8 items

- **PK Details measurement type** – A dropdown to select the PK details measurement type. All measurement types (compound and batch) that have been tagged with the measurement type category **PKDetail** will be displayed. If the **PK Detail** measurement type has already been configured as a detail measurement of the selected PK Parameters measurement type, the dropdown will automatically be set to the correct measurement type (recommended). If none have been tagged, then no entries will be listed. Refer to the section Configuring a Measurement Type as Details of another Measurement Type.
    - Select the plus-sign **Add** icon to open the **Match Columns** UI. Match columns from the **Required attributes** and **Available attributes** lists then select **Add items** to match the two elements from both lists. Matched items can be removed by selecting the entry in the **Matched items** list, then **Remove items**. Note that the following elements must be matched prior to selecting **Save**:
        - *Time*
        - *Concentration Value*

The attribute *Concentration Unit* may be optionally mapped.



Match Columns

Required attributes — Marked: 1

Concentration Unit – (Keyword, Keyword)

1 items

Available attributes — Marked: 1

Search

Animal ID – (Keyword)
The Animal ID (if available) for this In Vivo result

Assay Date – (Date)
The run date for an assay

Cohort – (Keyword)
The In Vivo cohort for these data

Concentration Unit – (Keyword)

Dose Route – (Keyword)

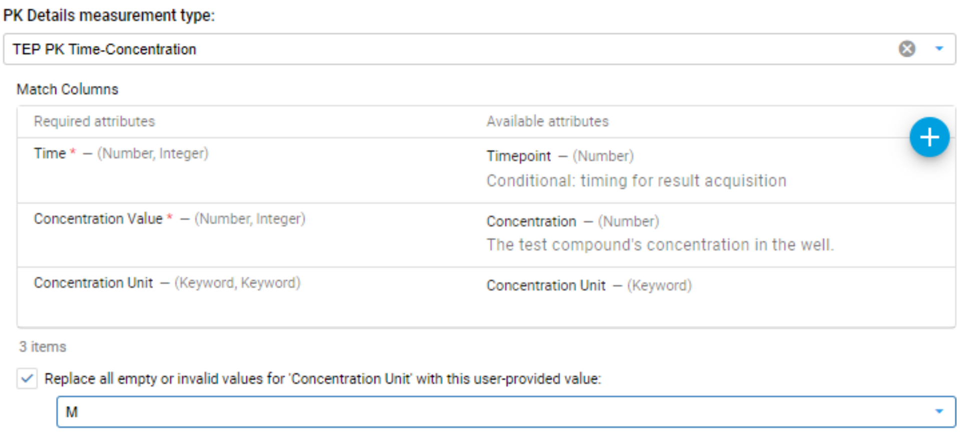
Viewing 9 of 9 items

Matched items

Time * – (Number, Integer)	Timepoint – (Number) Conditional: timing for result acquisition	☐
Concentration Value * – (Number, Integer)	Concentration – (Number) The test compound's concentration in the well.	☐

2 items

After selecting the **Save** button, the **Configuration** tab is updated with the matched columns.



PK Details measurement type:

TEP PK Time-Concentration

Match Columns

Required attributes	Available attributes
Time * – (Number, Integer)	Timepoint – (Number) Conditional: timing for result acquisition
Concentration Value * – (Number, Integer)	Concentration – (Number) The test compound's concentration in the well.
Concentration Unit – (Keyword, Keyword)	Concentration Unit – (Keyword)

3 items

☑ Replace all empty or invalid values for 'Concentration Unit' with this user-provided value:

M

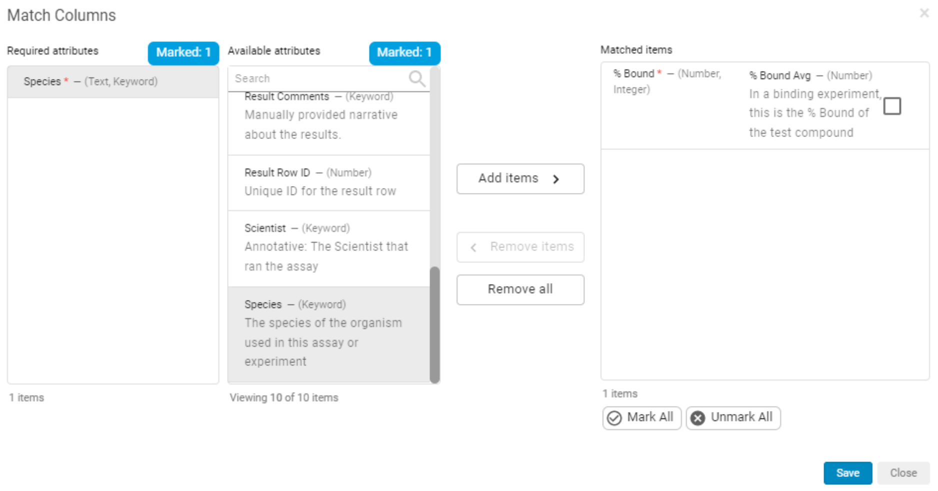
  - The checkbox *Replace all empty or invalid values for 'Concentration Unit' with this user-provided value* should be used in cases where an unsupported or no concentration unit has been specified and the user wishes to assign one of the supported units. These include g/L, mg/L, mg/mL, ug/mL, ng/mL, M, mM, uM, nM, pM, fM.

    Note: It is recommended that the user add a concentration unit column to their data and manually convert it to a supported concentration unit if one does not already exist.

- **Plasma Protein Binding measurement type** (Optional) – A dropdown to select the Plasma Protein Binding measurement type to perform normalization. All measurement types (compound and batch) that have been tagged with the measurement type category **Ppb** will be displayed. If none have been tagged, then no entries will be listed.

  - Select the plus-sign **Add** icon to open the **Match Columns** UI. Match columns from the **Required attributes** and **Available attributes** lists and select **Add items** to match the two elements from both lists. Matched items can be removed by selecting the entry in the **Matched items** list, then **Remove items**. Note that the following elements must be matched prior to selecting **Save**:

    - % Bound
    - Species



Required attributes: Species * – (Text, Keyword)

1 items

Available attributes:

Result Comments – (Keyword)
Manually provided narrative about the results.

Result Row ID – (Number)
Unique ID for the result row

Scientist – (Keyword)
Annotative: The Scientist that ran the assay

Species – (Keyword)
The species of the organism used in this assay or experiment

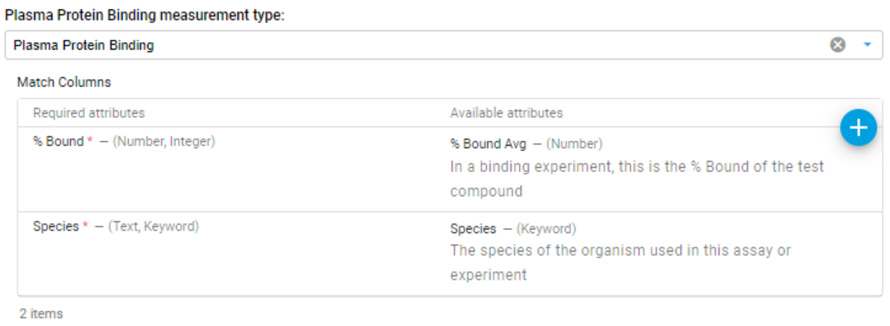
Viewing 10 of 10 items

Matched items:

% Bound * – (Number, Integer) | % Bound Avg – (Number) In a binding experiment, this is the % Bound of the test compound ☐

1 items

After selecting the **Save** button, the **Configuration** tab is updated with the matched columns.



Plasma Protein Binding measurement type:

Plasma Protein Binding

Match Columns

Required attributes	Available attributes
% Bound * – (Number, Integer)	% Bound Avg – (Number) In a binding experiment, this is the % Bound of the test compound
Species * – (Text, Keyword)	Species – (Keyword) The species of the organism used in this assay or experiment

2 items

- **Limit the Plasma Protein Binding by this query** (Optional) – A dropdown to select a saved **Global Search** query to limit the returned assays by a pre-defined criterion. Refer to the Saving a Global Search section for more information. Select the **X** icon to remove the selection, if desired.
- **Limit the Assay Endpoint Results based on this query** (Optional) – A dropdown to select a saved **Global Search** query to limit the returned assays by a pre-defined criterion. Refer to the Saving a Global Search section for more information. Select the **X** icon to remove the selection, if desired.

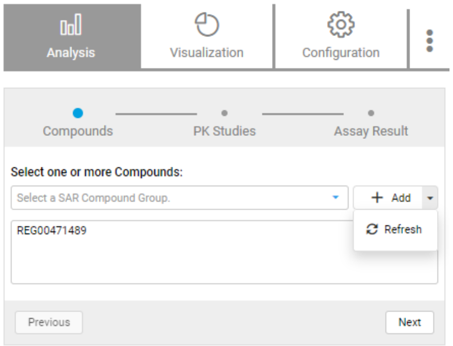
12.3 Analysis Tab

Once the user has completed the settings in the **Configuration** tab, select the **Analysis** tab to complete the *Compounds, PK Studies,* and *Assay Result* steps.

12.3.1 Compounds

In the *Compounds* step the user can specify one or more Compound IDs and/or Compound Batch IDs using the following methods to filter the **PK Parameters** measurement type to include only the desired IDs:

- **Select a SAR Compound Group** – This dropdown menu contains previously defined SAR Compound Groups. Refer to the Groups section under the SAR Analysis App for more information. Select the **+ Add** button to append the Compound IDs to a list in the textbox.
  - **Refresh** – This icon is available via the dropdown menu next to the **+ Add** button and will refresh the selected SAR Compound Group from the Signals Data Factory.
- **Input Compound IDs or Batch IDs** – This textbox allows users to manually input or copy/paste up to 2000 IDs.

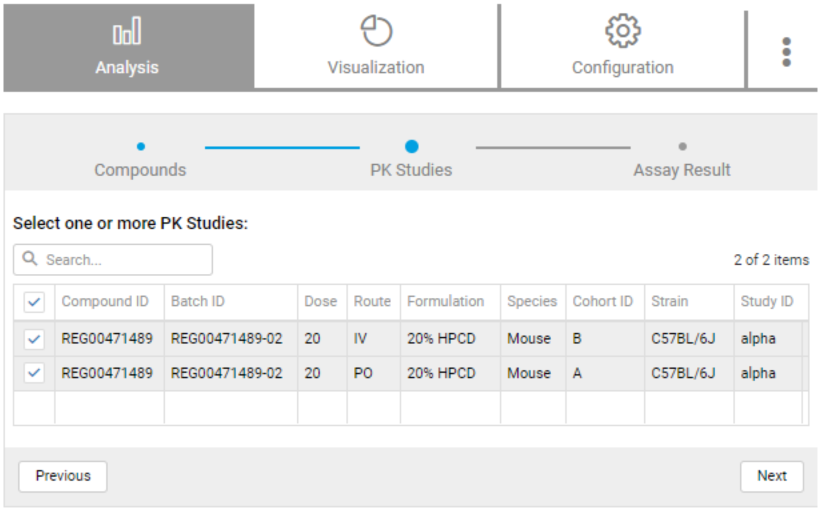


Select **Next** to move on the *PK Studies* step.

12.3.2 PK Studies

In the *PK Studies* step the user can specify one or more PK studies to include for downstream analysis via a summary table displaying the critical factors mapped in the **Configuration** tab. To remove a PK Study from the analysis, uncheck the box corresponding to the desired entry. Use the **Search** box to filter on any table value or click the column header to sort by a column.

Note: Only those PK studies with **PK Detail** level data and that are associated with the list of Compounds/Batches noted in the previous “Compounds” section will be displayed.



Select one or more PK Studies:

2 of 2 items

☑	Compound ID	Batch ID	Dose	Route	Formulation	Species	Cohort ID	Strain	Study ID
☑	REG00471489	REG00471489-02	20	IV	20% HPCD	Mouse	B	C57BL/6J	alpha
☑	REG00471489	REG00471489-02	20	PO	20% HPCD	Mouse	A	C57BL/6J	alpha

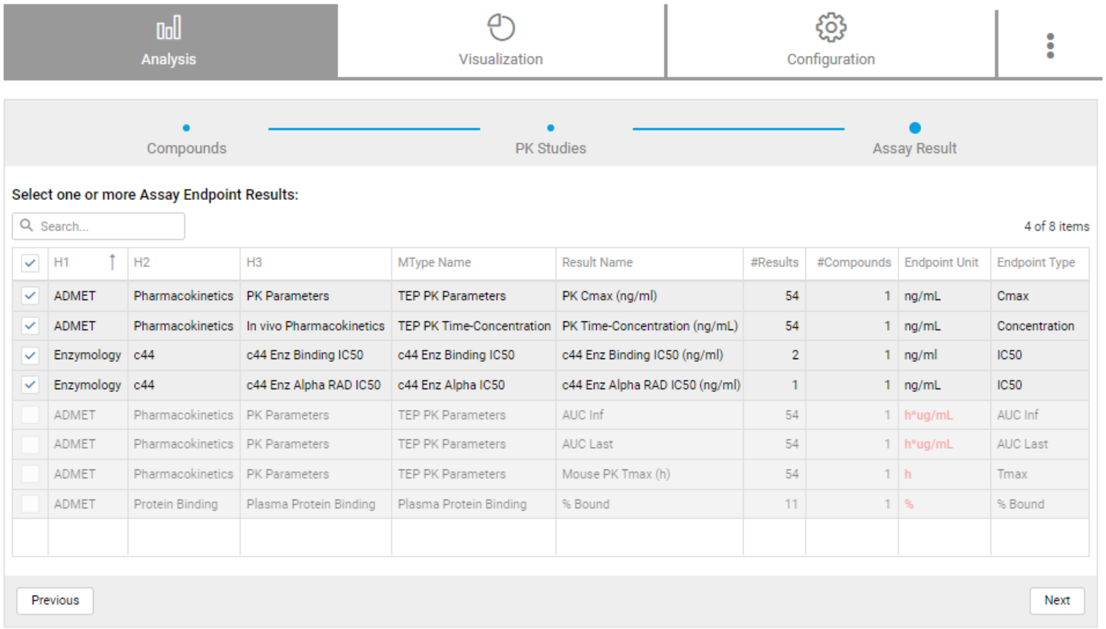
Select **Next** to move on the *Assay Result* step.

12.3.3 Assay Result

In the *Assay Result* step, the user can select the *in vitro* assays of interest. The displayed table consists of a list of endpoints that have been filtered by the previous two steps. Therefore, only those assay endpoints which have been tested with the compounds previously selected will be shown.

Note: All assays associated with *any* batch of a previously selected compound will be displayed.

Note: Endpoint units marked in red contain invalid units and will not be downloaded in the *Assay Endpoint Results* table. As such, the row containing the invalid endpoint unit is greyed out and cannot be included via the checkbox. To use this entry for downstream analysis, the user must manually convert the endpoint unit to one of the accepted units and then define the endpoint unit using the Managing Measurement Types Tool.



Select one or more Assay Endpoint Results:

4 of 8 items

☑	H1	H2	H3	MType Name	Result Name	#Results	#Compounds	Endpoint Unit	Endpoint Type
☑	ADMET	Pharmacokinetics	PK Parameters	TEP PK Parameters	PK Cmax (ng/ml)	54	1	ng/mL	Cmax
☑	ADMET	Pharmacokinetics	In vivo Pharmacokinetics	TEP PK Time-Concentration	PK Time-Concentration (ng/mL)	54	1	ng/mL	Concentration
☑	Enzymology	c44	c44 Enz Binding IC50	c44 Enz Binding IC50	c44 Enz Binding IC50 (ng/ml)	2	1	ng/ml	IC50
☑	Enzymology	c44	c44 Enz Alpha RAD IC50	c44 Enz Alpha IC50	c44 Enz Alpha RAD IC50 (ng/ml)	1	1	ng/mL	IC50
☐	ADMET	Pharmacokinetics	PK Parameters	TEP PK Parameters	AUC Inf	54	1	h*ug/mL	AUC Inf
☐	ADMET	Pharmacokinetics	PK Parameters	TEP PK Parameters	AUC Last	54	1	h*ug/mL	AUC Last
☐	ADMET	Pharmacokinetics	PK Parameters	TEP PK Parameters	Mouse PK Tmax (h)	54	1	h	Tmax
☐	ADMET	Protein Binding	Plasma Protein Binding	Plasma Protein Binding	% Bound	11	1	%	% Bound

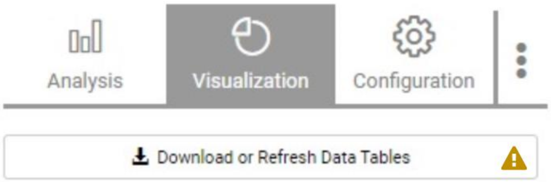
Note: In the above example, 4 of the 8 items will be downloaded to the *Assay Endpoint Results* table, as noted by the checkmark and black text. The remaining 4 items contain invalid endpoint units (highlighted in red text), the row has been greyed out and the checkbox cannot be enabled.

Select **Next** to move to the **Visualization** tab.

12.4 Visualizations Tab

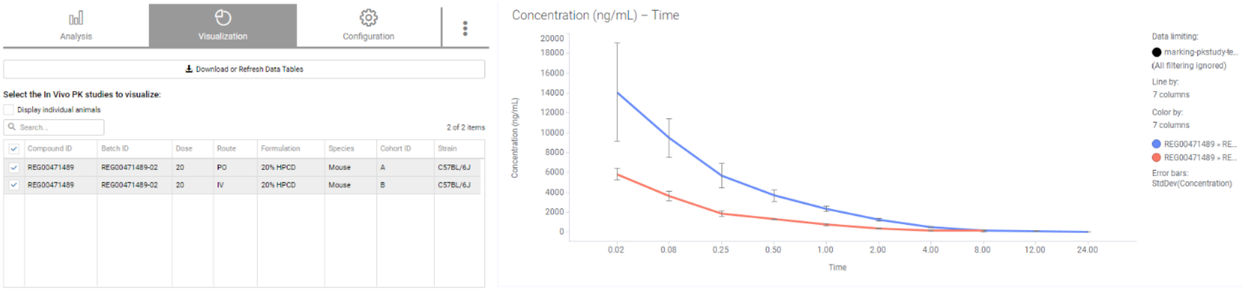
Once the user has completed the **Analysis** tab settings, the **Visualization** tab can be used to view and customize the *Concentration – Time* plot. The first time a user opens this tab no data will be loaded. To do so, select the **Download or Refresh Data Tables** button. This button may be used at any time to refresh the data tables from Signals Data Factory.

Note: The tables must be refreshed any time criteria set in the **Analysis** tab has been changed.



This tab contains the following options to customize the visualizations:

- **Select the In Vivo PK studies to visualize** – This section is used to control the PK studies displayed on the *Concentration – Time* plot by selecting the corresponding checkbox next to the PK Study of interest. By default, all entries in the table are selected.



Select the In Vivo PK studies to visualize:

☐ Display individual animals

Search... 2 of 2 items

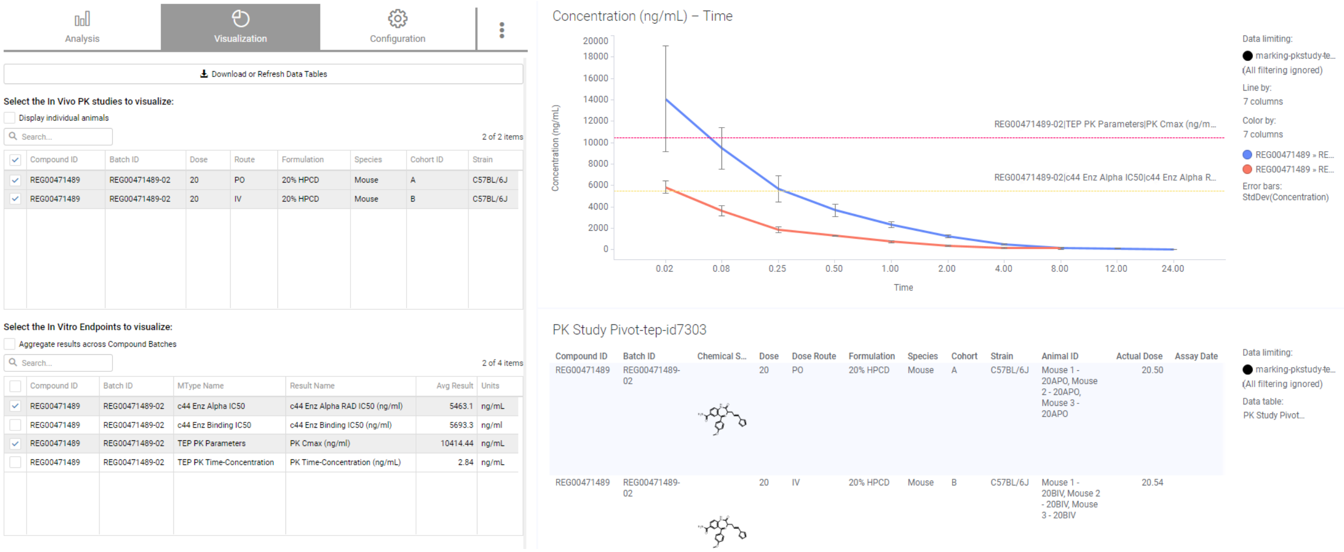
☑	Compound ID	Batch ID	Dose	Route	Formulation	Species	Cohort ID	Strain
☑	REG00471489	REG00471489-02	20	PO	20% HPCD	Mouse	A	C57BL/6J
☑	REG00471489	REG00471489-02	20	IV	20% HPCD	Mouse	B	C57BL/6J

Data limiting:
● marking-pkstudy-te...
(All filtering ignored)
Line by:
7 columns
Color by:
7 columns
● REG00471489 » RE...
● REG00471489 » RE...
Error bars:
StdDev(Concentration)

- ○ **Display individual animals** – By default the results for multiple animals are averaged (box unchecked). By selecting this checkbox, the table and plot in the right-hand panel will update to include details at the animal level.

- ○ **Search** – This textbox is used to filter PK studies for easier selection / deselection based on any table value. Selecting the checkbox next to the header 'Compound ID' will select/deselect only those rows displayed in the current view.

- **Select the In Vitro Endpoints to visualize** – This section is used to control the *in vitro* endpoints displayed on the *Concentration – Time* plot as a labelled horizontal line. Select the corresponding checkbox next to the endpoint of interest to add it to the plot. By default, no entries in the table are selected. If required, backend calculations are made such that the y-axis unit accurately represents the data.



Select the In Vivo PK studies to visualize:

☐ Display individual animals

Search... 2 of 2 items

☑	Compound ID	Batch ID	Dose	Route	Formulation	Species	Cohort ID	Strain
☑	REG00471489	REG00471489-02	20	PO	20% HPCD	Mouse	A	C57BL/6J
☑	REG00471489	REG00471489-02	20	IV	20% HPCD	Mouse	B	C57BL/6J

Select the In Vitro Endpoints to visualize:

☐ Aggregate results across Compound Batches

Search... 2 of 4 items

☐	Compound ID	Batch ID	MType Name	Result Name	Avg Result	Units
☑	REG00471489	REG00471489-02	c44 Enz Alpha IC50	c44 Enz Alpha RAD IC50 (ng/ml)	5463.1	ng/mL
☐	REG00471489	REG00471489-02	c44 Enz Binding IC50	c44 Enz Binding IC50 (ng/ml)	5693.3	ng/ml
☑	REG00471489	REG00471489-02	TEP PK Parameters	PK Cmax (ng/ml)	10414.44	ng/mL
☐	REG00471489	REG00471489-02	TEP PK Time-Concentration	PK Time-Concentration (ng/mL)	2.84	ng/mL

Data limiting:
● marking-pkstudy-te...
(All filtering ignored)
Line by:
7 columns
Color by:
7 columns
● REG00471489 » RE...
● REG00471489 » RE...
Error bars:
StdDev(Concentration)

PK Study Pivot-tep-id7303

Compound ID	Batch ID	Chemical S...	Dose	Dose Route	Formulation	Species	Cohort	Strain	Animal ID	Actual Dose	Assay Date
REG00471489	REG00471489-02		20	PO	20% HPCD	Mouse	A	C57BL/6J	Mouse 1 - 20APO, Mouse 2 - 20APO, Mouse 3 - 20APO	20.50	
REG00471489	REG00471489-02		20	IV	20% HPCD	Mouse	B	C57BL/6J	Mouse 1 - 20BIV, Mouse 2 - 20BIV, Mouse 3 - 20BIV	20.54	

Data limiting:
● marking-pkstudy-te...
(All filtering ignored)
Data table:
PK Study Pivot...

  - ○ **Aggregate results across Compound Batches** – By default different compound batches are displayed as individual endpoints (box unchecked). By selecting this checkbox, the table and plot in the right-hand panel will update to average endpoints using the same compound from different batches into a single endpoint.

  - ○ **Search** – This textbox is used to filter *in vitro* endpoints for easier selection / deselection based on any table value.

- **Calculation options** – This section provides options for instantly normalizing the data by including the selection of one of three radio buttons below, thus adjusting the *Concentration – Time* plot. Note that options 2 and 3 are only available if the Plasma Protein Binding measurement type was provided previously in the **Configuration** tab:

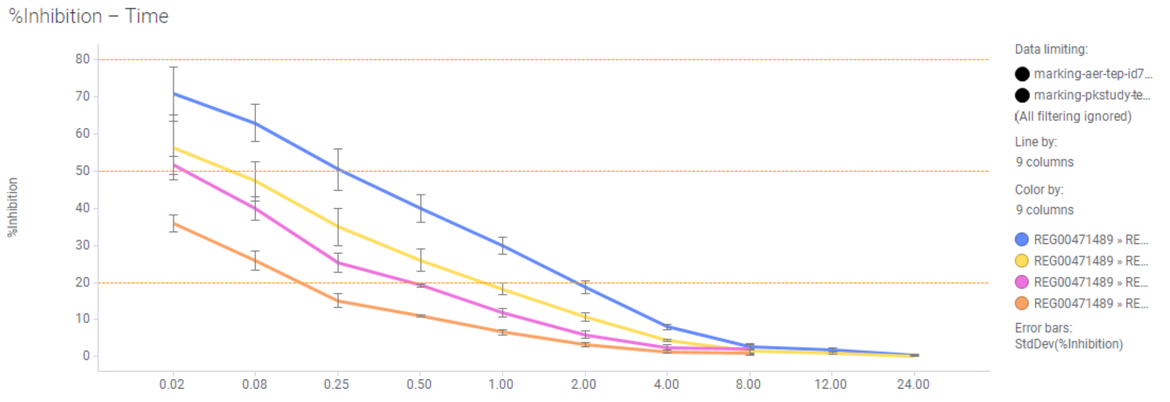
  1. Display raw PK Concentration values and raw Endpoint Results values (Default on)
  2. Adjust the Endpoint Results based on the Plasma Protein Binding
  3. Adjust the PK Concentration values based on the Plasma Protein Binding

  - **Calculate additional ICxx values based on the Hill slope of 1** – This textbox can be used to enter a desired IC value (1-99) to extrapolate and display as a horizontal line on the *Concentration – Time* plot. Note that multiple IC values can be added and should be separated by a comma or a space.

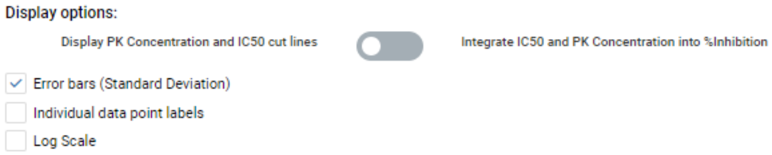
- **Display options** – The toggle can be used to adjust the axis of the plot to one of two options:
  - Display PK Concentration and IC50 cut lines (Default on)
  - Integrate IC50 and PK Concentration into % inhibition using the equation:

    % Inhibition = 100 / (1 + (10 ^ (Log10(Endpoint Result (ng/mL)) - Log10(Concentration (ng/mL)))))

    Note: The selected *in vitro* endpoints are not visible on the *%Inhibition – Time* plot, however by default a dotted line representing the IC50 is displayed, along with any ICxx values entered by the user. See example below where the IC20, IC50, and IC80 are displayed.



  - **Error bars (Standard Deviation) –** By default this setting is checked and displays the error bars for each data point in the *Concentration – Time* and *%Inhibition – Time* visualizations.
  - **Individual data point labels –** By default this setting is unchecked. When checked data points are added to the *Concentration – Time* and *%Inhibition – Time* visualizations.
  - **Log Scale –** By default this setting is unchecked. When checked the *Concentration – Time* visualization will be displayed in log scale for the y-axis.



Display options:

Display PK Concentration and IC50 cut lines ○ Integrate IC50 and PK Concentration into %Inhibition

☑ Error bars (Standard Deviation)

☐ Individual data point labels

☐ Log Scale

13 Appendix A: Workflows

A workflow is a formalization of both a set of Apps, their order of execution and their configuration. This concept allows the users to string several Apps together, run different types of analysis with the same app, create and maintain different variants of the same study, etc.

This feature allows to easily share ideas and collaborate to improve them. To achieve it, a workflow can have a private visibility (when set to Draft) or public (when set to Published). Draft workflows can only be seen by their creator (and thus only them can edit or publish them), whereas Published workflows are visible and editable by all members of the group.

Note: Only the original creator can set a workflow back to draft.

Workflows are a key concept within Signals Apps and thus can be accessed directly from the Signals Apps homepage.

Note: Certain apps may not support the use of multiple instances within the same document.

The Workflows storage must be configured by a Spotfire administrator.

13.1 Role Based Permissions

Workflow management can be limited to specific users or groups of users by setting up roles using the *Signals Apps Workflows Role - Admin* and *Signals Apps Workflows Role - Author* licenses. By default, everyone has a consumer role, unless any of the aforementioned licenses are granted, in which case, the least restrictive of the granted licenses will apply (thus setting the role).

When the user role does not allow a certain interaction, then the controls in the system will not be present.

Action	Roles		
	Consumer	Author	Admin
See and execute published owned Workflows	✓	✓	✓
See and execute draft owned Workflows	✓	✓	✓
See and execute published unowned Workflows	✓	✓	✓
See and execute draft unowned Workflows	✗	✗	✓
See and execute Out-of-the-Box Workflows	✓	✓	✓
Add a new Workflow	✗	✓	✓
Add a new Out-of-the-Box Workflow	✗	✗	✗
Delete an owned Workflow	✗	✓	✓
Delete an Out-of-the-Box Workflow	✗	✗	✗
Edit an owned Workflow	✗	✓	✓
Edit an Out-of-the-Box Workflow	✗	✗	✗
Clone an owned Workflow	✗	✓	✓
Clone an Out-of-the-Box Workflow	✗	✓	✓
Delete an unowned Workflow	✗	✗	✓
Edit an unowned Workflow	✗	✗	✓

Clone an unowned Workflow	✗	✓	✓

The optimal way of distributing licenses to a large number of users is to create groups and assign the users to the groups. That ensures that all users in a group are granted the same license.

Signals Inventa provides a framework in which to create analysis Workflows that can be easily applied to different datasets provided these datasets follow the same structure as the ones used to design the Workflow.

This framework can be used in three different manners that differentiate three clear user roles:

- **Consumer Role:** A user that is not necessarily an expert in the use of Spotfire® and will typically be an expert in the field that will execute the analysis Workflow created by the author and interpret the results. They will not modify the Workflow although they may add additional downstream analysis steps using either Spotfire®, or other analysis Apps. Consumers have access to all published (non-draft) Workflows, but cannot add new Workflows or delete, edit, or clone existing Workflows.

- **Author Role:** An expert Spotfire® user that understands the context of the analysis that needs to be performed and will create the standard analysis Workflows to be used by the Consumers. Authors have access to all published Workflows and their owned draft Workflows. Workflow authors can add new Workflows and are also able to delete and edit their owned Workflows. Lastly, they can clone any Workflow they have access to.

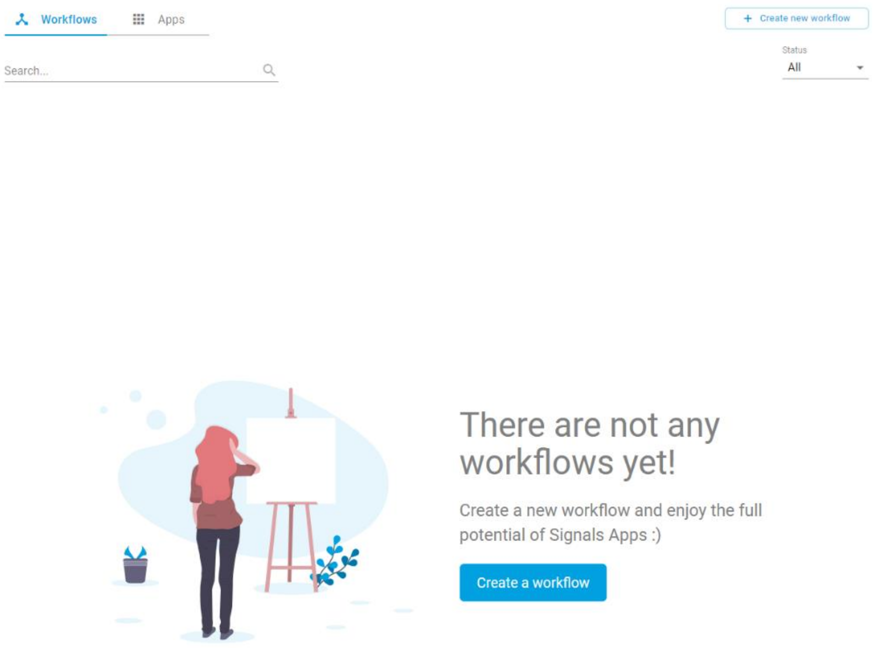
- **Admin Role:** Admins have full access to draft or published Workflows and can create, delete, edit (except Out-of-the-Box Workflows), or clone Workflows regardless of whether they own them.

13.2 Creating a workflow

This process will be performed by the author or admin roles.

A Signals Inventa Workflow consists of a series of Apps that are executed consecutively to produce the desired analysis. Standard apps can be added one after another in the document by simply clicking on them in the Signals Apps page and following the steps required in the App to perform the corresponding analysis. In most cases, Aps are restricted to one instance per document.

A workflow can be created using the **+ Create new workflow** button on the top right area of the Signals Apps homepage within the Workflows tab. Also, when there are no available workflows, another **Create a workflow** button will appear in the center of the page.



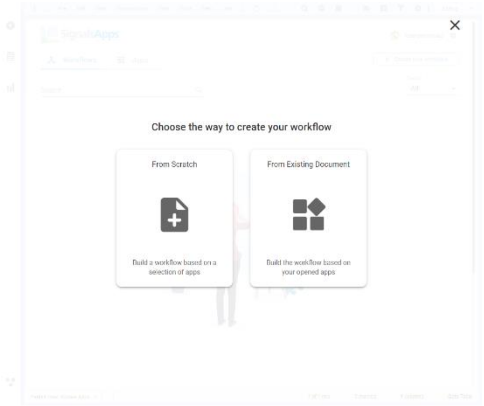
There are not any workflows yet!

Create a new workflow and enjoy the full potential of Signals Apps :)

When clicking on any of these buttons the user will be presented with an overlay to choose the workflow creation method. If the user wishes to cancel the creation, there's an "x" button on the top right corner.

This will display two different options for creating the workflow:

- **From Scratch:** Select this if you would like to create a workflow in an empty document.
- **From Existing Document:** Select this option if you have a set of apps already present in the document that you would like to save as a workflow.


Choose the way to create your workflow

From Scratch

Build a workflow based on a selection of apps

From Existing Document

Build the workflow based on your opened apps

13.2.1 Creating a workflow from scratch

After choosing to create a workflow from scratch, an App selection screen will appear.

Apps can be filtered using the “Search” filter and added to the workflow simply by clicking on them. All added Apps will be shown on the panel available on the right side, which also provides controls to reorder or remove them from the workflow.

The **Discard** button available at the top right corner of the app selection area cancels the creation process and returns the user to the homepage. Finally, at the bottom of the right panel there are two buttons: the **Clear** button removes all apps from the workflow and the **Configuration** button guides the user to the next step.

After clicking on the **Configuration** button, the user will be able to navigate the workflow configuring each App in the process. At the end of the navigation and configuration process, clicking on the **Summary & Save** button of the workflow navigator will lead you to the last stage.

In the last stage the user will have to provide a unique name, choose a (new or existing) category, write a description (optional) and choose whether the workflow will be saved as draft or be published. Once the user is ready, the blue **Save** button will save the workflow and the system will return to the homepage. Hitting the **Cancel** button will return the user to the homepage, discarding the workflow (a confirmation dialog will be shown to ensure nothing is accidentally lost).

13.2.2 Creating a workflow from an existing document

If the user has created an analysis workflow in the document using the different Apps, it can be saved in the App store by selecting the workflows tab and clicking on Save as workflow.

After choosing to create a workflow from existing document, the last stage of the workflow creation process will be shown.

Just like creating a workflow from scratch, the user will have to provide a unique name, choose a (new or existing) category, write a description (optional) and choose whether the workflow will be saved as draft or be published. Once the user is ready, the blue **Save** button will save the workflow and the system will return to the homepage. Hitting the **Cancel** button will return the user to the homepage, discarding the workflow (a confirmation dialog will be shown to ensure nothing is accidentally lost).

It is important to understand that when creating a workflow from existing document, it is not necessary to navigate the workflow. This occurs because the apps from the document, their configuration and their order are used to create and configure the workflow.

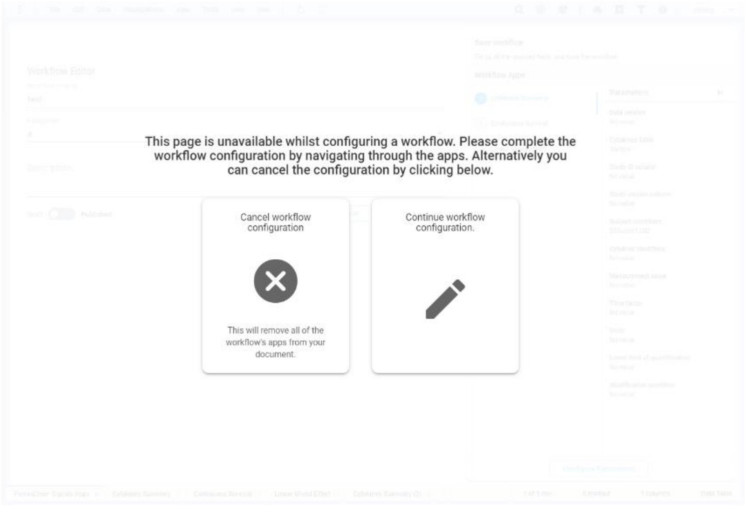
13.3 Workflow Navigation

When navigating a workflow, the workflow navigator panel will be embedded in the app and will allow the user to navigate (forwards and backwards) the workflow while configuring and executing the apps. Since a workflow can be executed in edition mode (creating from scratch, editing, cloning), in those cases the last app will include a **Summary & Save** button that records the changes made through the execution of the workflow. During normal executions, for the first and last app, the **Previous** and **Next** buttons will be disabled accordingly.

When moving forwards, the new apps’ pages will be added with all the settings configured to the same values as were used when initially saving the workflow. This allows the user to easily repeat the same type of analysis on different datasets with a minimum number of clicks.

Note: If a workflow contains one or more apps that do not support Web Player execution, then the workflow will not be supported in Web Player.

If during an execution in edition mode the user attempts to return to the homepage, an overlay will be shown to ensure the user continues the execution or correctly cancel the process (acknowledging the loss of changes).



This page is unavailable whilst configuring a workflow. Please complete the workflow configuration by navigating through the apps. Alternatively you can cancel the configuration by clicking below.

13.4 Editing a Workflow

The Workflow edition screen can be accessed through the **More actions** '…' icon on the Workflow card controls, or from the **Edit** button at the bottom of the Workflow's details panel. Note that this option is not available for Out-of-the-Box Workflows.

After choosing to edit a workflow, the system will navigate to the workflow edition screen.

Similarly to creating a workflow from scratch, the user will be able to edit the unique name, choose a (new or existing) category, edit the description and choose whether the workflow will be saved as draft or be Published.

The user can expand the **Instructions** area in the '**Save Workflow**' area to add App specific instructions for each App in the Workflow. Once the user is ready, the blue save button will save the Workflow and the system will return to the homepage. Selecting **Cancel** will return the user to the homepage, discarding the changes made to the Workflow (a confirmation dialog will be shown to ensure nothing is accidentally lost).

Also, the user can click the **Configure Parameters** button (located at the bottom of the right side panel) to execute the workflow in edition mode and reconfigure the App's parameters. The right-hand side panel also contains other controls that allow the user to further customize the workflow.

13.4.1 Parameter Locking

Parameters can be locked to edition (this prevents modification of their configured values during later executions) by clicking the App, hovering over the desired parameter and clicking on the corresponding Lock icon. Note that the parameter locking is only supported for SDK based Apps. The Global Search App does not support parameter locking.

Signals Inventa App	Support Parameters	Support Parameter Locking
Global Search	×	×
SAR Analysis	✓	✓
Publish Measurements	✓	✓
Assay Results Review	✓	✓
Target Engagement Profile	✓	✓

Note: Parameter Locking in Publish Measurements Apps

1. When the "Mapping name" is locked, the data grid UI for editing the map content is also locked.
2. Locking is done by disabling the UI components for the parameter, and the data model for the parameter is not locked. This means that a locked parameter may still be changed by other unlocked parameters depending on their relationship. For example, if the user locks "Mapping name", but does not lock the "Select Measurement Type", the "Mapping name" will be reset once the user changes "Select Measurement Type". In this case, user may need to also lock the "Select Measurement Type".

13.5 Cloning a workflow

The workflow cloning screen can be accessed through the workflow card controls or using the split button found at the bottom of the workflow's details panel.

After choosing to clone a workflow, the system will navigate to the workflow cloning screen.

Just like creating a workflow from scratch, the user will have to provide a unique name, choose a (new or existing) category, write a description (optional) and choose whether the workflow will be saved as draft or be published. Of course, since the workflow is being cloned, these values will be provided by default using the original workflow as template. Once the user is ready, the blue **Save** button will save the workflow and the system will return to the homepage. Hitting the **Cancel** button will return the user to the homepage, discarding the workflow (a confirmation dialog will be shown to ensure nothing is accidentally lost).

Also, the user can click the **Configure Parameters** button (located at the bottom of the right side panel) to execute the workflow in edition mode and reconfigure the App's parameters. Refer to Workflow Navigation section. As expected, once the workflow is saved, a new cloned workflow will be available in the homepage.

13.6 Deleting a workflow

The Workflow deletion button can be accessed through the workflow card controls and will ask for confirmation to ensure the workflow is not accidentally deleted. Note that this option is not available for Out-of-the-Box Workflows.

13.7 Running a workflow

Consumers can access those app workflows that have been created and stored in the app store by the authors and use them to perform complex analysis with a few simple clicks.

To use an Apps workflow the consumer should follow these steps:

- Have a dataset supported by the workflow available. This would be a dataset that has the equivalent columns/parameters to those that are needed in the workflow.
- Choose the desired workflow. A workflow can be executed using the **Execute workflow** button (that has a “play” icon) available in the workflow card controls or using the **Run** button found at the bottom of the workflow’s details panel.
- After clicking on either button, the workflow will be executed in normal mode (see Workflow navigation) and any changes made to the app’s configuration will only be present in the App’s pages corresponding to this specific workflow execution.
- In the first step of the workflow the user will need to either input the data in one of the data entry apps, which will automatically match the required data fields to the workflow requirements or match the data explicitly with the required fields if the first step of the workflow is a Calculations Explorer App (Signals VitroVivo) .
- After the initial data is matched, navigation through the workflow can be easily done by clicking on the forward and back arrows to move through the different steps. Adding when needed any extra input from the user required for the analysis.

13.7.1 Workflow Panel

The Workflow panel allows the user to review all the Workflow’s details and perform certain actions.

The Workflow panel can be accessed via the **Show/hide workflow panel** button located on the right-hand side of the Workflow navigator. The Workflow panel will appear on the right-hand side of the screen and its upper part will show the main information of the Workflow and its lower part will contain a list of the Apps that compose the workflow. Please note that:

- The active App is highlighted in blue.
- If any of the Apps’ parameters has been locked, the App will indicate it contains locked parameters by also displaying a lock next to it.

The upper part of the Workflow panel will include an ellipsis (…) button with some available actions:

- **Generate report**, which allows you to generate a pdf report of the Workflow execution.
- **Cancel Workflow**, which allows the user to cancel the Workflow execution and close all its Apps’ tabs.

13.8 Workflow Reports

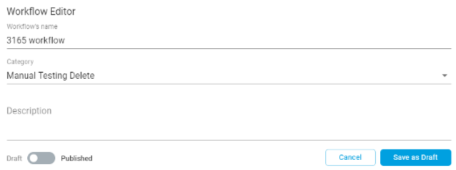
The user can configure the report that the Workflow will generate and will be able to choose which Apps and data to include. This can be accessed by clicking on the **Open Report Setup** button found on the top right of the right-hand side panel, located next to **Save workflow** available during Workflow edition. Refer to Editing a Workflow. Any user can check the report settings in read only mode by opening a Workflow and selecting the ⋮ icon, followed by **Report settings.**

The report can be generated using the “Generate report” button from the Workflow panel available during the execution of the Workflow.

13.9 Workflow Instructions

The user can work with the Workflow panel during the Workflow creation or edition phase to configure the instructions to be displayed in the Workflow panel (during use phase) and in the Workflow details sidebar (in the main Workflows page).

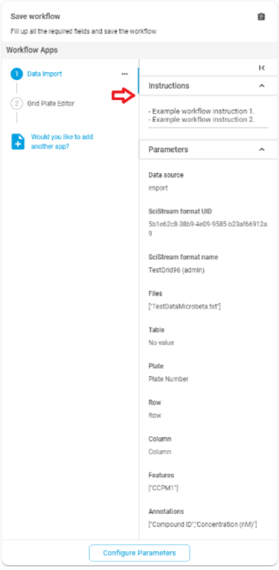
A Workflow developer may edit the Workflow instructions by simply opening the Workflow panel, then navigating to the relevant App and finally opening the Workflow panel and expanding the **Instructions** section. Please note that the format entered for the instructions will be used to display them later.



Workflow Editor

Workflow's name: 3165 workflow

Category: Manual Testing Delete



Save workflow

Fill up all the required fields and save the workflow

- Example workflow instruction 1.
- Example workflow instruction 2.

Data source: import

SciStream format UID: 5b1e62c8-38b9-4e09-9585-b23af66912a9

SciStream format name: TestGrid96 (admin)

Files: ["TestDataMicrobeta.txt"]

Table: No value

Plate: Plate Number

Row: Row

Column: Column

Features: ["CCPM1"]

Annotations: ["Compound ID","Concentration (nM)"]

13.10 Exporting Workflows

To export Workflows, select the **Settings** dropdown (*Cog Wheel icon*) and **Export workflows**. The user may also hover over the lower right-hand corner of a Workflow card to reveal a white circle which will activate selection mode when selected. Note the user can expect the same behavior with the “List mode” view active.

With the selection mode active, the user can select the Workflow(s) which they would like to export by selecting the corresponding Workflow card. Note the button with the text ‘**2 SELECTED WORKFLOWS’**, which displays the number of currently selected Workflow. Select the X next to the button to close the selection mode.

Additionally, note the checkbox in the lower right-hand corner of the Workflow card which indicates the Workflow has been selected for exporting, and is shown in full color so that it can be easily differentiated from the unselected Workflows.

If the user wants to see the Workflow details, select the information icon when hovering over a Workflow.

When the user is ready to export the selected Workflow(s), select **Export** and a popup appears to save the Workflow(s) as a local .zip file with the generic file name “exported-worflows.zip”, by default.

13.11 Importing Workflows

To import Workflows, select the **Settings** dropdown (*Cog Wheel icon*) and **Import workflows**.

An **Open File** dialog will appear, prompting users to navigate to and select a .json file with the Workflow definition or a .zip file containing one or more .json files with the Workflow definitions. Refer to Exporting Workflows for details on how to export Workflows.

Select **Open** to import the Workflow(s). When the process is complete, the imported Workflows will appear in the Workflows page.

13.12 Synchronizing Workflows for Offline Usage

If the user often works offline, it is in their best interest to keep the offline cache of Workflows synchronized. To do so, the user will have to select the **Settings** dropdown (*Cog Wheel* icon) located on the top right-hand corner of the Signals Apps page and select **Sync workflows for offline usage**. The system will then connect to the Spotfire® Library and synchronize all available Workflows.

Note: This process might take a while and may be canceled in the displayed progress dialog.

It is important to understand that the system will update the offline version of any Workflow interacted with, but there are certain cases (such as when configuring a system for the first time) that it will be useful to perform a full synchronization.

14 Appendix B: Signals Data Factory

Signals Data Factory (SDF) is an infrastructural component which provides data transforming, indexing and query capabilities for Signals Inventa. After the measurement metadata has been correctly defined and measurement data is in Spotfire, you are able to publish the measurements into the Signals Data Factory such that the measurement data can be transformed and indexed and then searched using complex queries in Signals Inventa's Global Search.

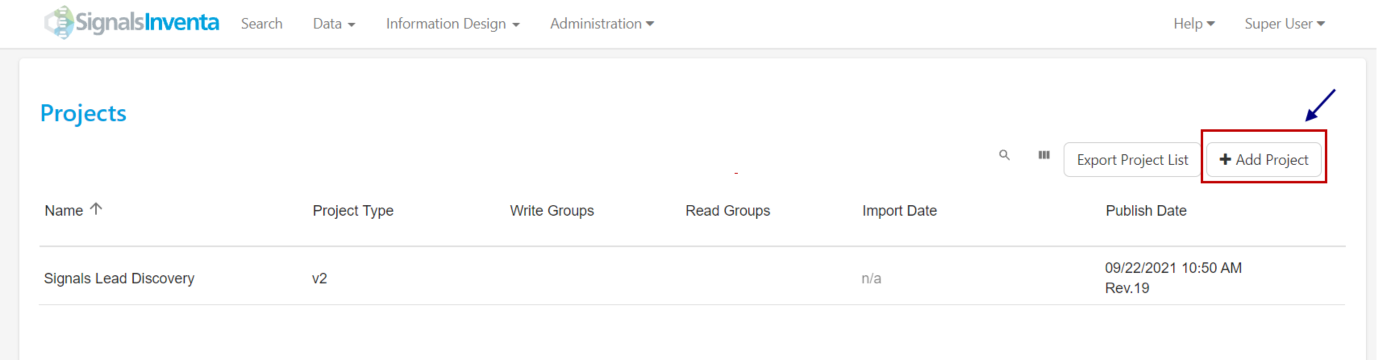
The Signals Data Factory version can be identified from **Help > About**.

14.1 Projects

In the Signals Data Factory, data is organized by project. Before you can publish measurement data into the Signals Data Factory, a project needs to be created.

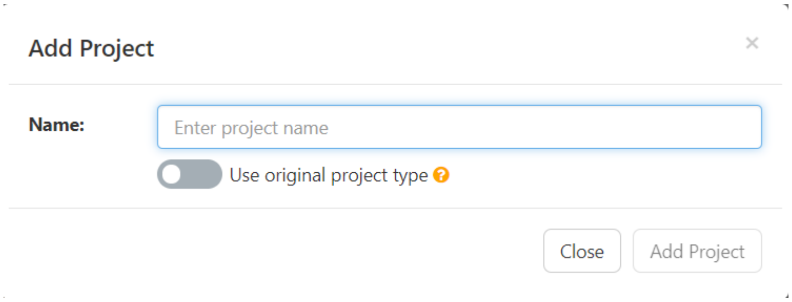
To create a project:

1. Log in to Signals Data Factory with username and password.
2. From **Data** menu, click **Projects.**
3. In the **Projects** page, in the upper-right corner of the project list, click **Add Project** button.



Name	Project Type	Write Groups	Read Groups	Import Date	Publish Date
Signals Lead Discovery	v2			n/a	09/22/2021 10:50 AM Rev.19

4. In the **Add Project** dialog, choose a name for your project.



5. A 'Use original project type' toggle is available for you to choose the project type. By default, this toggle is disabled and will create a V2 project type (incremental project) which includes load-new and datasets

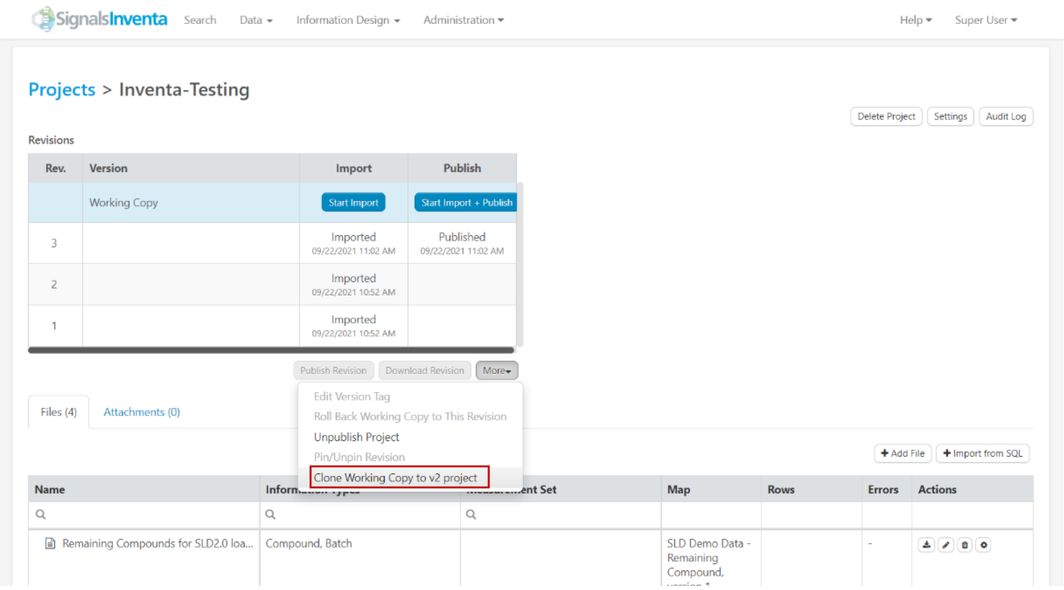
functionality. You can create an original project type (V1) by clicking the slider bar which excludes load-new and dataset functionalities. Use this toggle to define the project type.

6. Click on the **Add Project** button to append the Project to the Projects list. The Project Type will be listed as v1 (original) or v2 on the Projects page.

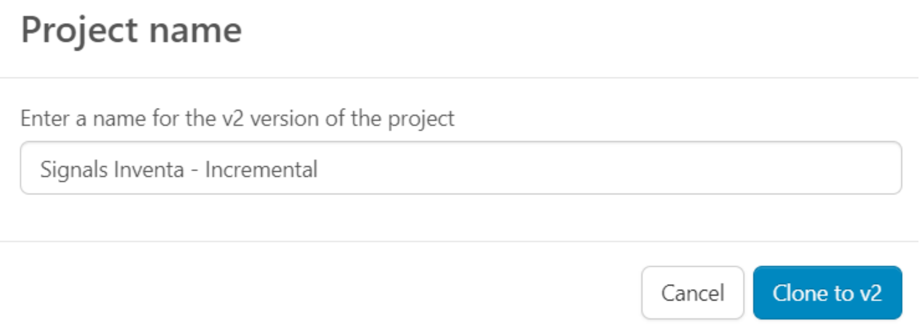
To convert a v1 (original) project to v2 (incremental project):

If you have an original project (v1) that you want to convert to an incremental project (v2), you have the option to do this from the original project.

1. From the Projects details page, select the ‘Clone Working Copy to v2 project’ sub-menu item from the More drop-down menu.



2. Enter a name for the v2 version of the project.



Enter a name for the v2 version of the project: Signals Inventa - Incremental

3. Click the **Clone to v2** button.

The v2 version of the product be appended to the Projects list page.

14.2 V1 Projects

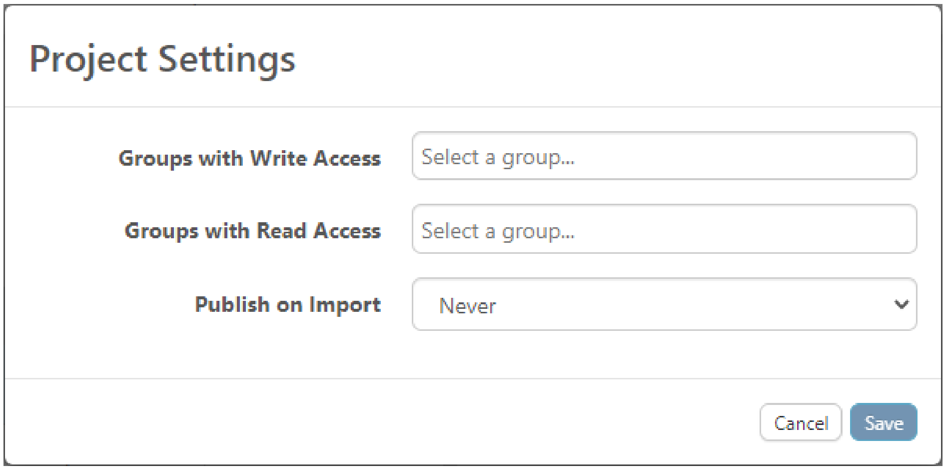
14.2.1 Configuring Project Permissions

Signals Data Factory also allows administrators to configure the permissions on projects, such that the projects can only be seen or be used by users belonging to specific groups.

To configure the project permission for V1 project:

1. Login Signals Data Factory with an administrator account.
2. From **Data** menu, click **Projects.**
3. In the project list, choose a project for which you want to configure the permission. This will open the project page.
4. From the upper-right corner of the page, click **Settings** button.

5. In the **Project Settings** pop-up dialog, specify the groups in the **Groups with Write Access** and **Groups with Read Access** text boxes. This grants the users under the specified group to have read or write permission on the current project.



Project Settings

Groups with Write Access: Select a group...

Groups with Read Access: Select a group...

Publish on Import: Never

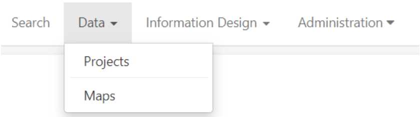
6. Click **Save** button to save the changes and close the dialog.

Note: By default, only administrative users (i.e. users who have ROLE_ADMIN or ROLE_SUPERADMIN) can see all the projects in Signals Data Factory. Non-administrative users will not be able to see any of the projects unless they have been granted permissions for the projects.

14.2.2 Adding a File

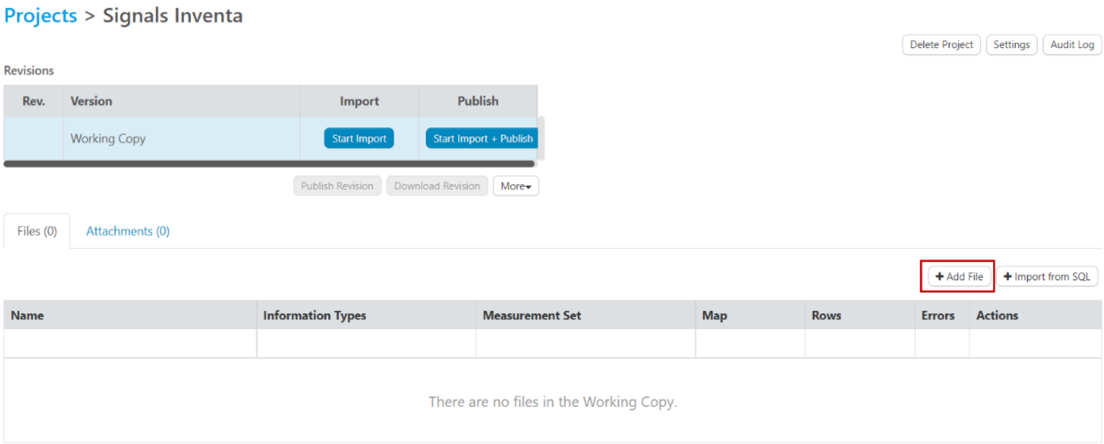
To add a new File to the project:

1. Click **Data > Projects**.



2. In the **Projects** page, click the name of the project to which you want to add a file.

3. In the Project Details page, click the **Add File** button in the upper-right corner of the Files list.



Rev.	Version	Import	Publish
	Working Copy	Start Import	Start Import + Publish

Name	Information Types	Measurement Set	Map	Rows	Errors	Actions

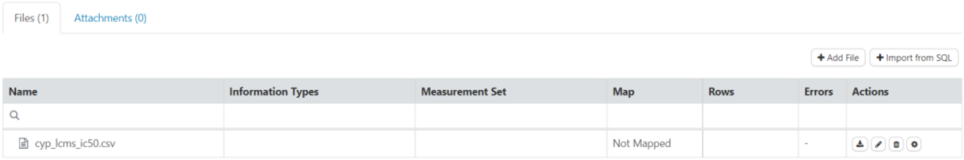
There are no files in the Working Copy.

4. In the **Upload Files to Project** dialog, either drag-and-drop the file into the dashed rectangle or click on the rectangle to choose the file to be uploaded

Drag and drop files here, or click here to select a file.

Note: Only text files in tabular format, such as comma-separated values (CSV), tab-separated values (TSV) are supported in Signals Inventa.

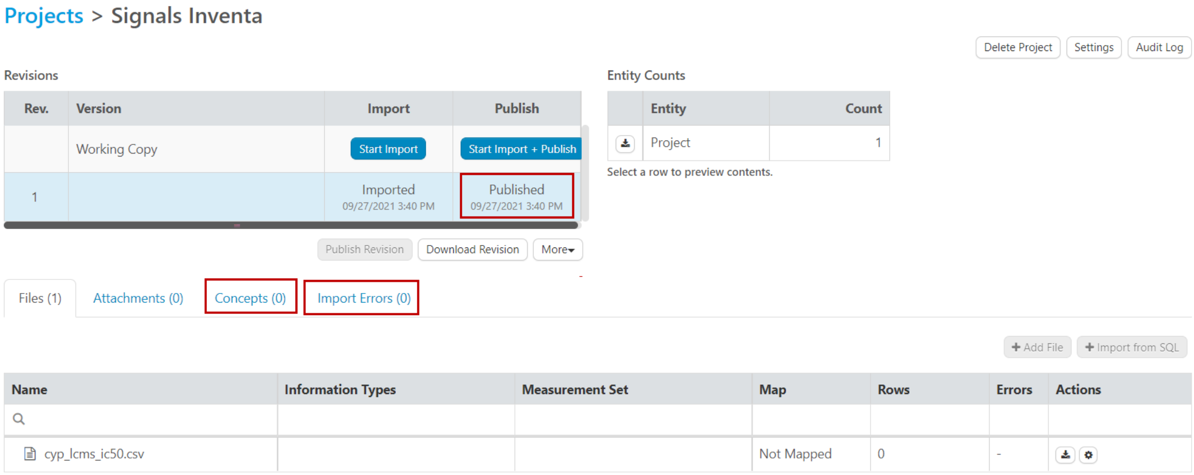
5. After the file has been added to the project, it will be displayed in the **Files** grid.



Name	Information Types	Measurement Set	Map	Rows	Errors	Actions
cyp_lcms_ic50.csv			Not Mapped		-	

For information on adding attachments to projects, refer to Attachments section.

If viewing a published version of a project, you will note that two additional tables are available: Concepts and Import Errors.



Revisions

Rev.	Version	Import	Publish
	Working Copy	Start Import	Start Import + Publish
1		Imported 09/27/2021 3:40 PM	Published 09/27/2021 3:40 PM

Entity Counts

	Entity	Count
	Project	1

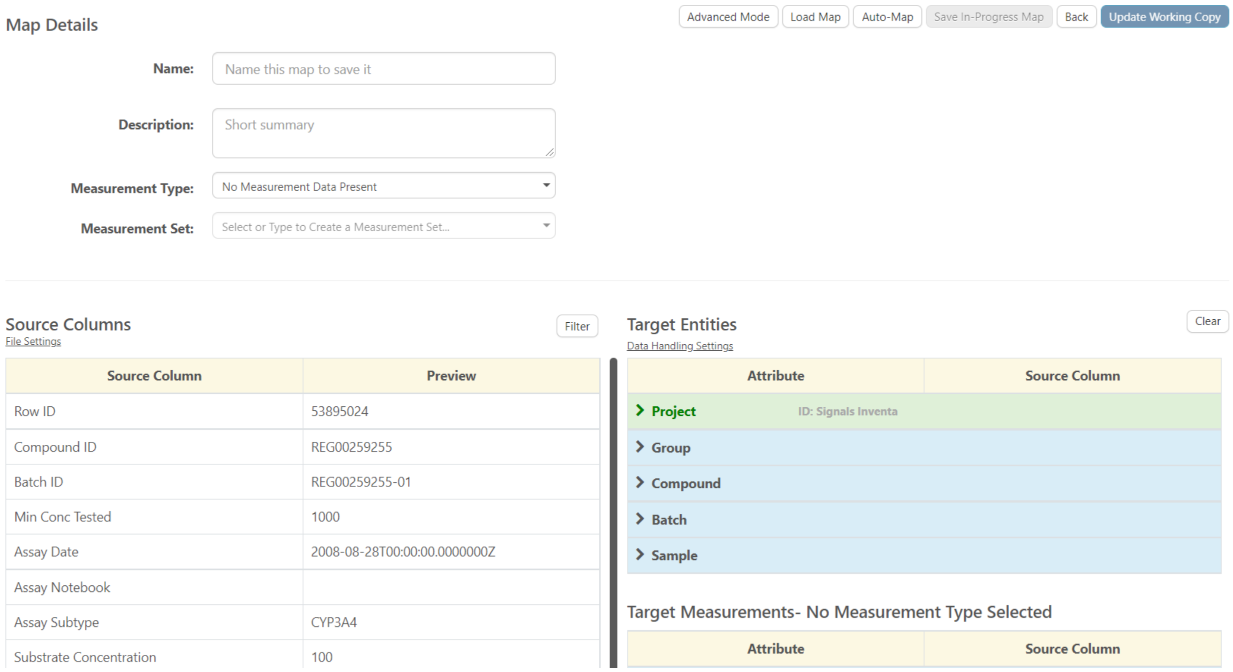
Select a row to preview contents.

Name	Information Types	Measurement Set	Map	Rows	Errors	Actions
cyp_lcms_ic50.csv			Not Mapped	0	-	

The Concepts tab allows you to verify the name of the source ontology file and the concept version being used. For further information on concepts, refer to the Ontologies section.

The errors which occur while importing file(s) can be tracked within the **Import Errors** tab. These errors may be file(s) specific.

6. To map the source details with the target entities, click the **Not Mapped** link.
7. The Map Details page is displayed.



Name: Name this map to save it

Description: Short summary

Measurement Type: No Measurement Data Present

Measurement Set: Select or Type to Create a Measurement Set...

Source Column	Preview
Row ID	53895024
Compound ID	REG00259255
Batch ID	REG00259255-01
Min Conc Tested	1000
Assay Date	2008-08-28T00:00:00.0000000Z
Assay Notebook	
Assay Subtype	CYP3A4
Substrate Concentration	100

Attribute	Source Column
Project	ID: Signals Inventa
Group	
Compound	
Batch	
Sample	

Target Measurements- No Measurement Type Selected

Attribute	Source Column

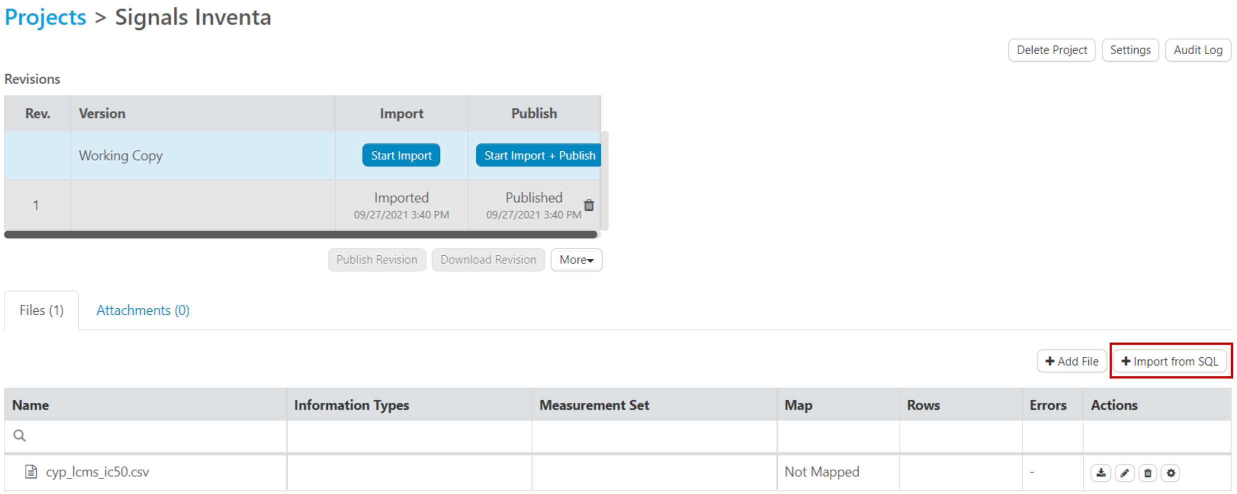
Note: To map source columns with the target entities, and for mapping details, refer to Mapping section.

14.2.3 Import from SQL

It is also possible to add files to a project using an External Connection rather than uploading files themselves.

Note: For more information on external connections, refer to the Connections – External Connection section.

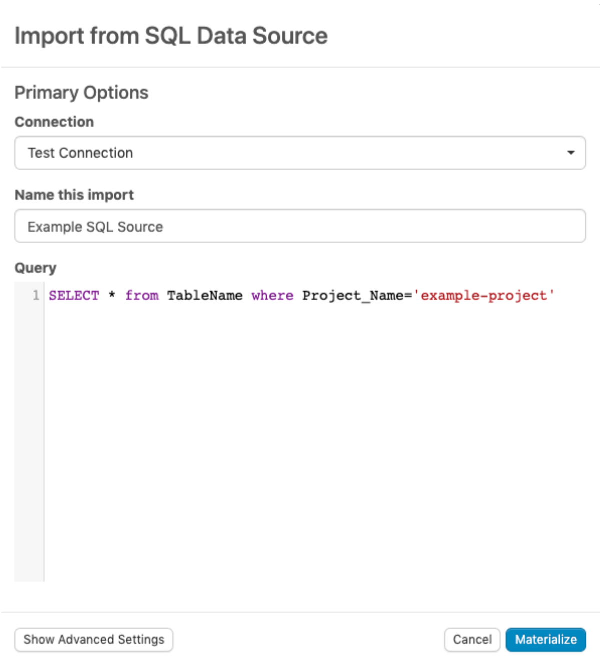
1. In the Project’s page, choose **Import from SQL**.



Rev.	Version	Import	Publish
	Working Copy	Start Import	Start Import + Publish
1		Imported 09/27/2021 3:40 PM	Published 09/27/2021 3:40 PM

Name	Information Types	Measurement Set	Map	Rows	Errors	Actions
cyp_lcms_ic50.csv			Not Mapped		-	

2. In the **Import from SQL Data Source** window, select the pre-configured connection and assign a name to the data being added.



```
SELECT * from TableName where Project_Name='example-project'
```

3. In the **Query** box, enter the SQL to run.

Note: To see advanced settings, refer to the Advanced Settings topic.

4. Once the settings are defined, click **Materialize** and it will materialize the results of the query and stage them as a file, which can then be mapped in the normal way.

Note: For more information on mapping, refer to the Mapping section.

14.2.3.1 Materialization Process

When the details for SQL retrieval are saved, a new process is started to materialize the results of the query.

Any modifications to the settings to the SQL retrieval will also begin a new materialization process.

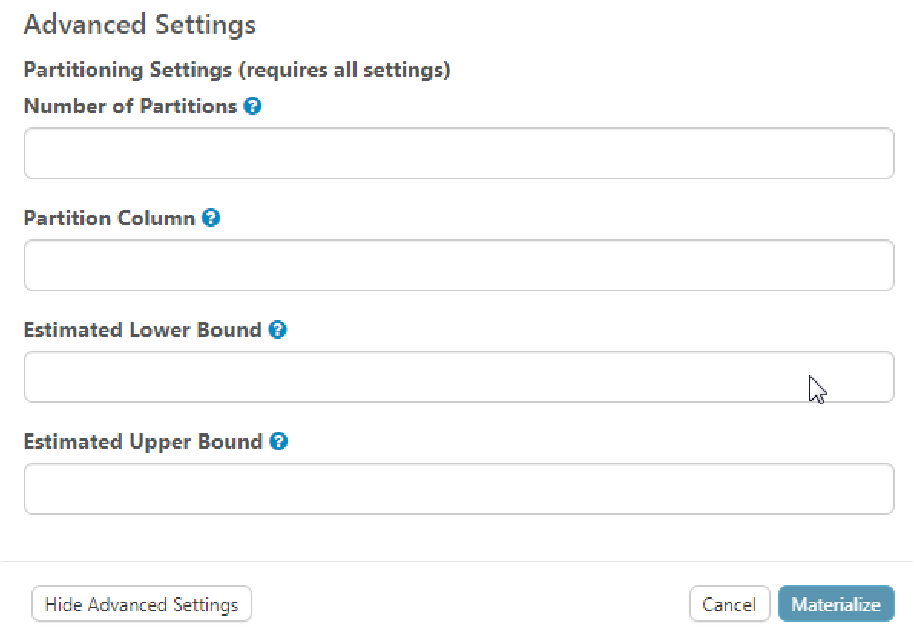
An active materialization will be indicated with a spinner alongside the file.

If there be any issues/errors in this process, the spinner will be replaced with a **!** Icon, which can be clicked to view the output log and diagnose the problem (there is also a shortcut to the log in the Actions column).

If an import job is started before materialization is complete, then a failed materialization will result in a failed import (and any dependent publish jobs).

14.2.3.2 Advanced Settings

For larger datasets it is possible to tune the retrieval mechanism via the ‘Advanced Settings’ option.



Here you can specify

- **Custom Schema**: can be used to override column types when Spark misinterprets the connected data. A comma separated list of column names (from the SQL definition) and desired data type, e.g.

  'Sample ID' LONG, Age INTEGER

  Common target data types are

  - INTEGER
  - LONG
  - DOUBLE
  - STRING

  ***Note**: The datatype must be in CAPS.*

- Partition Settings (if used, all of the settings are required)

  When provided with a partition column along with an estimated lower and upper value, Signals Data Factory will split the data according to the number partitions requested and run these queries in parallel. This can result in significant performance improvements when materializing the data for large datasets.

  - **Number of Partitions**: The number of queries to run in parallel
  - **Partition Column**: A numeric or date column to use to split the query into multiple parts.
  - **Estimated Lower Bound**: An estimate of the lower bound of the partition columns' values
  - **Estimated Upper Bound**: An estimate of the upper bound of the partition columns' values

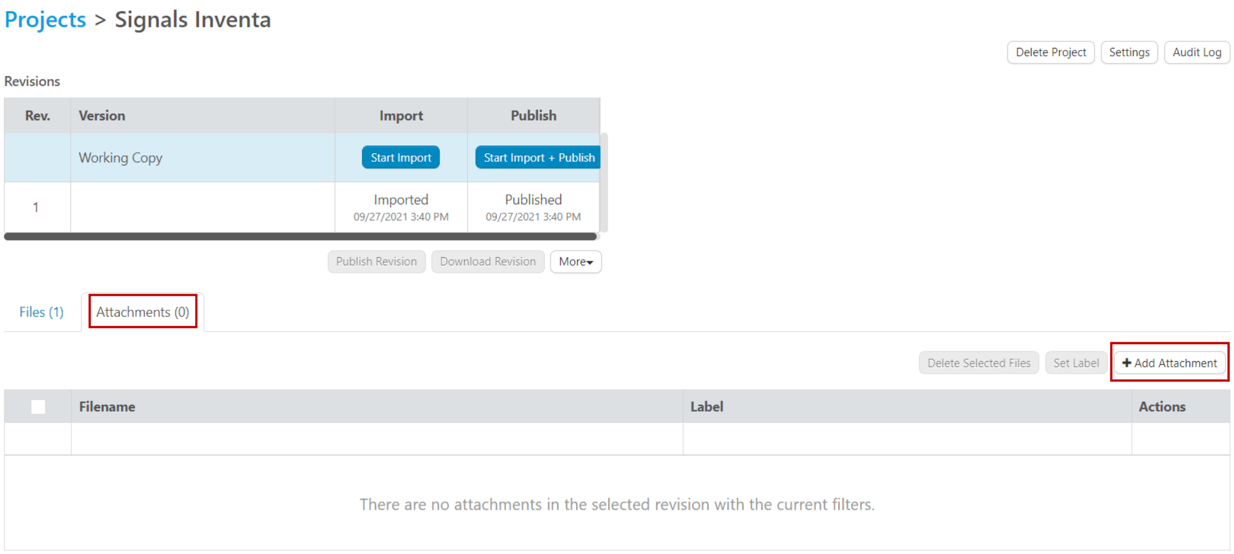
14.2.4 Attachments

Using attachments, you can attach various file formats to the working copy of a project without any mapping requirements. Attachments can be in any file format (PDF, DOC, XLS, JPG, etc.) and behave as part of the project.

After publishing a project, an attachment must be downloaded to make an update; the attachments are not manageable from within the Signals Data Factory interface.

To add attachments:

1. In the Project's page, select a working copy of the project.
2. From the Attachments tab, select the **+ Add Attachments** button.

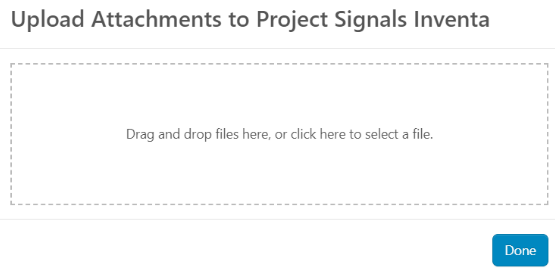


Rev.	Version	Import	Publish
	Working Copy	Start Import	Start Import + Publish
1		Imported 09/27/2021 3:40 PM	Published 09/27/2021 3:40 PM

☐	Filename	Label	Actions

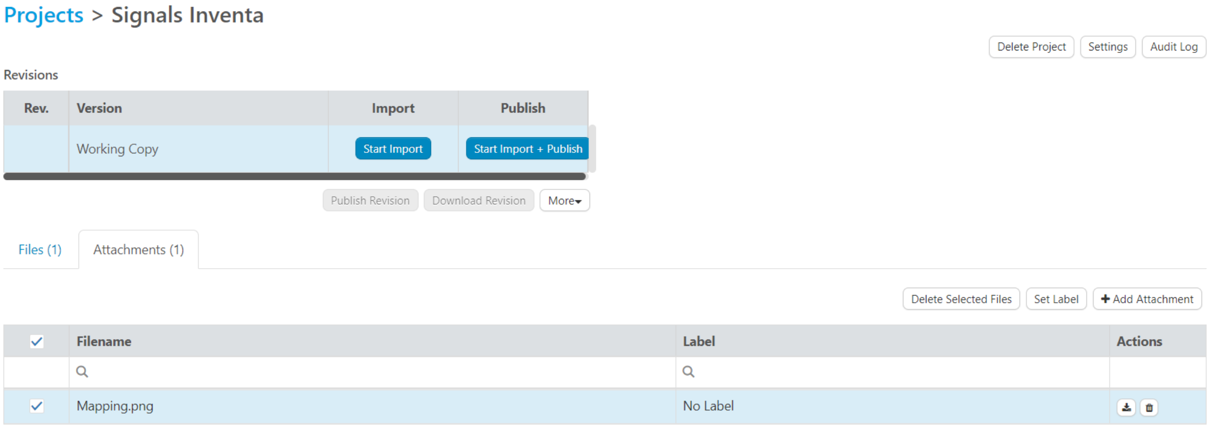
There are no attachments in the selected revision with the current filters.

3. In the **Upload Attachments to Project** dialog, either drag-and-drop the file into the dashed rectangle or click on the rectangle to choose the attachment to be uploaded.



Drag and drop files here, or click here to select a file.

4. Click **Done**.

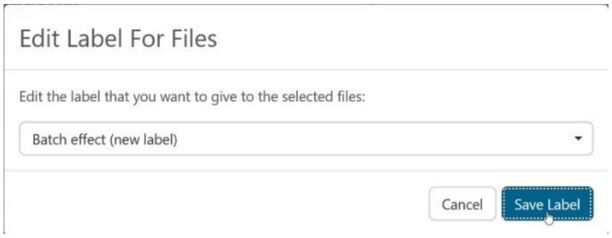


Rev.	Version	Import	Publish
	Working Copy	Start Import	Start Import + Publish

✓	Filename	Label	Actions
✓	Mapping.png	No Label	

5. The attachment is appended to the Attachments grid.

6. If you want to edit label of an attachment, select the attachment file and click the **Set Label** button.



Edit the label that you want to give to the selected files:

Batch effect (new label)

7. Edit the label that you want to give to the selected files and click **Save Label**.

14.3 V2 Projects

14.3.1 Configuring Project Permissions

Signals Data Factory also allows administrators to configure the permissions on projects, such that the projects can only be seen or be used by users belonging to specific groups.

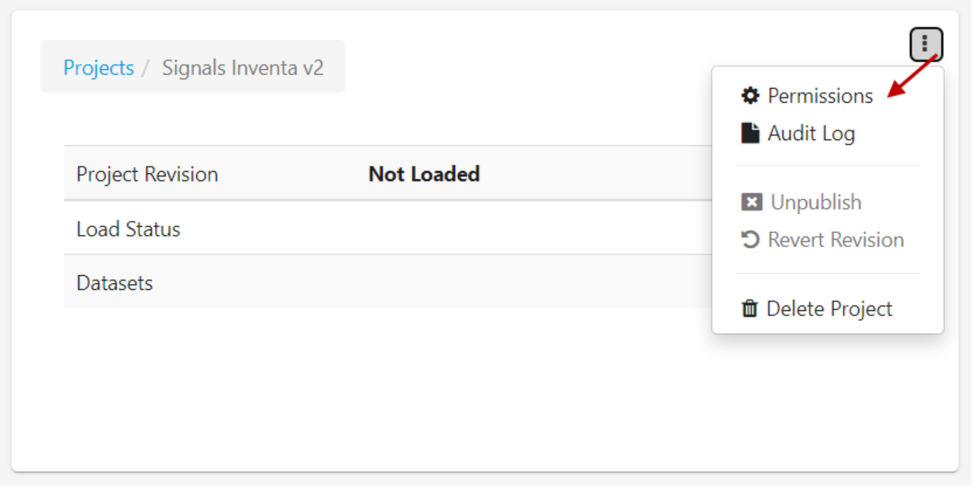
To configure the project permission for V2 project:

1. Login Signals Data Factory with an administrator account.

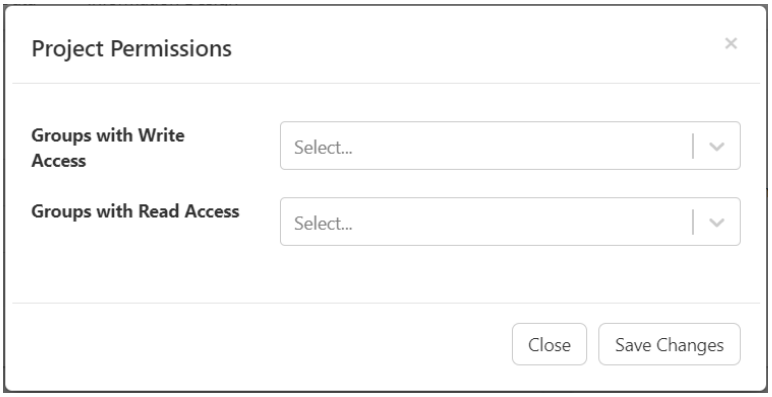
2. From **Data** menu, click **Projects.**

3. In the project list, choose a project for which you want to configure the permission. This will open the project page.

4. From the upper-right corner of the project summary panel, click the ellipse icon, then in the drop-down menu, click **Permissions**



5. In the **Project Permissions** pop-up dialog, specify the groups in the **Groups with Write Access** and **Groups with Read Access** text boxes. This grants the users under the specified group to have read or write permission on the current project.

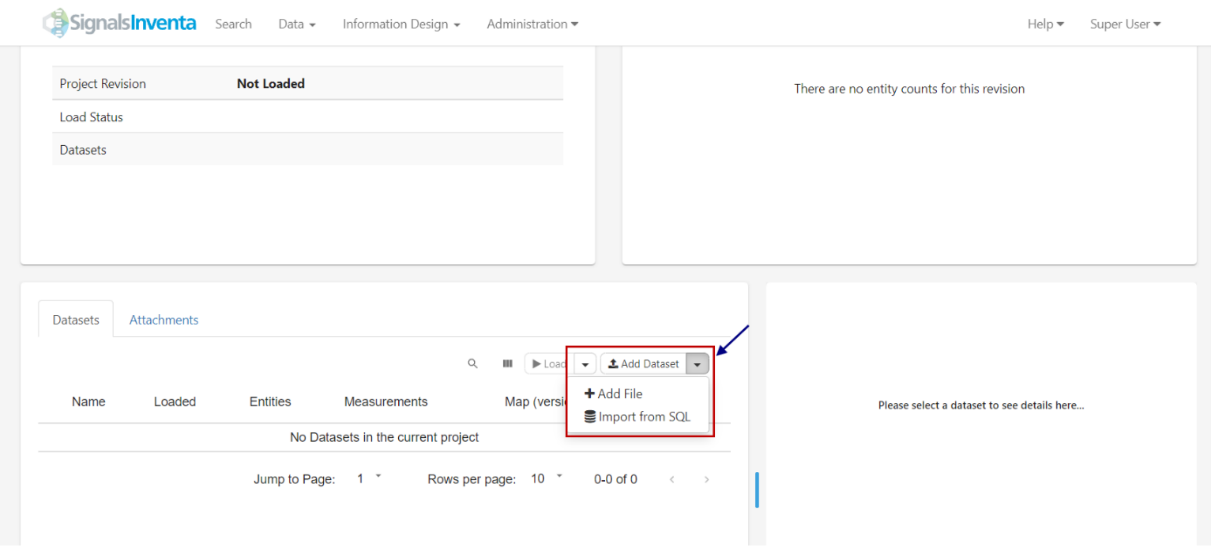


6. Click **Save Changes** button to save the changes and close the dialog.

Note: By default, only administrative users (i.e. users who have ROLE_ADMIN or ROLE_SUPERADMIN) can see all the projects in Signals Data Factory. Non-administrative users will not be able to see any of the projects unless they have been granted permissions for the projects.

14.3.2 Adding Datasets, Files and SQL Files

On the Project details page for an incremental project (v2), there is the option to Add Dataset, Add File and Add SQL File from the **Add Dataset** drop-down button.



Project Revision Not Loaded

Load Status

Datasets

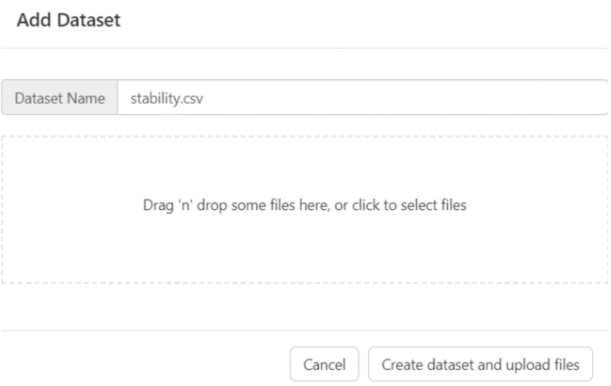
There are no entity counts for this revision

No Datasets in the current project

Please select a dataset to see details here...

To create a dataset:

1. Click on the **Add Dataset** button.



Dataset Name: stability.csv

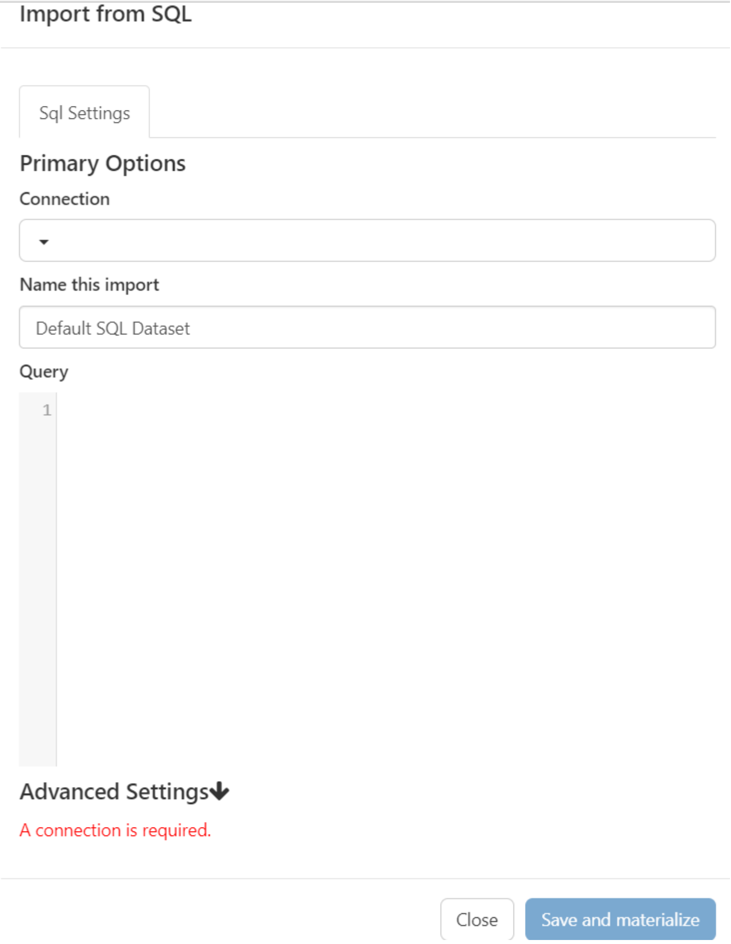
2. Enter a Dataset Name.
3. Drag ‘n’ drop files or click to select files.
4. Click on the **Create dataset and upload files** button.

To add files to a dataset:

1. Select the data from the Dataset list to which you want to add file(s).
2. Click on the **Add File** menu from the Add Dataset drop-down button to open the Add file window.
3. Drag ‘n’ drop files or click to select files.
4. Click **Close**.

To import from SQL to dataset:

1. Select the data from the Dataset list to which you want to import SQL file(s).
2. Click on the **Import from SQL** menu from the Add Dataset drop-down button to open the Import from SQL window.



A connection is required.

Refer to the section ‘Import from SQL’ for v1 projects for information on defining the primary optins and advanced settings as well as materialization.

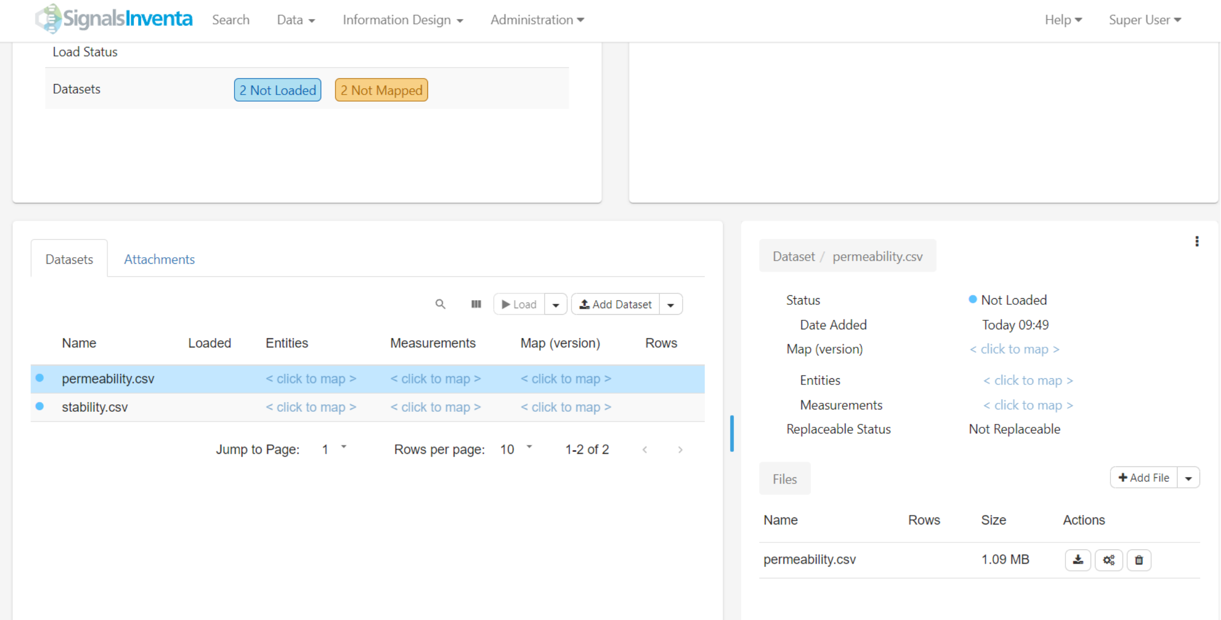
14.3.3 Attachments

Using attachments, you can attach various file formats to the working copy of a project without any mapping requirements. Attachments can be in any file format (PDF, DOC, XLS, JPG, etc.) and behave as part of the project.

After publishing a project, an attachment must be downloaded to make an update; the attachments are not manageable from within the Signals Data Factory interface.

Refer to the section ‘Attachments’ for v1 projects for more information.

14.3.4 Mapping Incremental Projects



Load Status

Datasets: 2 Not Loaded, 2 Not Mapped

Name	Loaded	Entities	Measurements	Map (version)	Rows
permeability.csv		< click to map >	< click to map >	< click to map >	
stability.csv		< click to map >	< click to map >	< click to map >	

Jump to Page: 1 Rows per page: 10 1-2 of 2

Dataset / permeability.csv

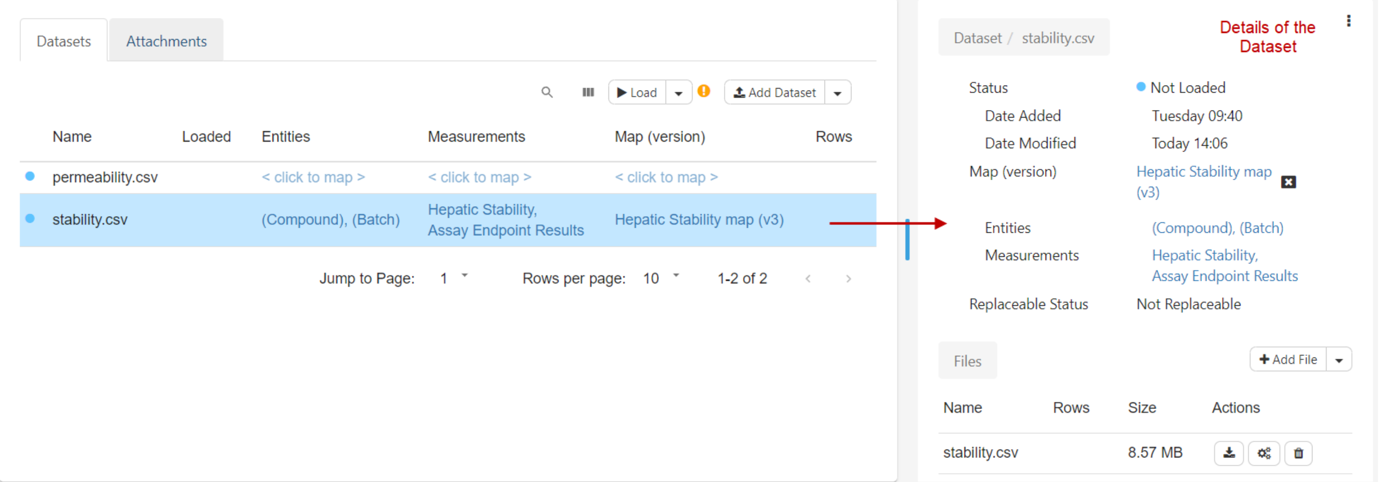
Status	Not Loaded
Date Added	Today 09:49
Map (version)	< click to map >
Entities	< click to map >
Measurements	< click to map >
Replaceable Status	Not Replaceable

Name	Rows	Size	Actions
permeability.csv		1.09 MB	

The <click to map> link exists in several places on the Project details page. Clicking on any of these links will display the mapping page. The mapping workflow is the same for v1 and v2 (incremental) projects. Refer to the Mapping section for further information.

14.3.5 Details of a Dataset

Selecting a dataset displays the details of the dataset in a separate panel. From here, you can add new files to a dataset, delete files from a dataset, modify file properties, apply file properties to all files in a dataset at once, download a file from a dataset, navigate to the warnings page if applicable, and navigate to the dataset mapping page.



Name	Loaded	Entities	Measurements	Map (version)	Rows
permeability.csv		< click to map >	< click to map >	< click to map >	
stability.csv		(Compound), (Batch)	Hepatic Stability, Assay Endpoint Results	Hepatic Stability map (v3)	

Jump to Page: 1 Rows per page: 10 1-2 of 2

Dataset / stability.csv

Details of the Dataset

Status	Not Loaded
Date Added	Tuesday 09:40
Date Modified	Today 14:06
Map (version)	Hepatic Stability map (v3)
Entities	(Compound), (Batch)
Measurements	Hepatic Stability, Assay Endpoint Results
Replaceable Status	Not Replaceable

Name	Rows	Size	Actions
stability.csv		8.57 MB	

14.3.6 Loading a Dataset

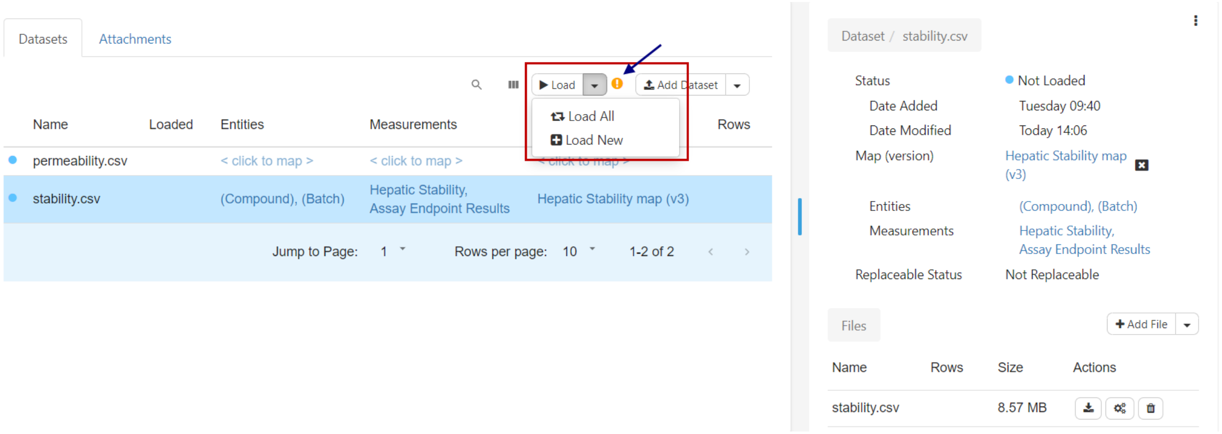
When mapping is complete, you have the option to **Load**, **Load All** or **Load New** (depending on the state of the project).

Loading will automatically Load New if it can and Load All if it can't.

Clicking Load All will re-process all data in the project. Clicking Load New will only re-process those datasets that are new, modified or deleted. If the project does not contain new, modified or deleted datasets, the Load New option is not available. You can override the system by clicking Load All.

If applicable, hovering over the ❗ icon will display load notifications. For example, Load New is not available for the following reasons:

- The project contains no new, modified or deleted datasets
- The Information design has changed (e.g an attribute has changed, and therefore you will be forced to Load All)
- The project has datasets that are not replacable
- You cannot load an empty dataset



Name	Loaded	Entities	Measurements		Rows
permeability.csv		< click to map >	< click to map >	< click to map >	
stability.csv		(Compound), (Batch)	Hepatic Stability, Assay Endpoint Results	Hepatic Stability map (v3)	

Jump to Page: 1 Rows per page: 10 1-2 of 2

Status	Not Loaded
Date Added	Tuesday 09:40
Date Modified	Today 14:06
Map (version)	Hepatic Stability map (v3)
Entities	(Compound), (Batch)
Measurements	Hepatic Stability, Assay Endpoint Results
Replaceable Status	Not Replaceable

Name	Rows	Size	Actions
stability.csv		8.57 MB	

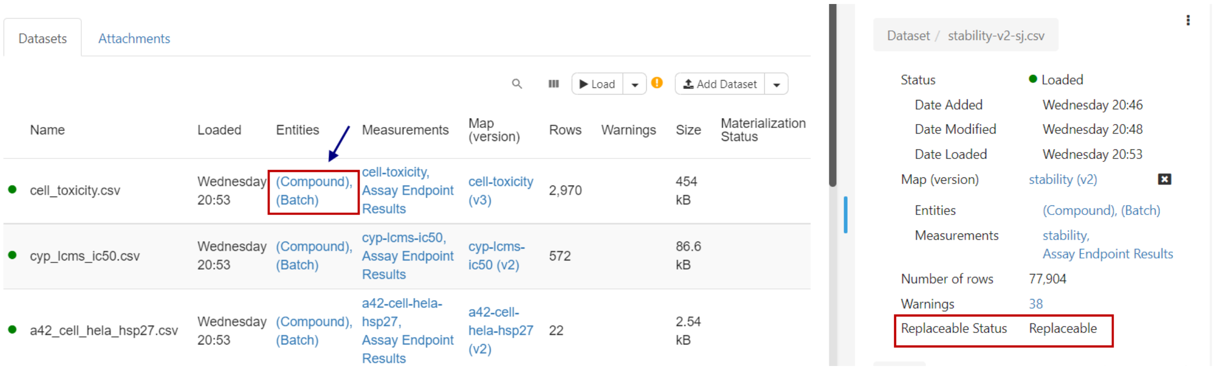
14.3.7 Replaceable Datasets

It is possible to replace most loaded datasets after modifying data and/or maps without reloading the entire project. This is automatic when loading or via Load New. This allows an individual dataset (set of files) to be modified and reprocessed as a distinct set of data.

A dataset is replaceable if it does not map any entity (batch, compound) attributes. This is because the same batch attributes may be updated earlier or later in the list and therefore you cannot guarantee the results if they are loaded out of order.

The Replaceable Status for the selected dataset is indicated in the details section for the dataset. Also, the Compound and Batch are entities in brackets (Entities column) if there are no entity attributes mapped indicating that the dataset is replaceable. The brackets mean you are referencing the entity but not updating it.

If brackets are not present, then that means compound and/or batch attributes are mapped and the dataset is not replaceable.



	Name	Loaded	Entities	Measurements	Map (version)	Rows	Warnings	Size	Materialization Status
●	cell_toxicity.csv	Wednesday 20:53	(Compound), (Batch)	cell-toxicity, Assay Endpoint Results	cell-toxicity (v3)	2,970		454 kB	
●	cyp_lcms_ic50.csv	Wednesday 20:53	(Compound), (Batch)	cyp-lcms-ic50, Assay Endpoint Results	cyp-lcms-ic50 (v2)	572		86.6 kB	
●	a42_cell_hela_hsp27.csv	Wednesday 20:53	(Compound), (Batch)	a42-cell-hela-hsp27, Assay Endpoint Results	a42-cell-hela-hsp27 (v2)	22		2.54 kB	

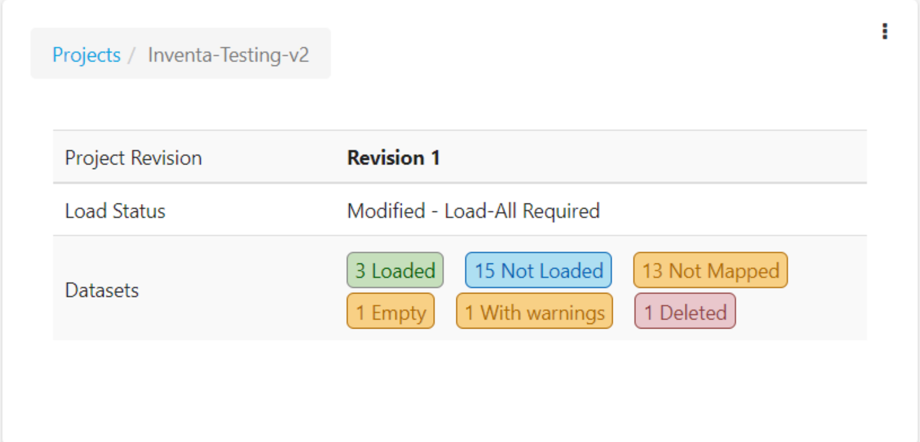
Dataset / stability-v2-sj.csv

Status	● Loaded
Date Added	Wednesday 20:46
Date Modified	Wednesday 20:48
Date Loaded	Wednesday 20:53
Map (version)	stability (v2)
Entities	(Compound), (Batch)
Measurements	stability, Assay Endpoint Results
Number of rows	77,904
Warnings	38
Replaceable Status	Replaceable

14.3.8 Project Details

The Project Details displays the Project Revision and the Load Status. If there is an error when loading, a link is available for you to click on to see the job log.

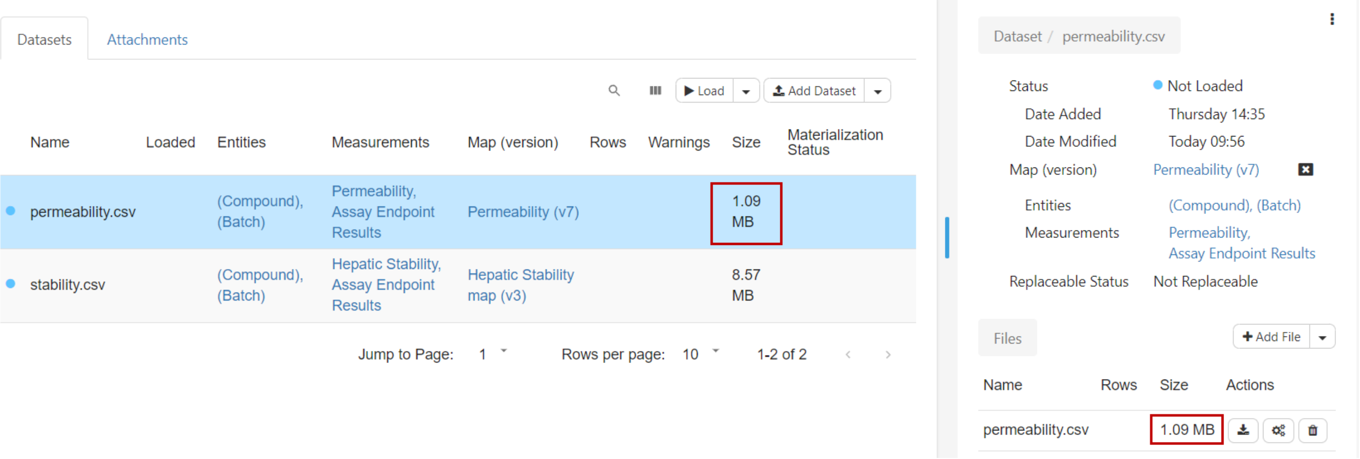
The Project Details page includes a quick filter/status for datasets that are ‘Loaded’, ‘Not Loaded’, ‘Not Mapped’, ‘Empty’, ‘With Warnings’ or ‘Deleted’. This allows you to quickly locate datasets of interest (for example, datasets with warnings) without having to page through all datasets.



Projects / Inventa-Testing-v2

Project Revision	**Revision 1**
Load Status	Modified - Load-All Required
Datasets	3 Loaded 15 Not Loaded 13 Not Mapped 1 Empty 1 With warnings 1 Deleted

The Project Details page displays the sizes of datasets and individual file.



Name	Loaded	Entities	Measurements	Map (version)	Rows	Warnings	Size	Materialization Status
permeability.csv		(Compound), (Batch)	Permeability, Assay Endpoint Results	Permeability (v7)			1.09 MB	
stability.csv		(Compound), (Batch)	Hepatic Stability, Assay Endpoint Results	Hepatic Stability map (v3)			8.57 MB	

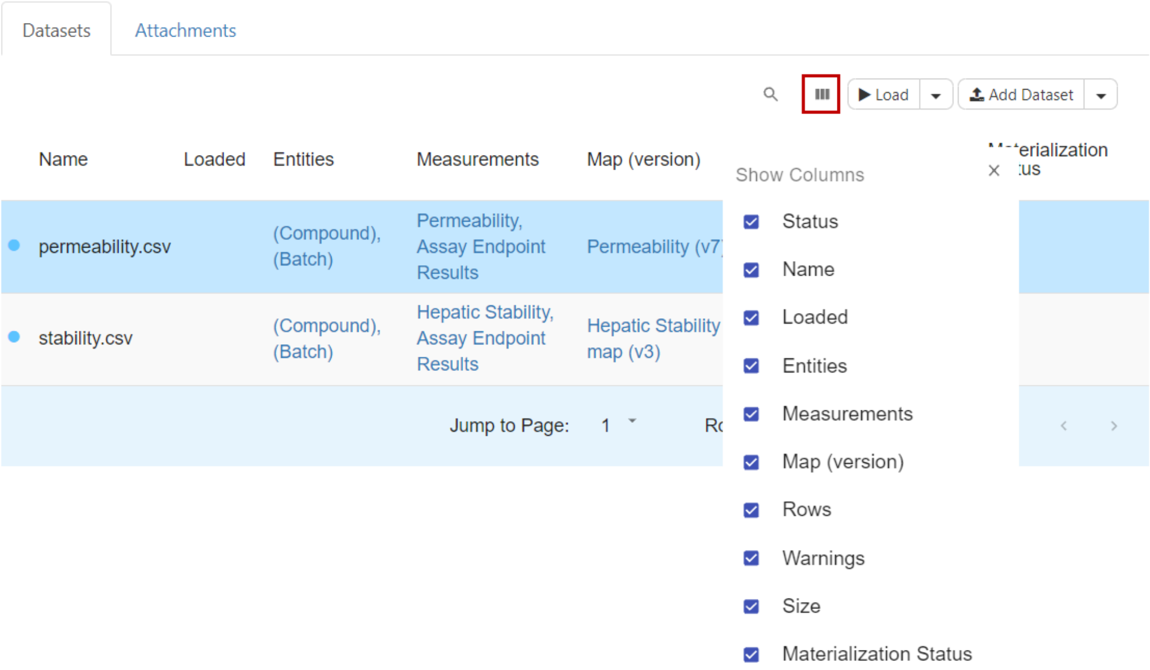
Jump to Page: 1 Rows per page: 10 1-2 of 2

Dataset / permeability.csv

Status	● Not Loaded
Date Added	Thursday 14:35
Date Modified	Today 09:56
Map (version)	Permeability (v7)
Entities	(Compound), (Batch)
Measurements	Permeability, Assay Endpoint Results
Replaceable Status	Not Replaceable

Name	Rows	Size	Actions
permeability.csv		1.09 MB	

Note: You can define the columns visible in the Datasets list by clicking on the ▥ View Columns icon. From here, you can specify the columns to display.



Name	Loaded	Entities	Measurements	Map (version)
permeability.csv		(Compound), (Batch)	Permeability, Assay Endpoint Results	Permeability (v7
stability.csv		(Compound), (Batch)	Hepatic Stability, Assay Endpoint Results	Hepatic Stability map (v3)

Jump to Page: 1

Show Columns

- ☑ Status
- ☑ Name
- ☑ Loaded
- ☑ Entities
- ☑ Measurements
- ☑ Map (version)
- ☑ Rows
- ☑ Warnings
- ☑ Size
- ☑ Materialization Status

If you choose to show the Filenames column, only the first three files will be displayed along with an indicator of the total number of total files.

Note: The ‘Publish’ option does not exist for incremental projects as both Load options will also push the data to Search.

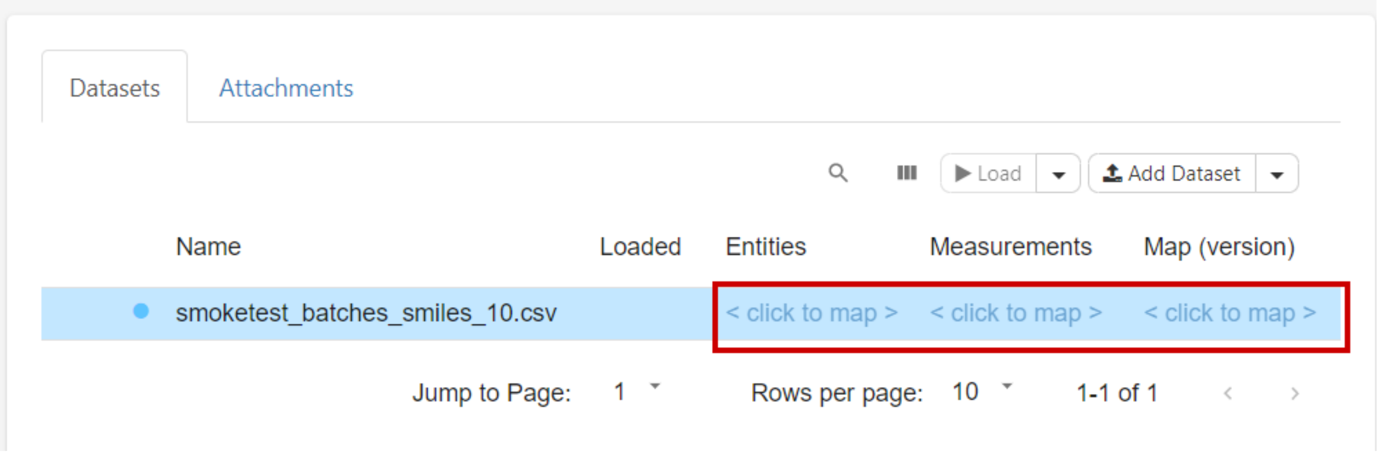
14.4 Mapping

14.4.1 Manual Mapping

After batch data has been uploaded to the project either by adding a tabular text file or importing from SQL, it is necessary to map the source details with the target entities.

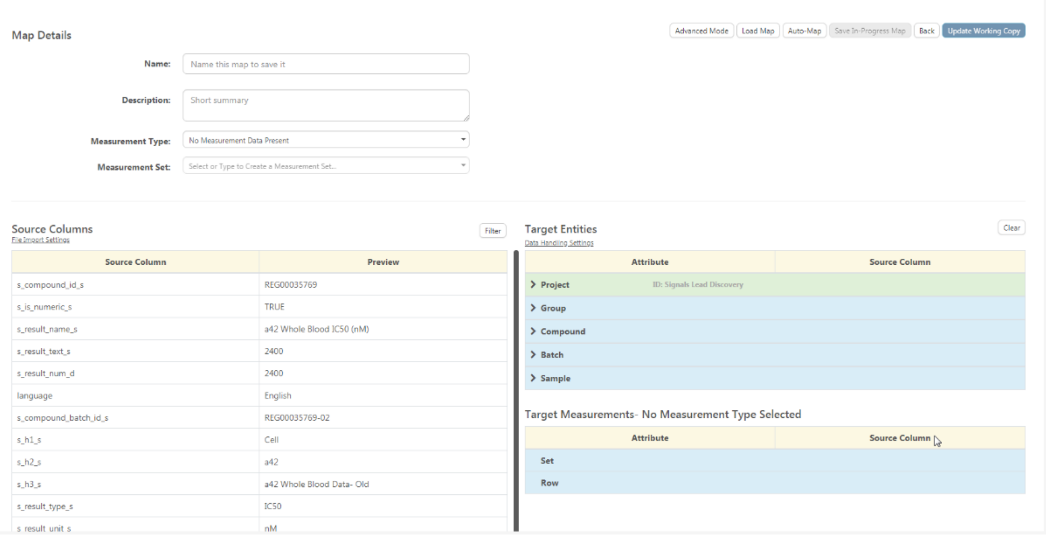
To map columns manually:

1. In the Project's page, click the **click to map** link.



Name	Loaded	Entities	Measurements	Map (version)
smoketest_batches_smiles_10.csv		< click to map >	< click to map >	< click to map >

2. The Map Details page is displayed.



Map Details

Name: Name this map to save it

Description: Short summary

Measurement Type: No Measurement Data Present

Measurement Set: Select or Type to Create a Measurement Set...

Source Columns
File Import Settings

Source Column	Preview
s_compound_id_s	REG00035769
s_is_numeric_s	TRUE
s_result_name_s	a42 Whole Blood IC50 (nM)
s_result_text_s	2400
s_result_num_d	2400
language	English
s_compound_batch_id_s	REG00035769-02
s_h1_s	Cell
s_h2_s	a42
s_h3_s	a42 Whole Blood Data- Old
s_result_type_s	IC50
s_result_unit_s	nM

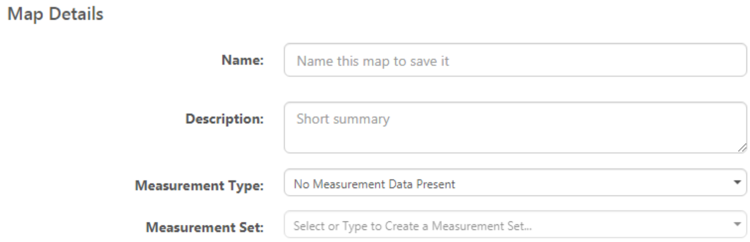
Target Entities
Data Handling Settings

Attribute	Source Column
> Project	ID: Signals Lead Discovery
> Group	
> Compound	
> Batch	
> Sample	

Target Measurements- No Measurement Type Selected

Attribute	Source Column
Set	
Row	

Note: It is mandatory to select the measurement type before initiating manual mapping of Measurement related columns (attributes).



Map Details

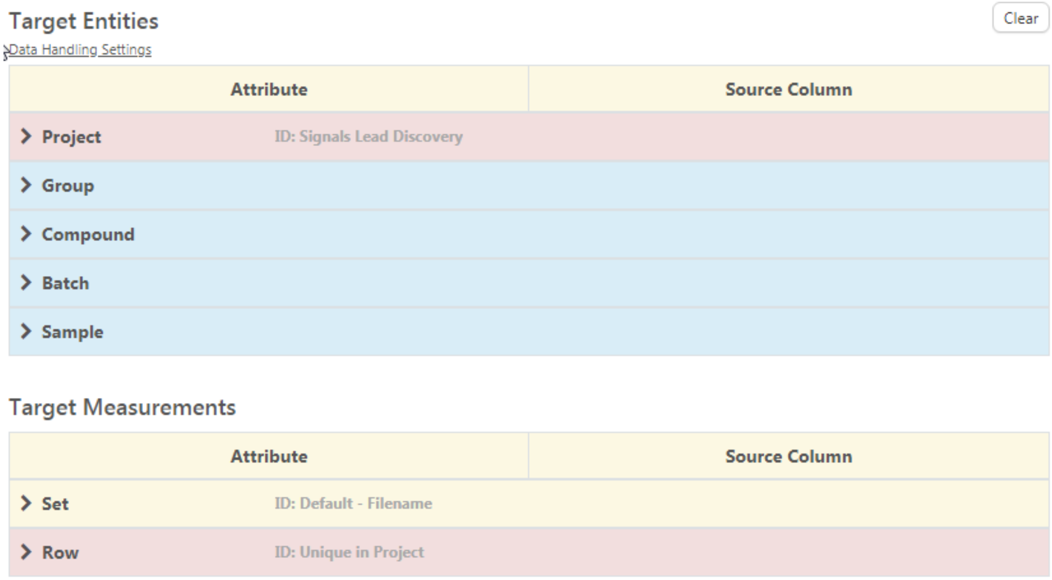
Name: Name this map to save it

Description: Short summary

Measurement Type: No Measurement Data Present

Measurement Set: Select or Type to Create a Measurement Set...

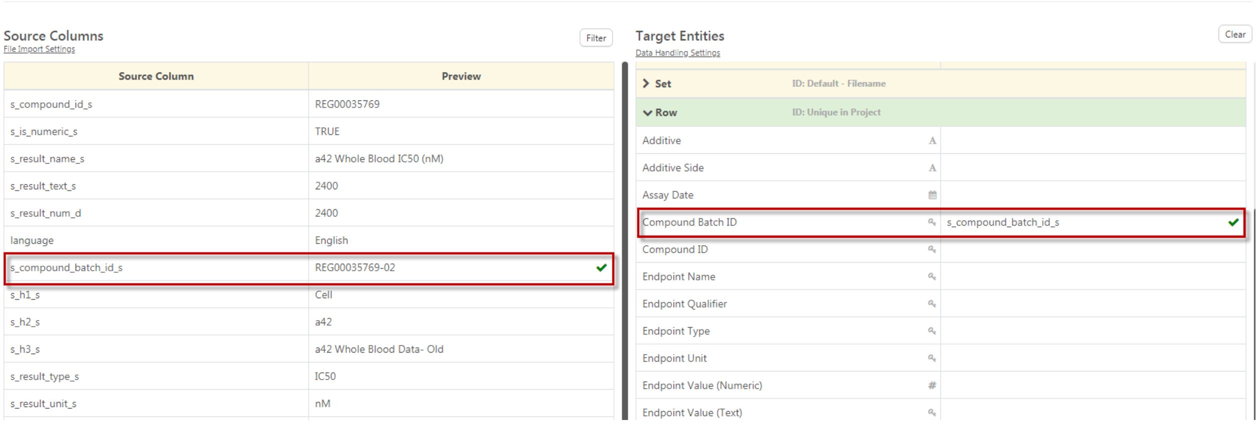
3. Enter name and description for the map. A name must be supplied to save the map.
4. Select the **Measurement Type**. The **Measurement Se**t field is enabled with the relevant measurement set details. For example, in the **Target Entities** area, the **Set** and **Row** data fields are enabled.



Attribute	Source Column
Project ID: Signals Lead Discovery	
Group	
Compound	
Batch	
Sample	

Attribute	Source Column
Set ID: Default - Filename	
Row ID: Unique in Project	

5. Select a file column heading on the left-hand pane and click on the target column heading to map.
6. The columns appear selected with a green checkmark indicating that the source and target columns are mapped.



Source Columns
File Import Settings

Source Column	Preview
s_compound_id_s	REG00035769
s_is_numeric_s	TRUE
s_result_name_s	a42 Whole Blood IC50 (nM)
s_result_text_s	2400
s_result_num_d	2400
language	English
s_compound_batch_id_s	REG00035769-02 ✓
s_h1_s	Cell
s_h2_s	a42
s_h3_s	a42 Whole Blood Data- Old
s_result_type_s	IC50
s_result_unit_s	nM

Target Entities
Data Handling Settings

Set	ID: Default - Filename
Row	ID: Unique in Project
Additive	
Additive Side	
Assay Date	
Compound Batch ID	s_compound_batch_id_s ✓
Compound ID	
Endpoint Name	
Endpoint Qualifier	
Endpoint Type	
Endpoint Unit	
Endpoint Value (Numeric)	
Endpoint Value (Text)	

Note: The **Target Entities** displayed here are created from within **Information Design** > **Entities and Attributes**. These attributes work differently based on the data type.

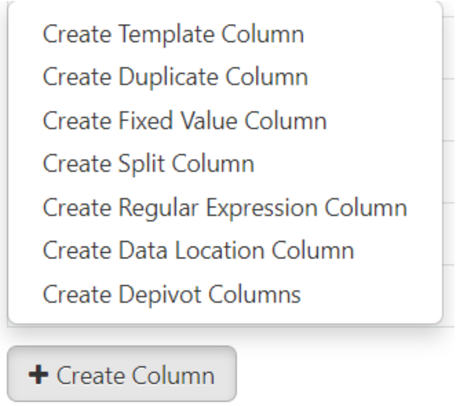
Note: For more information about adding Entity Attributes, refer the Entities and Attributes topic of the document.

7. Click **Save In Progress Map** to save the mapping details.

8. After mapping, click **Add File to Project.** The mapped file is be added to the project's list.

14.4.1.1 Create Columns

Using the 'Create Columns' feature, it is possible to create different column types for use when mapping source columns to target entities.



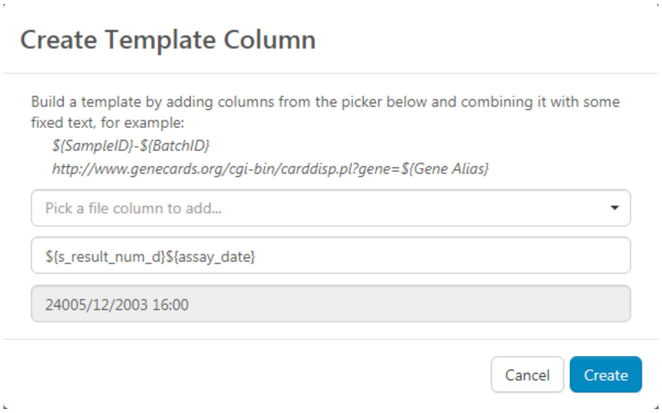
Note: If a selected column is already created, you will not be permitted to re-create the same column.

Create Template Column

Using 'Create Template Column', you can build a column value which includes one or more columns (irrespective of the order) of the source columns into a single column. This column can be used to map to a target entity.

To create a Template column:

1. Select **Create Column** > **Create Template Column**.
2. Select columns to combine from the drop-down list.



Create Template Column

Build a template by adding columns from the picker below and combining it with some fixed text, for example:

${SampleID}-${BatchID}

http://www.genecards.org/cgi-bin/carddisp.pl?gene=${Gene Alias}

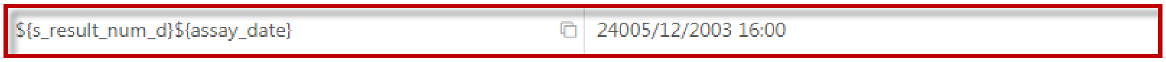
Pick a file column to add...

${s_result_num_d}${assay_date}

24005/12/2003 16:00

3. Click **Create**. The Template column is created in the source columns list as follows.

For example,



${s_result_num_d}${assay_date} | 24005/12/2003 16:00

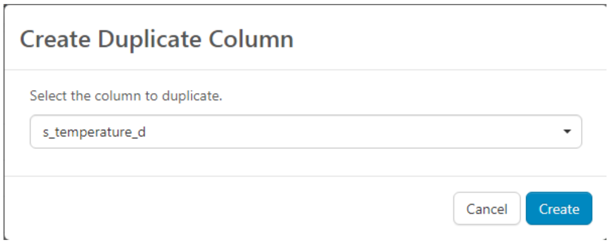
Note: These columns are separated as per the character set in the Data Handling Settings. For more information, refer to the [Data Handling Settings]() section.

Create Duplicate Column

Using the 'Duplicate Columns' feature, it is possible to duplicate source columns.

To create a duplicate column:

1. Select **Create Column > Create Duplicate Column**.
2. Select a column from the drop-down list.



Create Duplicate Column

Select the column to duplicate.

s_temperature_d

3. Click **Create**. The duplicated column is created in the Source columns list.

Source Columns

File Import Settings

s_result_num_d	2400
language	English
s_compound_batch_id_s	REG00035769-02
s_h1_s	Cell
s_h2_s	a42
s_h3_s	a42 Whole Blood Data- Old
s_result_type_s	IC50
s_result_unit_s	nM
s_result_qualifier_s	>=
s_temperature_d	11
assay_date	5/12/2003 16:00 Format - Month, Day, Year
salt_name_s	no_salt
lit_ref_s	TH2201:U07
salt_mw_d	0
s_compound_batch_id_s	REG00035769-02
s_compound_id_s	REG00035769
${s_result_num_d}${assay_date}	24005/12/2003 16:00
s_temperature_d	11

Create Fixed Value Column

Using ‘Create Fixed Value Column’, you can create a column with a fixed value to be used when mapping a source column that is missing from the project. If mapped to a target entity, each value of the target column is replaced with the fixed value column.

To create a fixed value column:

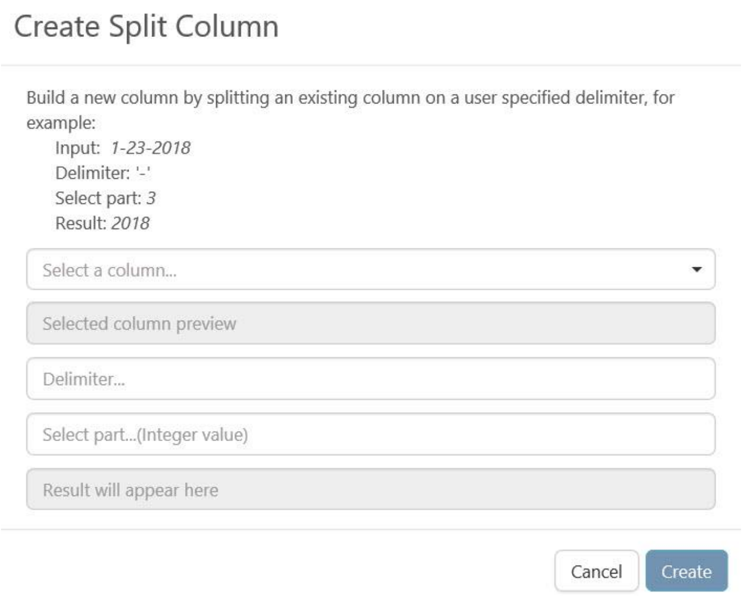
1. Select **+Create Column > Create Fixed Value Column**.
2. Enter value for fixed column.
3. Click **Create.** A Fixed Value Column is appended to the Source Column list and can be mapped to a target entity.

Create Split Column

You can build a new column by splitting an existing column using a user specified delimiter or multiple characters of that column.

To create split column:

1. Select **+Create Column > Create Split Column**.



Create Split Column

Build a new column by splitting an existing column on a user specified delimiter, for example:
Input: *1-23-2018*
Delimiter: '-'
Select part: *3*
Result: *2018*

2. Select the column to split (e.g. 1-23-2018). The column preview is displayed.
3. Enter delimiter to separate selected column
4. Enter part (integer value) to split the column,
5. Click Create to create new column.

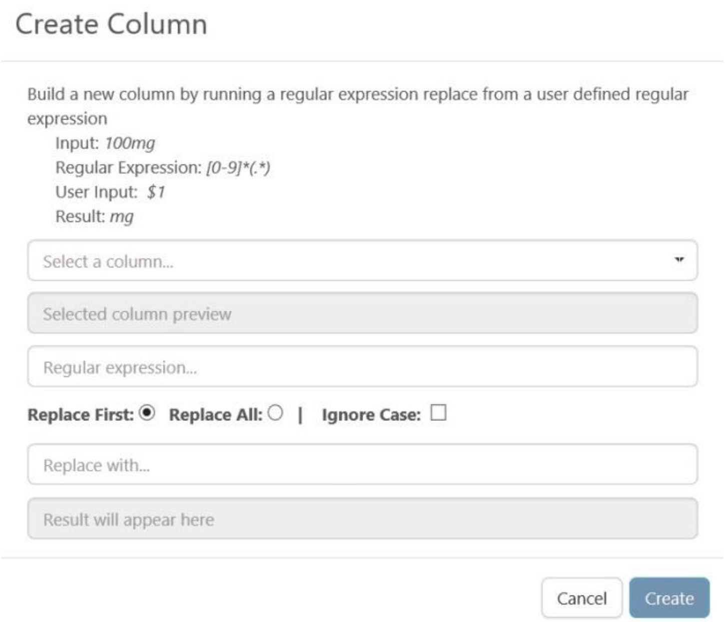
Create Regular Expression Column

You can build a new column by executing a regular expression replace from a user defined regular expression.

Regular Expression Column allows the user to input a search and replace pattern that will be executed on the string value of a field to produce a new column.

To create regular expression column:

1. Click the **+Create Column > Create Regular Expression Column**.



Create Column

Build a new column by running a regular expression replace from a user defined regular expression
Input: *100mg*
Regular Expression: *[0-9]*(.*)*
User Input: *$1*
Result: *mg*

2. Select a column to use as the input for the regular expression.
3. Enter a Regular Expression.

Note: More information on the format of Regular Expressions search patterns is available here: https://docs.oracle.com/javase/8/docs/api/java/util/regex/Pattern.html

4. You can optionally choose to 'Replace First', or 'Replace All' matching patterns. You can choose to Ignore Case when matching the pattern.
5. In the **Replace with…** field, you can enter a numeric or string value that will replace the first value of the matching (or all values if selected) pattern.

Note: Leaving the **Replace with** field blank will result in the match(es) being deleted from the source value.

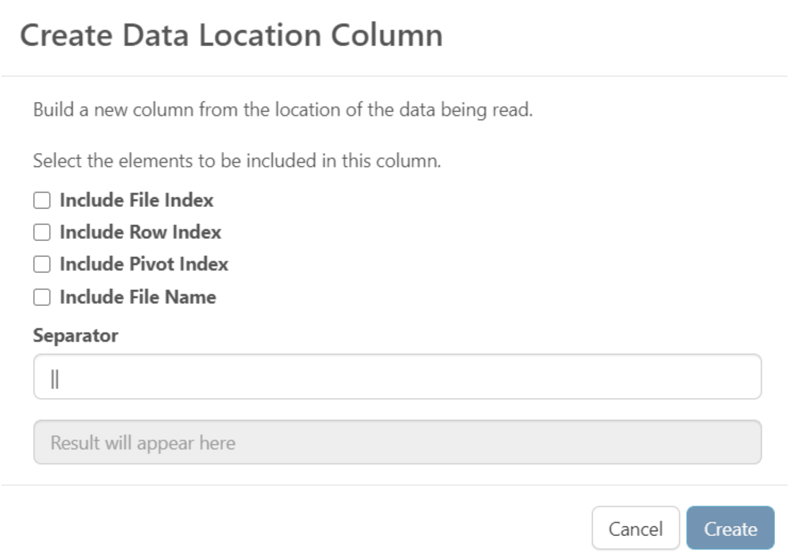
6. Click **Create** to create new column.

Create Data Location Column

You can build a new column from the location of the data being read.

To create Data Location Column:

1. Click the **+Create Column** button and choose **Create Data Location Column**.



Create Data Location Column

Build a new column from the location of the data being read.

Select the elements to be included in this column.

☐ **Include File Index**
☐ **Include Row Index**
☐ **Include Pivot Index**
☐ **Include File Name**

Separator: ||

Result will appear here

2. Select the elements to be included in this column.

This locator can be used to generate unique values relating to the source location of the data (e.g. for use when generating a unique identifier).

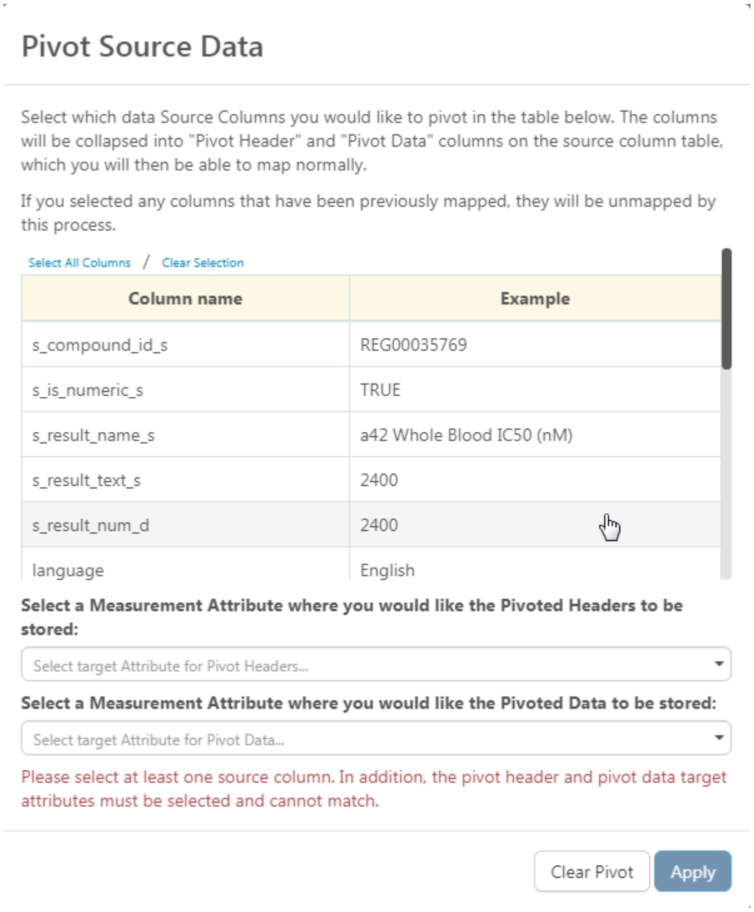
- File and Row Index will generate unique values according to which file in the project and/or which row in the file the data came from.
- Pivot index will always be ‘0’, unless the depivot option is used in the mapping, in which case the index of the depivoted item will be used (starting at 1).
- The filename of the source data can be included.

One or more of these values can be added, and a separator can be specified to be used when concatenating multiple values.

Create Depivot Columns

To create Depivot Columns:

1. Select **+Create Column > Create Depivot Column**.
2. Select the source columns to pivot. The columns will be collapsed into ‘Pivot Header’ and ‘Pivot Data’ columns on the source columns table which you can then map to a target entity.



Pivot Source Data

Select which data Source Columns you would like to pivot in the table below. The columns will be collapsed into "Pivot Header" and "Pivot Data" columns on the source column table, which you will then be able to map normally.

If you selected any columns that have been previously mapped, they will be unmapped by this process.

Column name	Example
s_compound_id_s	REG00035769
s_is_numeric_s	TRUE
s_result_name_s	a42 Whole Blood IC50 (nM)
s_result_text_s	2400
s_result_num_d	2400
language	English

Select a Measurement Attribute where you would like the Pivoted Headers to be stored:

Select a Measurement Attribute where you would like the Pivoted Data to be stored:

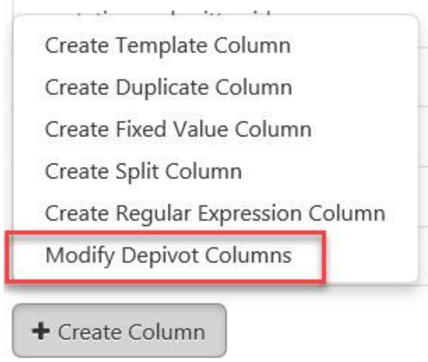
Please select at least one source column. In addition, the pivot header and pivot data target attributes must be selected and cannot match.

3. Select a measurement attribute from the dropdown list to store the pivoted headers.
4. Select a measurement attribute from the dropdown list to store the pivoted data.

You much select at least one source column. In addition, the pivot header and pivot target attributes must be selected and cannot be the same atttribute.

5. Click **Apply.**

Using the Modify Depivot Columns menu item, you can modify the Pivot Source Data.



14.4.2 Auto Mapping

Automapping allows you to automatically map source and target columns with the same name.

To auto map column headers:

1. From the Map Details page for a project, click **Auto-Map** to map source columns with target columns.

Map source and target columns with the same name

2. Click **Filter** to filter the mapped or unmapped columns.

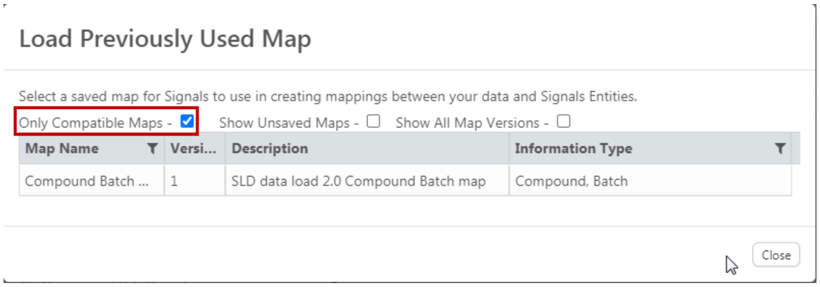
3. Click **Save In Progress Map** to save the auto mapped entities.

14.4.3 Load Map

The **Load Map** feature loads a previously configured used map to create mappings between source and target columns.

To load a map:

1. From the Map Details page for a project, click **Load Map** to load a previously created and saved map to the project.



Load Previously Used Map

Select a saved map for Signals to use in creating mappings between your data and Signals Entities.

Only Compatible Maps - ☑ Show Unsaved Maps - ☐ Show All Map Versions - ☐

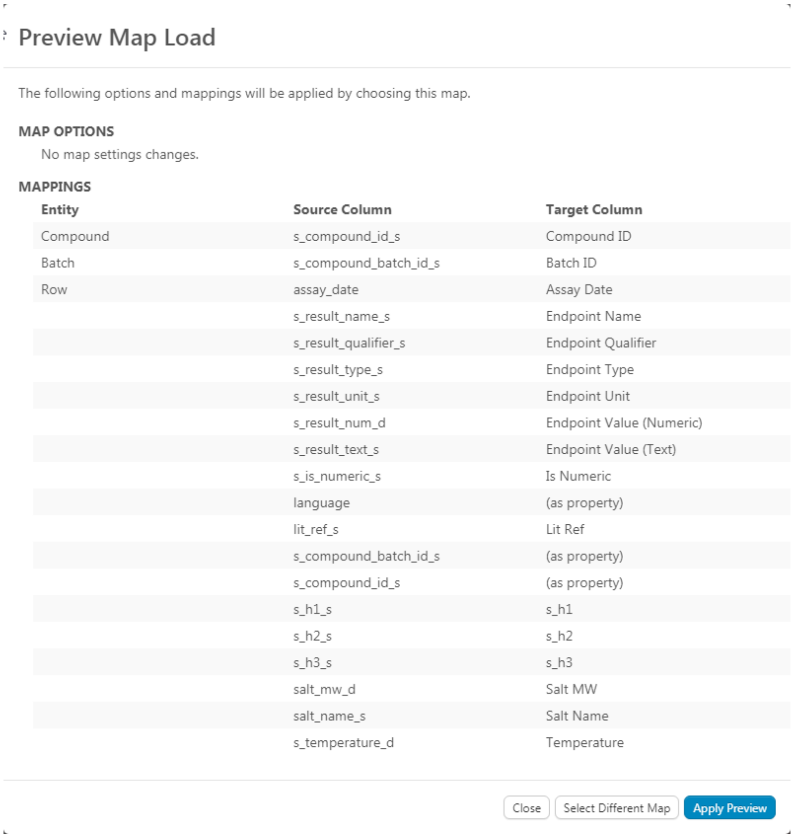
Map Name	Versi...	Description	Information Type
Compound Batch ...	1	SLD data load 2.0 Compound Batch map	Compound, Batch

By default, ony maps that are compatible with the current file and its available source columns will be displayed. To view all available maps, de-select the ‘Only Compatible Maps’ checkbox.

For a map to be compatible with a file:

- Any columns mapped to an ID in the map must be found in the source file currently being mapped.
- All de-pivot columns referenced by the map must be found.
- If a measurment type is referenced, at least one column mapped to a measurement attribute must be found.

A Preview Map Load indicates the options and mapping that will be applied if the selected map is applied.



Preview Map Load

The following options and mappings will be applied by choosing this map.

MAP OPTIONS

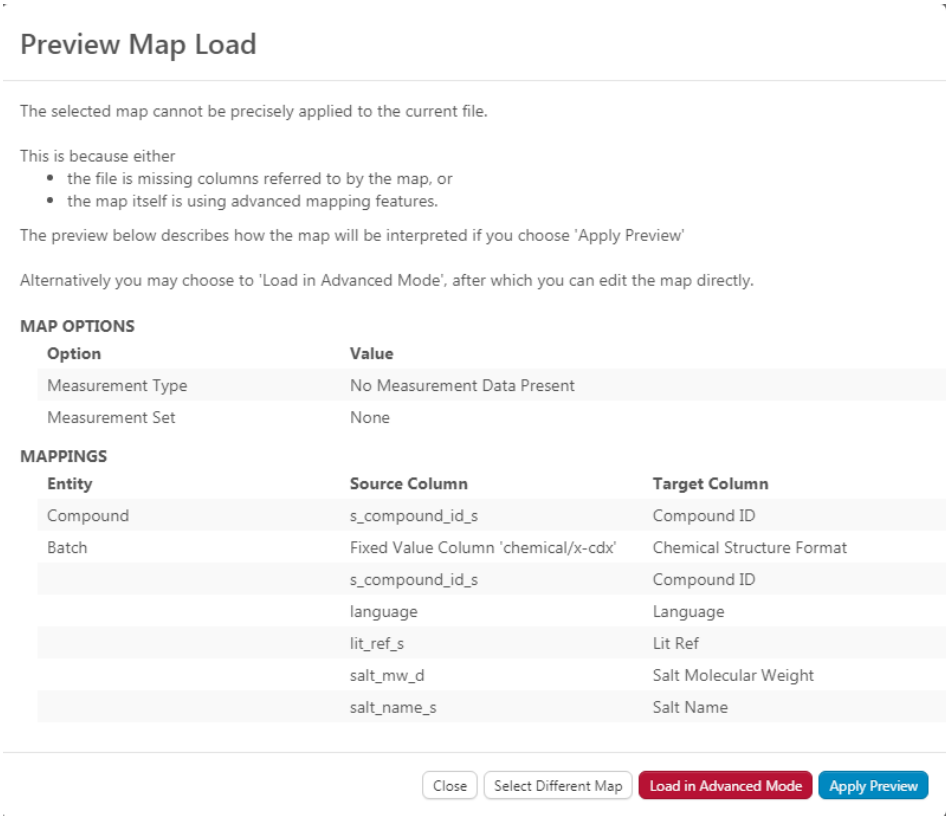
No map settings changes.

MAPPINGS

Entity	Source Column	Target Column
Compound	s_compound_id_s	Compound ID
Batch	s_compound_batch_id_s	Batch ID
Row	assay_date	Assay Date
	s_result_name_s	Endpoint Name
	s_result_qualifier_s	Endpoint Qualifier
	s_result_type_s	Endpoint Type
	s_result_unit_s	Endpoint Unit
	s_result_num_d	Endpoint Value (Numeric)
	s_result_text_s	Endpoint Value (Text)
	s_is_numeric_s	Is Numeric
	language	(as property)
	lit_ref_s	Lit Ref
	s_compound_batch_id_s	(as property)
	s_compound_id_s	(as property)
	s_h1_s	s_h1
	s_h2_s	s_h2
	s_h3_s	s_h3
	salt_mw_d	Salt MW
	salt_name_s	Salt Name
	s_temperature_d	Temperature

2. To load a different map, click on the **Select Different Map** button.
3. Once satisfied with the map selection, click **Apply Preview,** to load the selected map details to the project.
4. Click **Save in Progress Map** to save the mapping updates.

In certain cases, the selected map cannot be precisely applied to the project. This can occur if the project is missing columns referred to by the map, or the map is using advanced mapping features.



Preview Map Load

The selected map cannot be precisely applied to the current file.

This is because either
- the file is missing columns referred to by the map, or
- the map itself is using advanced mapping features.

The preview below describes how the map will be interpreted if you choose 'Apply Preview'

Alternatively you may choose to 'Load in Advanced Mode', after which you can edit the map directly.

MAP OPTIONS

Option	Value
Measurement Type	No Measurement Data Present
Measurement Set	None

MAPPINGS

Entity	Source Column	Target Column
Compound	s_compound_id_s	Compound ID
Batch	Fixed Value Column 'chemical/x-cdx'	Chemical Structure Format
	s_compound_id_s	Compound ID
	language	Language
	lit_ref_s	Lit Ref
	salt_mw_d	Salt Molecular Weight
	salt_name_s	Salt Name

If this situation, you can choose to apply this map using the previewed interpretation, select a different map or load the map in advanced mode.

If you choose to apply the selected map, you may lose some advanced mapping options if applicable.

Note: For more details on the Advanced Mapping feature, refer to the Advanced Mode topic of the document.

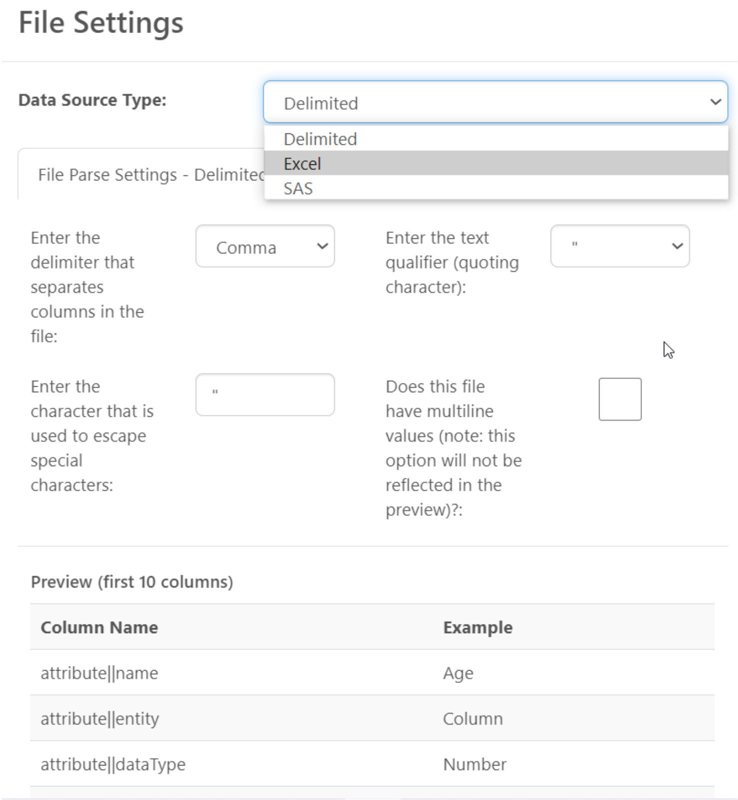
14.4.4 File Settings

The Signals Data Factory supports UTF-8 encoding format therefore imported data formats or symbols must be converted to UTF-8 format using an external program.

To configure file settings:

1. From the Map Details page for a project, click on the **File Settings** link.

The File Settings dialog allows you to define the data source type and, file parse settings and immediately preview the changes.



File Settings

Data Source Type: Delimited

File Parse Settings - Delimited

Enter the delimiter that separates columns in the file: Comma

Enter the text qualifier (quoting character): "

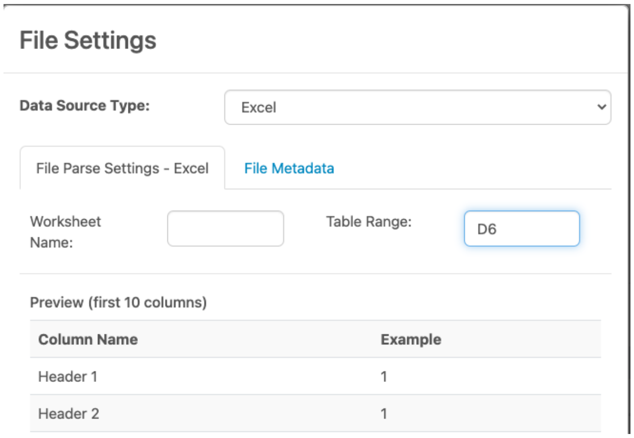
Enter the character that is used to escape special characters: "

Does this file have multiline values (note: this option will not be reflected in the preview)?: ☐

Preview (first 10 columns)

Column Name	Example
attribute||name	Age
attribute||entity	Column
attribute||dataType	Number

2. For Excel files, you can specify the Worksheet to load and, if required, a range offset for the data location.



File Settings

Data Source Type: Excel

Worksheet Name:

Table Range: D6

Preview (first 10 columns)

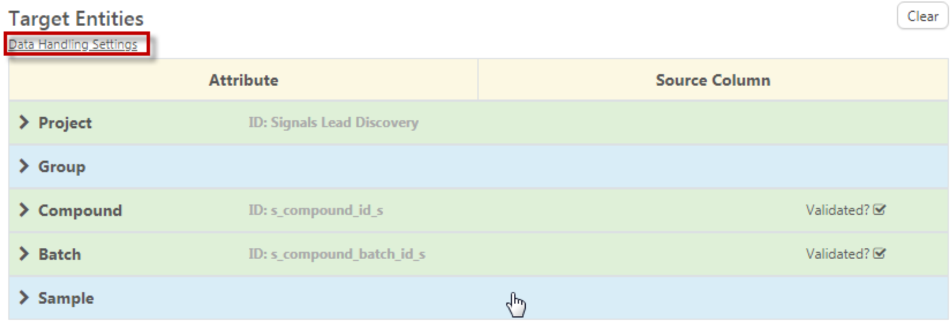
Column Name	Example
Header 1	1
Header 2	1

- **Worksheet Name** (optional) – by default the first Worksheet is loaded.
- **Worksheet Range (optional)** - it can be used to offset the start position by specifying the start cell of the header row. Note that a cell specification is the required input for this field (e.g., D6).

3. Click **Save.**

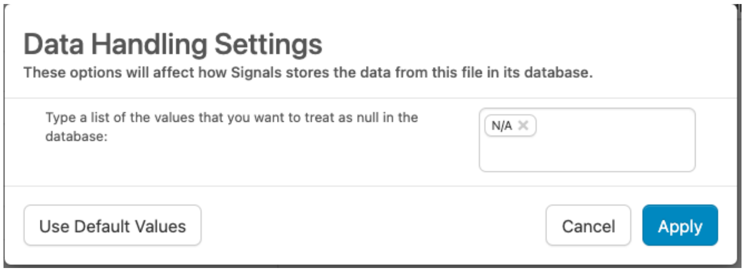
14.4.5 Data Handling Settings

1. From the Map Details page for a project, click **Data Handling Settings** link to verify the data settings.



Attribute	Source Column
Project	ID: Signals Lead Discovery
Group	
Compound	ID: s_compound_id_s Validated? ☑
Batch	ID: s_compound_batch_id_s Validated? ☑
Sample	

2. The **Data Handling Settings** screen allows you to specify values in the file to be ignored and therefore to be interpreted as a null value.



These options will affect how Signals stores the data from this file in its database.

Type a list of the values that you want to treat as null in the database: N/A

3. Click **Apply**. You can choose to use default values by clicking **Use Default Values**.

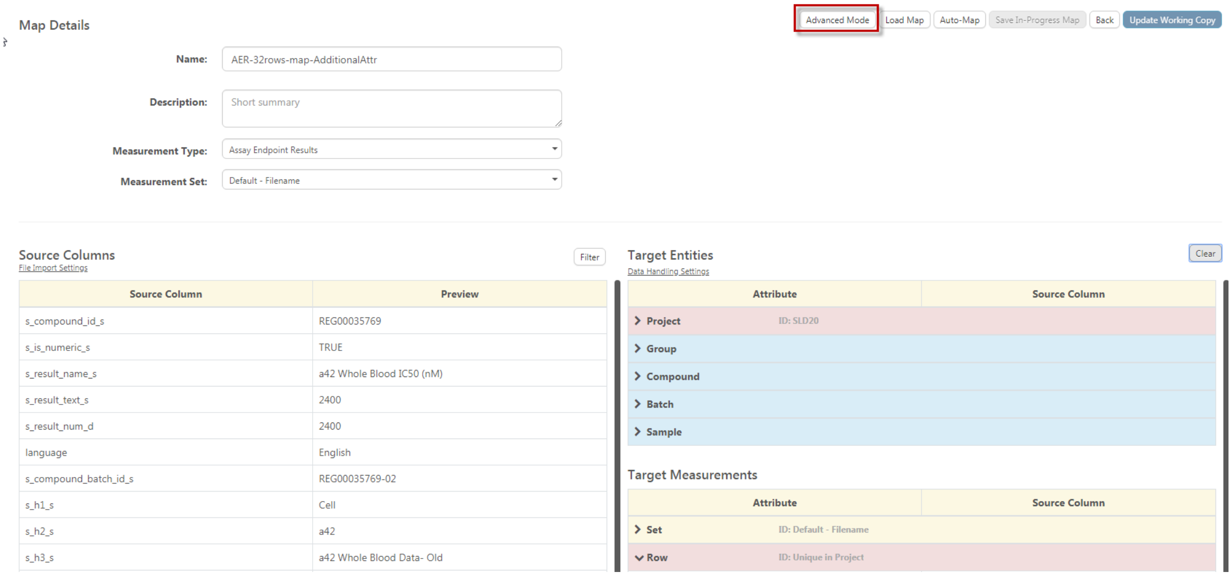
14.4.6 Advanced Mode

Some mapping features cannot be displayed or configured using the standard mapping interface.

When editing a map that uses advanced mapping features, an advanced mode interface allows you to edit the JSON document representing the map.

To edit a map using the Advanced Mode feature:

1. From the Map Details page for a project, click on the **Advanced Mode** button.



Map Details

Name: AER-32rows-map-AdditionalAttr

Description: Short summary

Measurement Type: Assay Endpoint Results

Measurement Set: Default - Filename

Source Columns

Source Column	Preview
s_compound_id_s	REG00035769
s_is_numeric_s	TRUE
s_result_name_s	a42 Whole Blood IC50 (nM)
s_result_text_s	2400
s_result_num_d	2400
language	English
s_compound_batch_id_s	REG00035769-02
s_h1_s	Cell
s_h2_s	a42
s_h3_s	a42 Whole Blood Data- Old

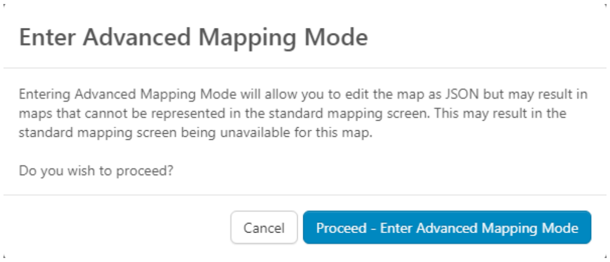
Target Entities

Attribute	Source Column
› Project ID: SLD20	
› Group	
› Compound	
› Batch	
› Sample	

Target Measurements

Attribute	Source Column
› Set ID: Default - Filename	
⌄ Row ID: Unique in Project	

You will be notified that entering Advanced Mapping Mode allows you to edit the map as JSON but may result in maps that cannot be represented in the standard mapping mode and therefore standard mapping may not be available for this map.

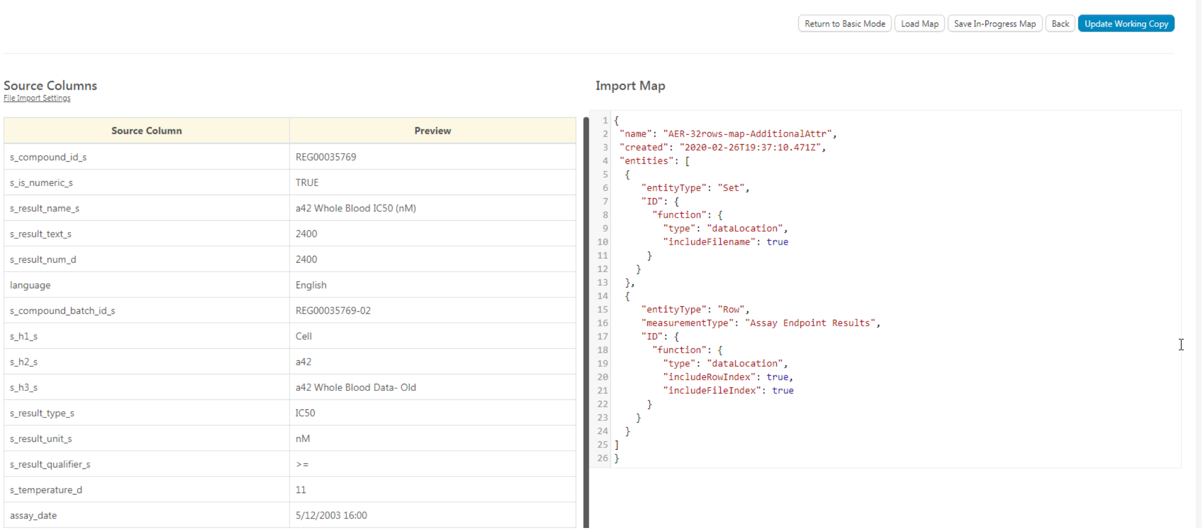


Enter Advanced Mapping Mode

Entering Advanced Mapping Mode will allow you to edit the map as JSON but may result in maps that cannot be represented in the standard mapping screen. This may result in the standard mapping screen being unavailable for this map.

Do you wish to proceed?

Clicking **Proceed – Enter Advanced Mapping Mode** will open the Advanced Mapping page, similar to the example shown below.



Source Columns

Source Column	Preview
s_compound_id_s	REG00035769
s_is_numeric_s	TRUE
s_result_name_s	a42 Whole Blood IC50 (nM)
s_result_text_s	2400
s_result_num_d	2400
language	English
s_compound_batch_id_s	REG00035769-02
s_h1_s	Cell
s_h2_s	a42
s_h3_s	a42 Whole Blood Data- Old
s_result_type_s	IC50
s_result_unit_s	nM
s_result_qualifier_s	>=
s_temperature_d	11
assay_date	5/12/2003 16:00

Import Map

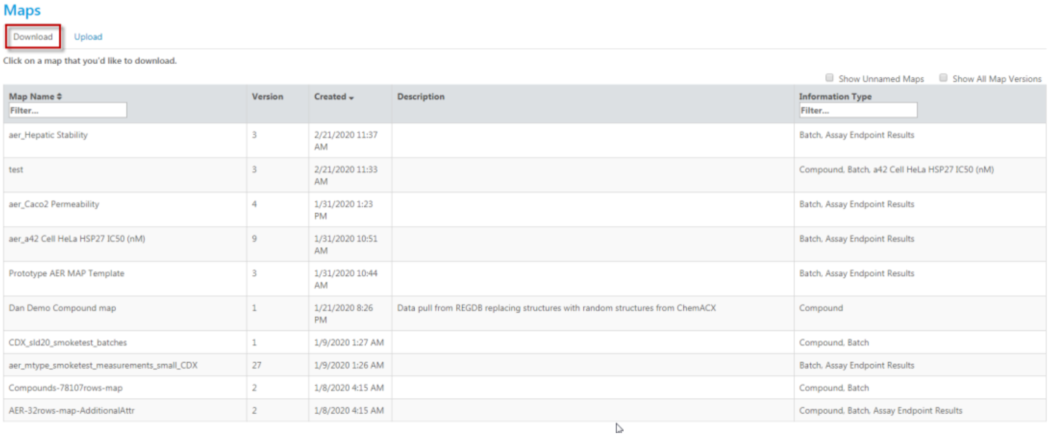
```
{
 "name": "AER-32rows-map-AdditionalAttr",
 "created": "2020-02-26T19:37:10.471Z",
 "entities": [
  {
     "entityType": "Set",
     "ID": {
       "function": {
         "type": "dataLocation",
         "includeFilename": true
        }
      }
  },
  {
     "entityType": "Row",
     "measurementType": "Assay Endpoint Results",
     "ID": {
       "function": {
         "type": "dataLocation",
         "includeRowIndex": true,
         "includeFileIndex": true
        }
      }
  }
 ]
}
```

It is possible to switch between the Advanced Mapping Mode and the Basic Mode, however some of the advanced mapping features may be lost.

An example of an advanced mapping feature is the Advanced Depivot feature. Using the standard mapping interface, it is not possible to group multiple columns when depivoting, however this operation can be performed editing the JSON in the Advanced Mapping Mode.

14.4.7 Downloading a Map

1. From the **Data** drop-down list box, select **Maps**.
2. From the Download tab, select **Show Unnamed Maps** and /or **Show All Map Versions** to view unnamed maps and/or all map versions.



Click on a map that you'd like to download.

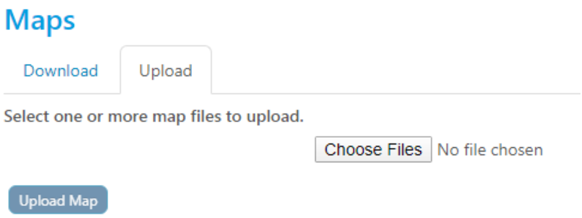
☐ Show Unnamed Maps ☐ Show All Map Versions

Map Name ⇕ Filter...	Version	Created ▾	Description	Information Type Filter...
aer_Hepatic Stability	3	2/21/2020 11:37 AM		Batch, Assay Endpoint Results
test	3	2/21/2020 11:33 AM		Compound, Batch, a42 Cell HeLa HSP27 IC50 (nM)
aer_Caco2 Permeability	4	1/31/2020 1:23 PM		Batch, Assay Endpoint Results
aer_a42 Cell HeLa HSP27 IC50 (nM)	9	1/31/2020 10:51 AM		Batch, Assay Endpoint Results
Prototype AER MAP Template	3	1/31/2020 10:44 AM		Batch, Assay Endpoint Results
Dan Demo Compound map	1	1/21/2020 8:26 PM	Data pull from REGDB replacing structures with random structures from ChemACX	Compound
CDX_sld20_smoketest_batches	1	1/9/2020 1:27 AM		Compound, Batch
aer_mtype_smoketest_measurements_small_CDX	27	1/9/2020 1:26 AM		Batch, Assay Endpoint Results
Compounds-78107rows-map	2	1/8/2020 4:15 AM		Compound, Batch
AER-32rows-map-AdditionalAttr	2	1/8/2020 4:15 AM		Compound, Batch, Assay Endpoint Results

3. Click on a map to download it.

14.4.8 Uploading a Map

1. From the **Data** drop-down list box, select **Maps**
2. From the Upload, select one or more maps to upload.



Select one or more map files to upload.

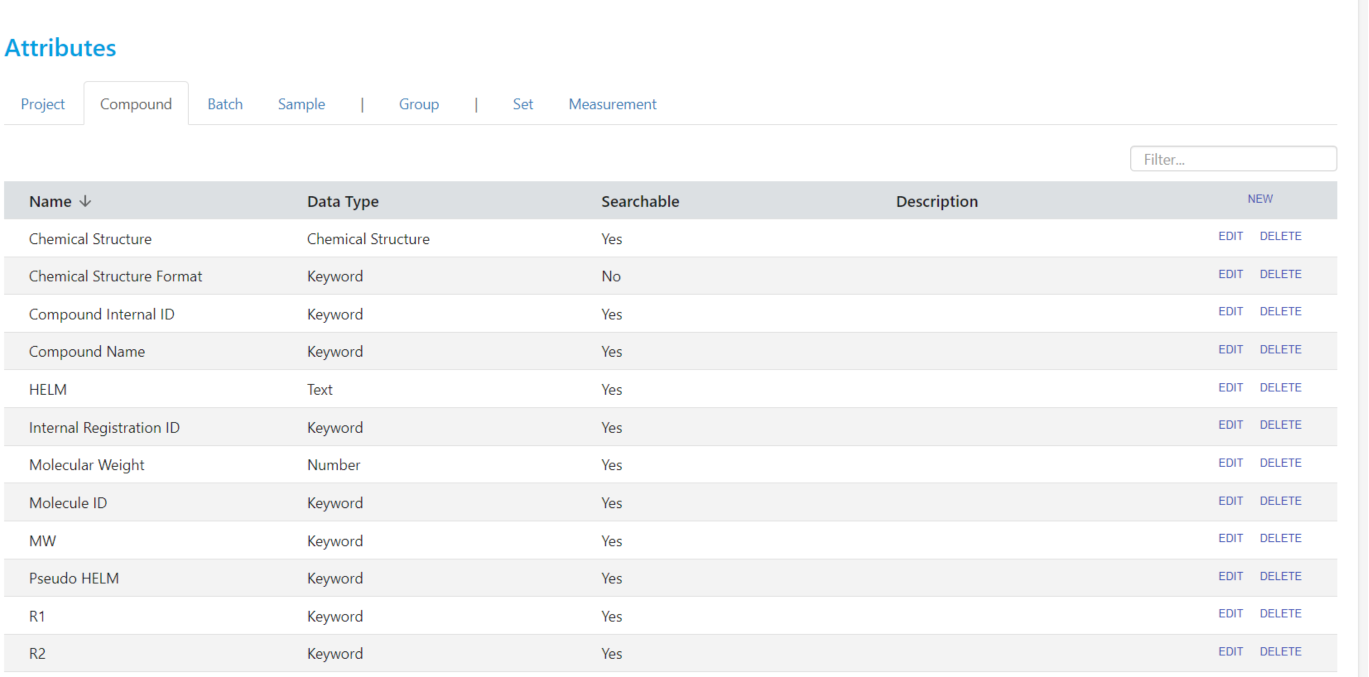
3. Click **Upload Map**.

14.5 Information Design

14.5.1 Entities and Attributes

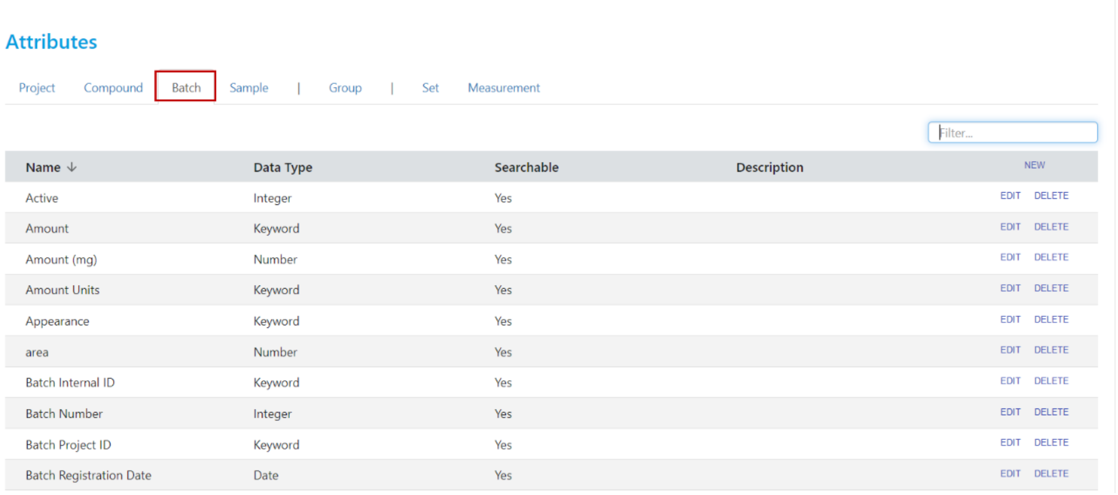
There is a single unified page that allows you to manage entity and measurement attributes.

1. Navigate to **Information Design > Entities and Attributes**.



Name ↓	Data Type	Searchable	Description	
Chemical Structure	Chemical Structure	Yes		EDIT DELETE
Chemical Structure Format	Keyword	No		EDIT DELETE
Compound Internal ID	Keyword	Yes		EDIT DELETE
Compound Name	Keyword	Yes		EDIT DELETE
HELM	Text	Yes		EDIT DELETE
Internal Registration ID	Keyword	Yes		EDIT DELETE
Molecular Weight	Number	Yes		EDIT DELETE
Molecule ID	Keyword	Yes		EDIT DELETE
MW	Keyword	Yes		EDIT DELETE
Pseudo HELM	Keyword	Yes		EDIT DELETE
R1	Keyword	Yes		EDIT DELETE
R2	Keyword	Yes		EDIT DELETE

The Attributes page is single page application for querying, adding, editing and deleting entity and measurement attributes. For example, from within the Compound and Batch tabs, you can manage the entity attributes. From the Measurement tab, you can manage the measurement attributes.



Name ↓	Data Type	Searchable	Description	NEW
Active	Integer	Yes		EDIT DELETE
Amount	Keyword	Yes		EDIT DELETE
Amount (mg)	Number	Yes		EDIT DELETE
Amount Units	Keyword	Yes		EDIT DELETE
Appearance	Keyword	Yes		EDIT DELETE
area	Number	Yes		EDIT DELETE
Batch Internal ID	Keyword	Yes		EDIT DELETE
Batch Number	Integer	Yes		EDIT DELETE
Batch Project ID	Keyword	Yes		EDIT DELETE
Batch Registration Date	Date	Yes		EDIT DELETE

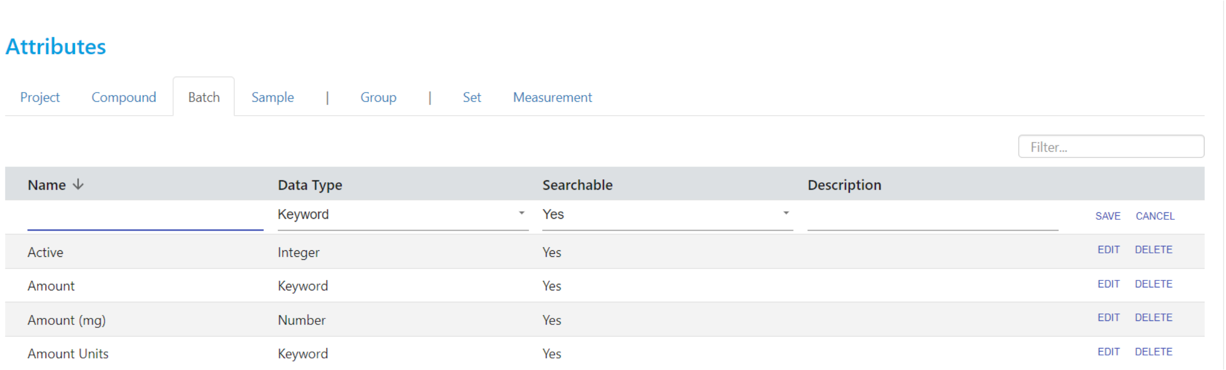
The table lists all currently defined attributes for the selected entity or measurement. Each row represents an attribute template. From the table, attributes can be edited or deleted.

Note: You can enter a query string in the text box located above the table on the right-hand side to filter the attributes in the table.

14.5.1.1 Defining a New Entity or Measurement Attribute

To add a new attribute:

1. Select entity or measurement tab to which you want to add a new attribute.
2. Click the **NEW** button to add a new row to the top of the table



Name ↓	Data Type	Searchable	Description	
	Keyword	Yes		SAVE CANCEL
Active	Integer	Yes		EDIT DELETE
Amount	Keyword	Yes		EDIT DELETE
Amount (mg)	Number	Yes		EDIT DELETE
Amount Units	Keyword	Yes		EDIT DELETE

3. Enter a unique Attribute Name in the Name field. .
4. Select the Data Type from the drop down list. An optional description can be entered. By default, the attribute is Searchable.
5. Click **SAVE**. You will be notified if the attribute fails to save.
6. Repeats steps 1-4 to add additional attributes.

14.5.1.2 Editing an Existing Attribute

To edit an attribute:

1. Click the **EDIT** button for the attribute you want to edit. .
2. Make the necessary modifications.
3. Click **SAVE**.

14.5.1.3 Deleting an Attribute

To delete an attribute:

1. Hover the mouse over the attribute to delete. An 🗑 icon appears in the last column for that row.
2. Click the 🗑 icon. The attribute is deleted.

NOTE: Signals Data Factory also provides the features and user interface components for managing measurement types, and attributes. However, these are general features that support common scientific data transformation use cases. With the exception of Compound/Batch attribute management, it is ***strongly recommended*** you use the measurement type and attributes management features in **Signals Inventa** to accomplish information design, as the features in Signals Inventa may provide you advanced capabilities such as assay endpoint mapping definition, guided measurement type creation, etc.

14.5.1.4 Custom Entities

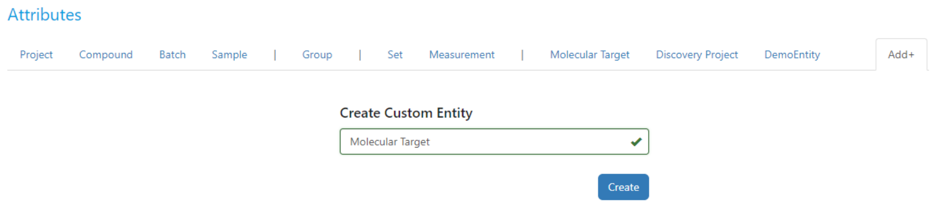
Signals Data Factory supports the addition of custom entities (or related entities). Related entities are an optional feature in Signals Inventa. They allow you to associate entity tables to your core entity (e.g. Compound, Batch) tables and then leverage those relationships while querying data.

The following section describes creating custom entities and relationships in Signals Data Factory.

A custom entity does not have a parent/child relationship (i.e. it is not a core entity), but it does have some relationship to a core entity (e.g. Compound, Batch). Often there is more information that is related to a core entity. Custom entities allow you to have another table (entity) in the system that describes the custom entity.

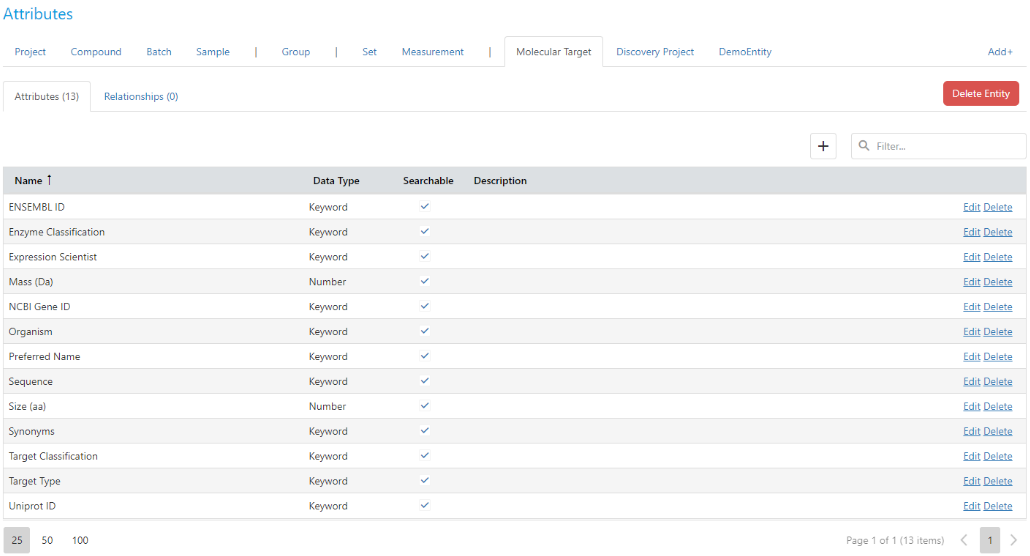
Adding Custom Entities

1. From the main tool bar, select **Information Design > Entities and Attributes > Add+**.
2. Enter the desired Entity name. Click on the **Create** button. The custom entity will be added as a tab next to the core entities.



Create Custom Entity
Molecular Target

3. Select the tab with the newly added custom entity and click on the + button. A new entry will be added as a row (column in the table). Enter the desired attribute Name, Data Type, Searchable, Description, then click on the **Save** button**.** Continue to add attributes as desired.



Name	Data Type	Searchable	Description	
ENSEMBL ID	Keyword	✓		Edit Delete
Enzyme Classification	Keyword	✓		Edit Delete
Expression Scientist	Keyword	✓		Edit Delete
Mass (Da)	Number	✓		Edit Delete
NCBI Gene ID	Keyword	✓		Edit Delete
Organism	Keyword	✓		Edit Delete
Preferred Name	Keyword	✓		Edit Delete
Sequence	Keyword	✓		Edit Delete
Size (aa)	Number	✓		Edit Delete
Synonyms	Keyword	✓		Edit Delete
Target Classification	Keyword	✓		Edit Delete
Target Type	Keyword	✓		Edit Delete
Uniprot ID	Keyword	✓		Edit Delete

Now there is a Custom Entity table that can relate to a core entity table.

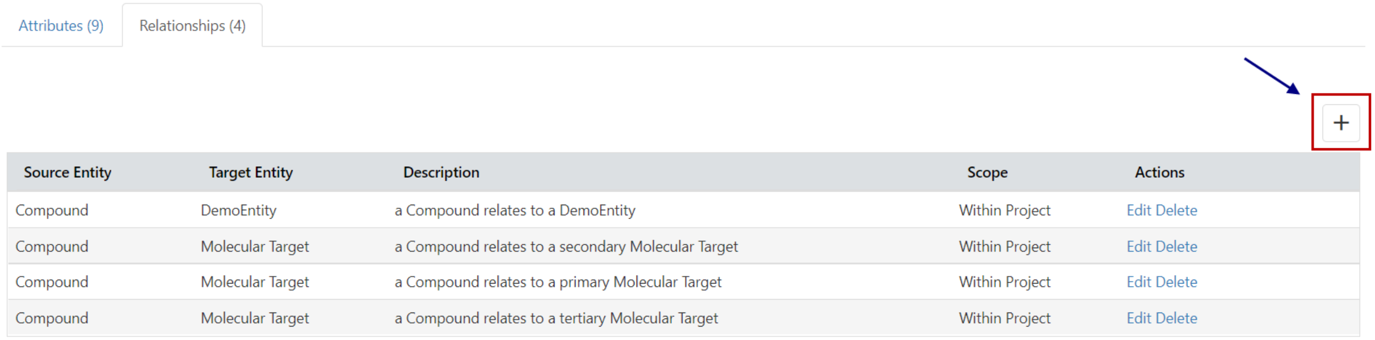
Defining Relationships and Dynamic Joins

Relationships between core entities and custom entities are defined from the core entity menus.

1. Signals Inventa only supports relationships defined on core entities (Compound, Batch). From the main tool bar, select **Information Design > Entities and Attributes,** then the desired core entity (e.g. Compound). Signals Inventa only supports relationships between core tables (Compounds and Batches) and custom entity tables.

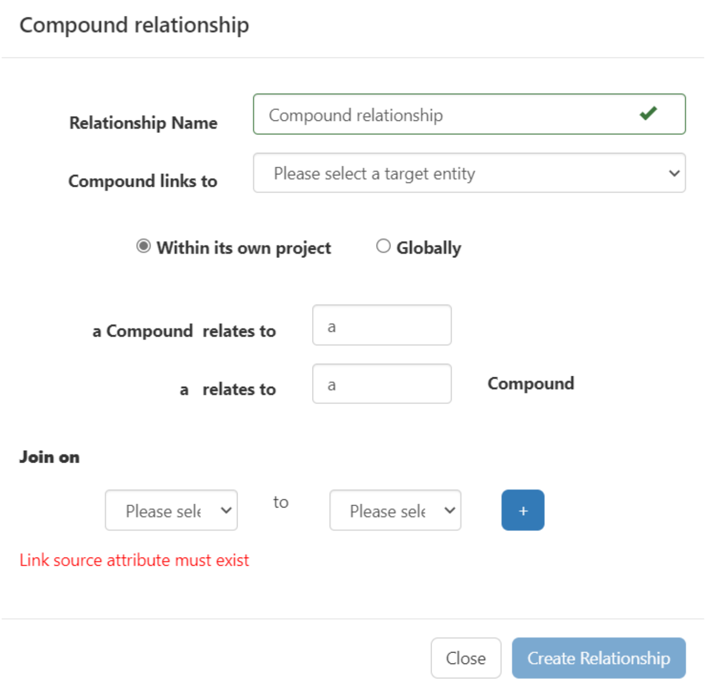
Note: The user may need to add the desired attribute to the core entity which will be linked to the custom entity if it does not already exist.

2. Select the **Relationships** tab > + button.



Source Entity	Target Entity	Description	Scope	Actions
Compound	DemoEntity	a Compound relates to a DemoEntity	Within Project	Edit Delete
Compound	Molecular Target	a Compound relates to a secondary Molecular Target	Within Project	Edit Delete
Compound	Molecular Target	a Compound relates to a primary Molecular Target	Within Project	Edit Delete
Compound	Molecular Target	a Compound relates to a tertiary Molecular Target	Within Project	Edit Delete

The Core Entity (e.g. Compound) Relationship window opens.



Compound relationship

Relationship Name Compound relationship ✓

Compound links to Please select a target entity

● **Within its own project** ○ **Globally**

a Compound relates to a

a relates to a **Compound**

Join on

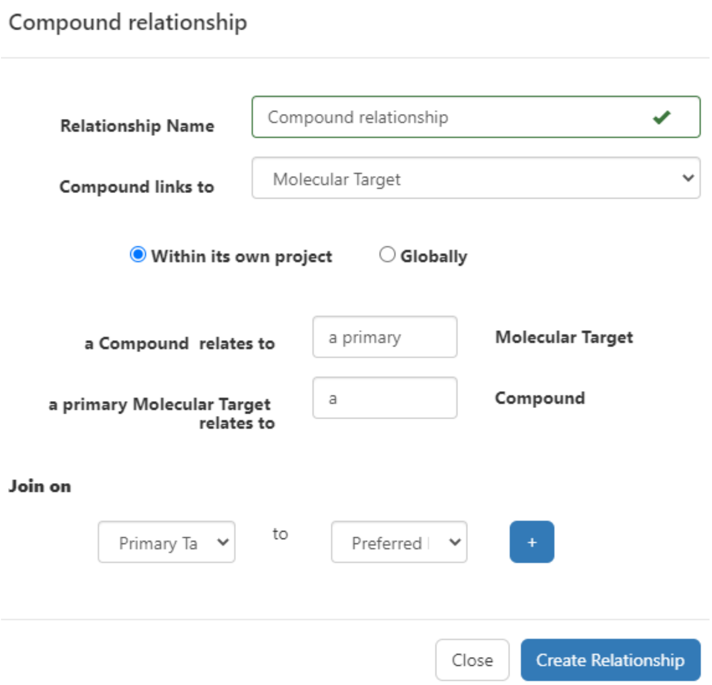
Please sele to Please sele

Link source attribute must exist

3. Specify a unique Relationship Name. Select the target entity (e.g. Molecular Target) from the ‘Compound links to’ dropdown list. The relationship can exist within its own project or globally. In the case that you want to load your custom entities in a different project, you would need to link ‘Globally’ here. By default, ‘Within its own project’ is selected.

4. The textboxes allow you to describe the relationship in more detail to drive the query capabilities in Signals Inventa. For example, you can add an adjective (e.g. primary). This is useful when two relationships are linked to the same custom entity. This allows you to define the relationship in more detail, for example primary target and secondary target. These descriptions will drive the Global Search interface when you are doing queries in Signals Inventa and therefore it is important to describe the relationship. However, this is optional and can simply be left as ‘a’.

5. The **Join on** dropdown menus allows the user to define what columns you are going to join. The first dropdown is the list of columns from the core entity (e.g. Compound) table. The link source attribute must exist. The second dropdown is the list of columns from the custom entity (e.g. Molecular Target) table. Select **Create Relationship** to save the settings and close the menu.



Compound relationship

Relationship Name	Compound relationship ✓
Compound links to	Molecular Target

● Within its own project ○ Globally

a Compound relates to	a primary	Molecular Target
a primary Molecular Target relates to	a	Compound

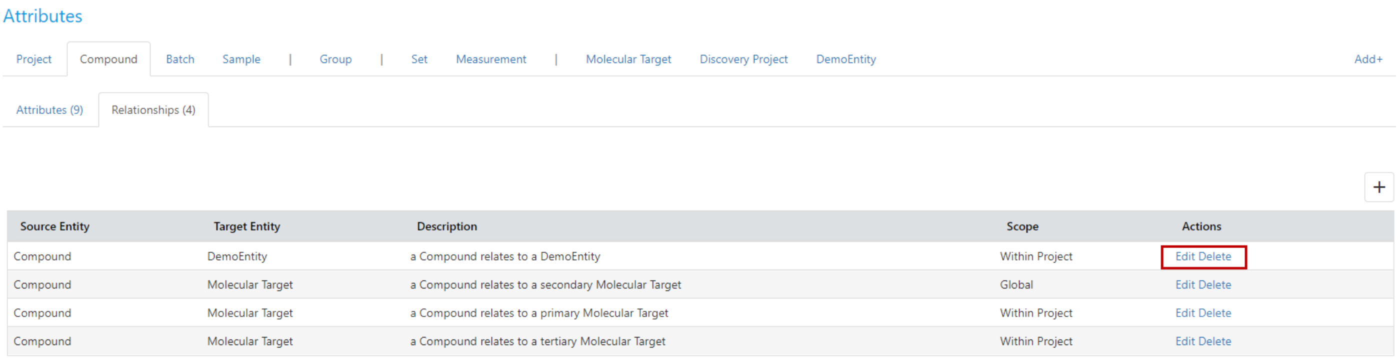
Join on

Primary Ta to Preferred

Note: It is recommended that the second attribute to be linked is unique (i.e. $$*attribute*ID).

Note: Composite joins can be created by adding additional joins via the + button. This describes one way to join where all items must match to be returned in a query.

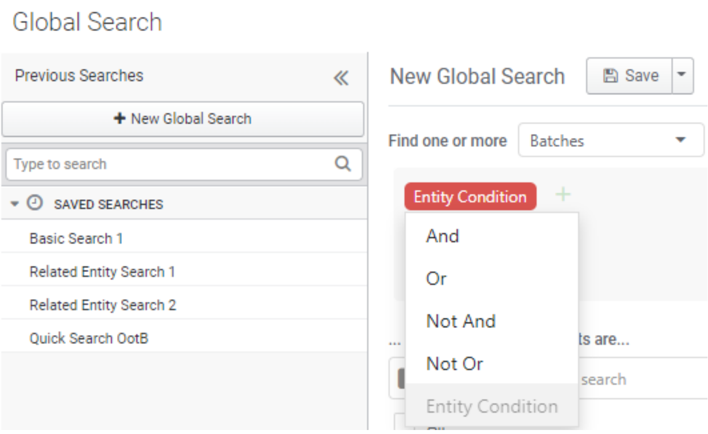
Individual relationships can be edited or deleted via the **Edit** and **Delete** buttons under **Actions** in the table.



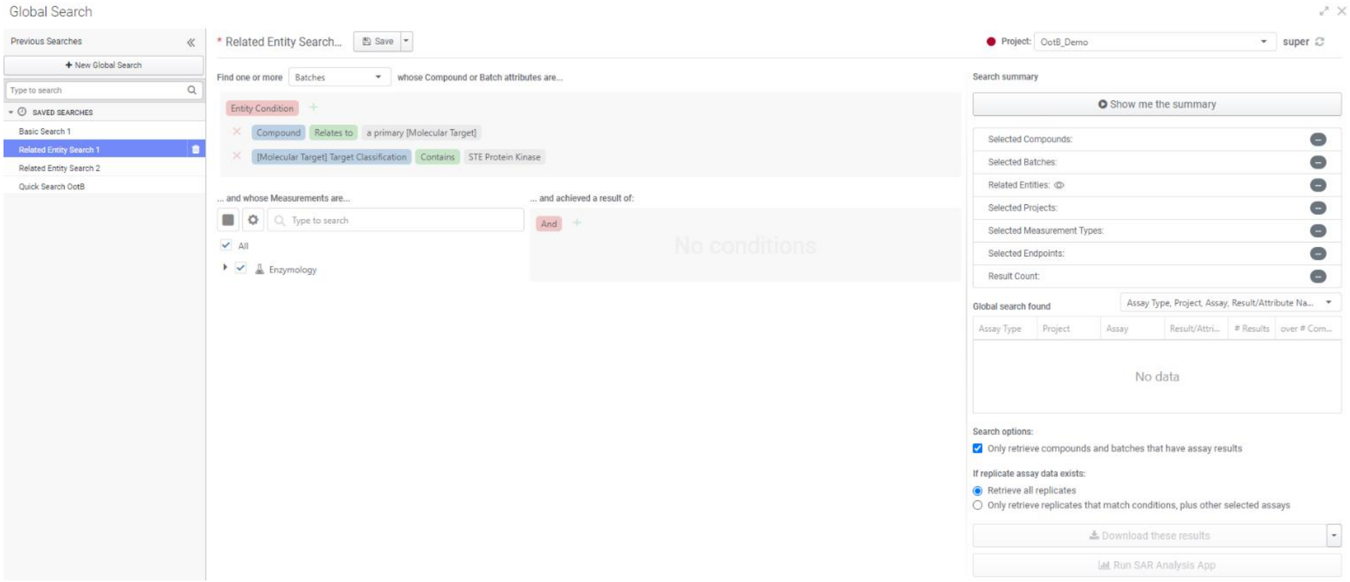
Source Entity	Target Entity	Description	Scope	Actions
Compound	DemoEntity	a Compound relates to a DemoEntity	Within Project	Edit Delete
Compound	Molecular Target	a Compound relates to a secondary Molecular Target	Global	Edit Delete
Compound	Molecular Target	a Compound relates to a primary Molecular Target	Within Project	Edit Delete
Compound	Molecular Target	a Compound relates to a tertiary Molecular Target	Within Project	Edit Delete

Custom Entities in Global Search

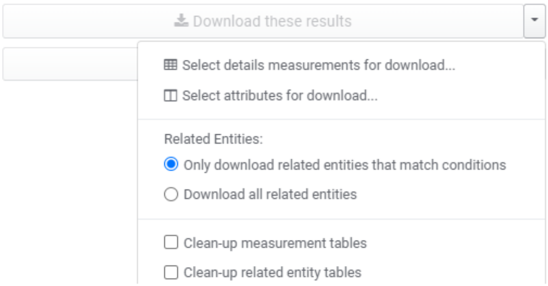
1. Custom entities can be added as a table and mapped in the same way that core entities are and can be viewed in Signals Inventa's Global Search via the Entity Condition tag**.** Refer to the Global Search section for more details using custom entities in Global Search.



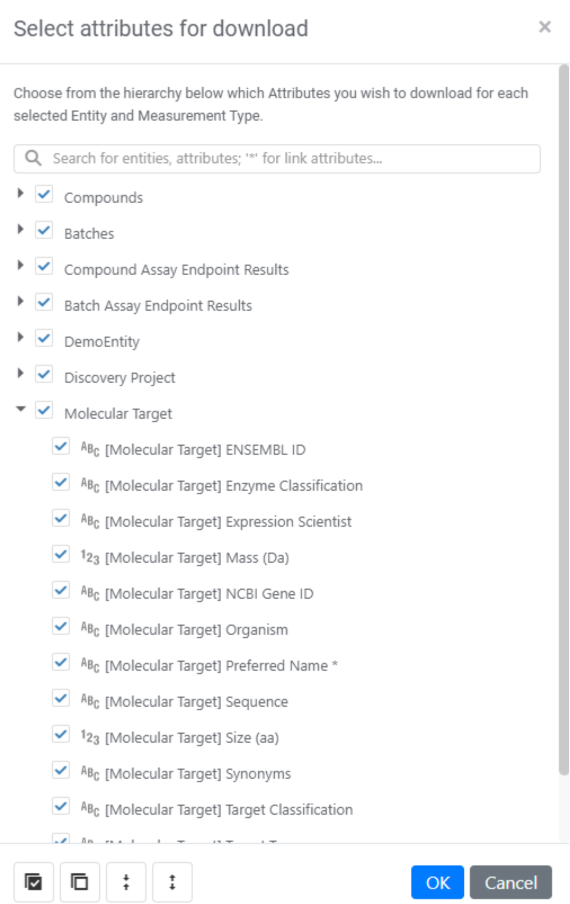
2. Select the + icon > **Add Condition,** then select the desired relationship in the **<enter a value>** dropdown. Continue to add conditions as desired.



3. Select the arrow next to **Download these results** to view additional options.



4. The user can select the desired related entities from the **Select attributes for download** menu.



Select attributes for download

Choose from the hierarchy below which Attributes you wish to download for each selected Entity and Measurement Type.

Search for entities, attributes; '*' for link attributes...

- ☑ Compounds
- ☑ Batches
- ☑ Compound Assay Endpoint Results
- ☑ Batch Assay Endpoint Results
- ☑ DemoEntity
- ☑ Discovery Project
- ☑ Molecular Target
  - ☑ ABC [Molecular Target] ENSEMBL ID
  - ☑ ABC [Molecular Target] Enzyme Classification
  - ☑ ABC [Molecular Target] Expression Scientist
  - ☑ 123 [Molecular Target] Mass (Da)
  - ☑ ABC [Molecular Target] NCBI Gene ID
  - ☑ ABC [Molecular Target] Organism
  - ☑ ABC [Molecular Target] Preferred Name *
  - ☑ ABC [Molecular Target] Sequence
  - ☑ 123 [Molecular Target] Size (aa)
  - ☑ ABC [Molecular Target] Synonyms
  - ☑ ABC [Molecular Target] Target Classification

Refer to the Search by Related Entity section for more information on custom entities in Global Search.

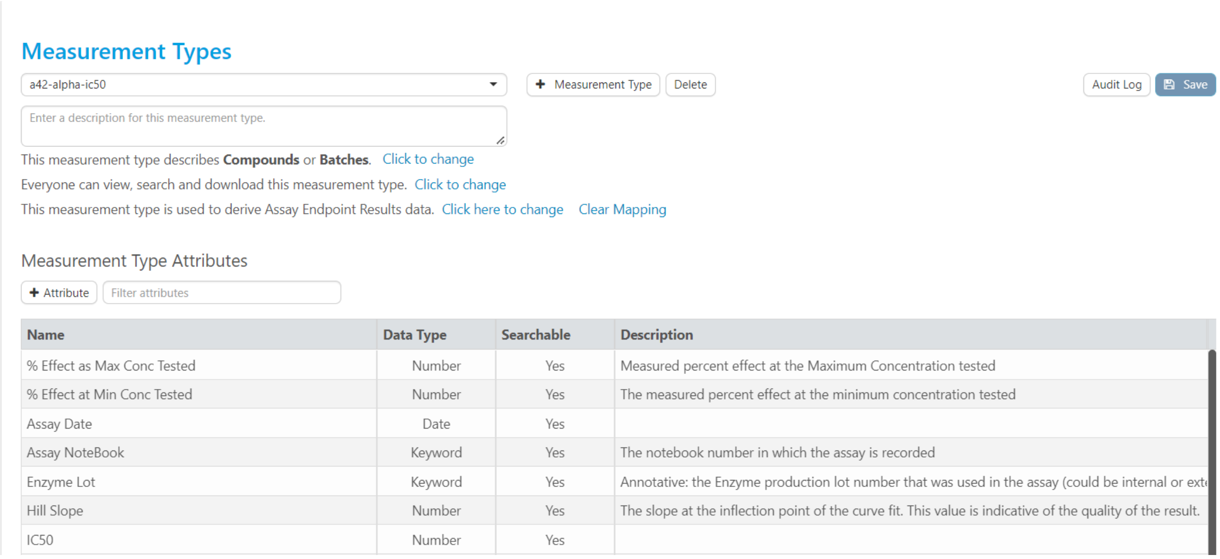
14.5.2 Measurement Types

Measurement Types are a category of similar measurements and are managed on the **Measurement Types** page. From this page, you can define and manage measurement types.

To access the Measurement Types page:

1. From the **Information Design** drop-down list box, select **Measurement Types**.

The Measurement Types page opens, similar to the example shown below.



This measurement type describes **Compounds** or **Batches**. Click to change

Everyone can view, search and download this measurement type. Click to change

This measurement type is used to derive Assay Endpoint Results data. Click here to change Clear Mapping

Measurement Type Attributes

Name	Data Type	Searchable	Description
% Effect as Max Conc Tested	Number	Yes	Measured percent effect at the Maximum Concentration tested
% Effect at Min Conc Tested	Number	Yes	The measured percent effect at the minimum concentration tested
Assay Date	Date	Yes	
Assay NoteBook	Keyword	Yes	The notebook number in which the assay is recorded
Enzyme Lot	Keyword	Yes	Annotative: the Enzyme production lot number that was used in the assay (could be internal or ext
Hill Slope	Number	Yes	The slope at the inflection point of the curve fit. This value is indicative of the quality of the result.
IC50	Number	Yes	

From the Measurement Types page you can define new measurement types or manage existing ones.

Note: Do NOT delete the ‘Assay Endpoint Results’ measurement type. This measurement type is added by Signals Inventa and required for functionality (e.g. Global Search hierarchy display, SAR table generation, endpoint management, etc) to work properly.

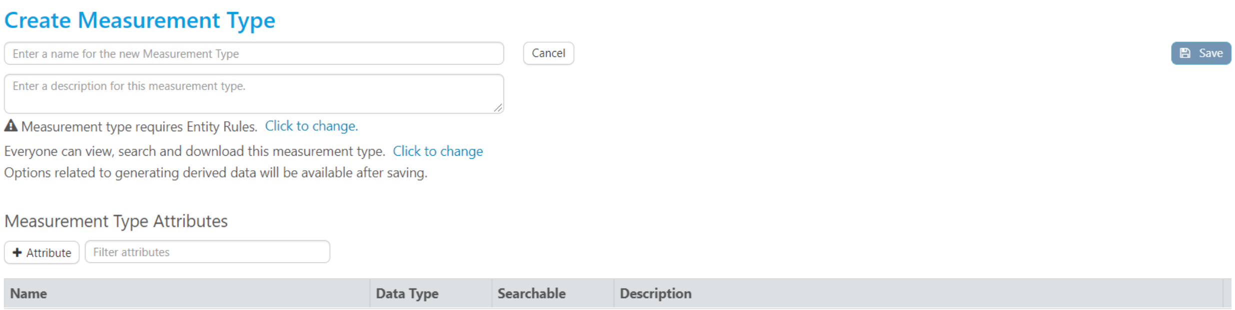
Measurement attributes can be added or removed, applicable entities specified, privileges for accessing the sensitive measurement type data can be defined.

The table lists all currently defined measurement attributes for the selected measurement type. Each row represents an attribute template.

14.5.2.1 Add Measurement Types

To add a new measurement type:

1. Click the +**Measurement Type** button.
2. The **Create Measurement Type** page opens similar to the example shown below.



⚠ Measurement type requires Entity Rules. Click to change.

Everyone can view, search and download this measurement type. Click to change

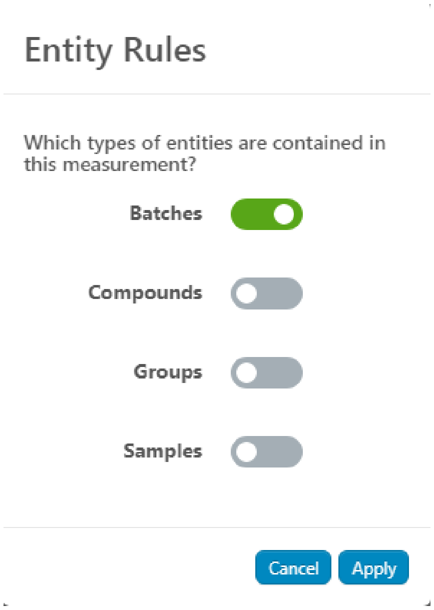
Options related to generating derived data will be available after saving.

Measurement Type Attributes

Name	Data Type	Searchable	Description

Note: Within Signals Data Factory, there are some symbols which should not be used when specifying names especially in the case of Measurement Types and Attributes. Refer to Signals Data Factory Restricted Characters.

3. Enter a unique name and optional description.
4. The Measurement Type requires Entity Rules. Click '**Click to change**' to add entity rules. The **Entity Rules** screen appears.



Entity Rules

Which types of entities are contained in this measurement?

Batches ☑
Compounds ☐
Groups ☐
Samples ☐

Note: At least one entity must be selected. Also, measurements associated with Groups cannot be associated with any other entity.

5. Select the types of entities to be contained in the measurement type and click **Apply**.
6. Optionally, specify security settings (defining who can view/search and download the measurement type.

Note: For more information. refer to the Measurement Types - Security Settings section.

7. Click the **Save** button.

14.5.2.2 Measurement Type – Security Settings

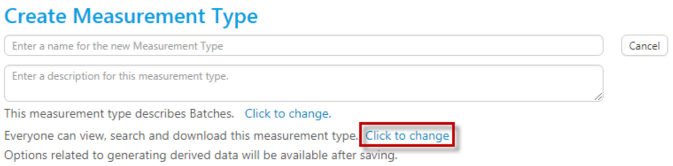
By default, there are no restrictions on who can view, search or download data for specific measurement types.

However, it is possible to restrict both the visibility and downloadability of a measurement type independently.

Note: These restrictions do not apply to Administrators, who will always be able to view/download all data.

To apply restrictions for a measurement:

1. Click the **Click to change** link, you can grant access rights to groups.

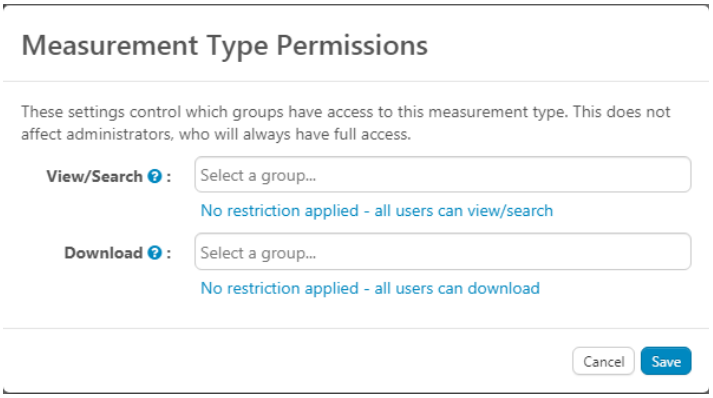


This measurement type describes Batches.

Everyone can view, search and download this measurement type.

Options related to generating derived data will be available after saving.

2. From the Measurement Type Permissions page, you can define which groups have access to the measurement type.



These settings control which groups have access to this measurement type. This does not affect administrators, who will always have full access.

No restriction applied - all users can view/search

No restriction applied - all users can download

3. There are 2 settings that can be controlled. View/Search and Download.

- In the **View/Search** setting, if no group is selected then everyone can view/search the measurement type details. Selecting one or more group(s) in this field means that you have restricted the view/search permission to users that are members of any of the selected groups.

- In the **Download** setting, it is possible to restrict the download of the measurement type. This will not impact any user's ability to View/Search the measurement type (unless specified above).

Note: Restricting View/Search will disable download of the measurement type for all users. To re-enable download, it is necessary to assign a group to the download setting. To download in this situation, users must be a member of a group assigned View/Search permissions and a group assigned Download permissions – this does not have to be the same group. (i.e. they must be able to View/Search in order to be able to Download).

4. Click the **Save** button.

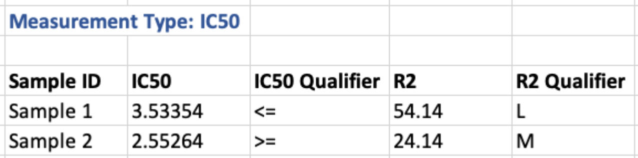
Note: Download permission for a measurement type is required to perform any of the following functions:

- Map new files to the measurement type, or change maps for files already mapped to the measurement type (including, on the file mapping page, loading a map associated with that measurement type)
- Download or preview the measurement type's data directly from the Project details page.
- Download the measurement type from a completed export (this does not restrict you from including the data in an export).

14.5.2.3 Derived Data

In some circumstances, if can be beneficial to store a measurement type in 2 formats. For example, data may be presented in both a short-wide and a tall-skinny format.

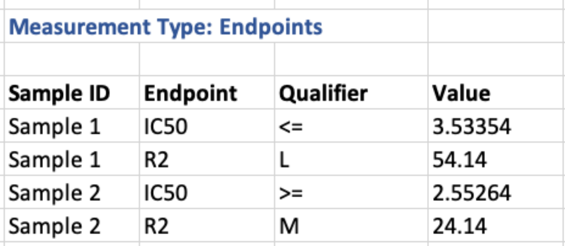
Consider a case where a measurement type contains multiple endpoints.



Measurement Type: IC50

Sample ID	IC50	IC50 Qualifier	R2	R2 Qualifier
Sample 1	3.53354	<=	54.14	L
Sample 2	2.55264	>=	24.14	M

It may be desirable to also store the data in a different (in this case de-pivoted) format, e.g.:

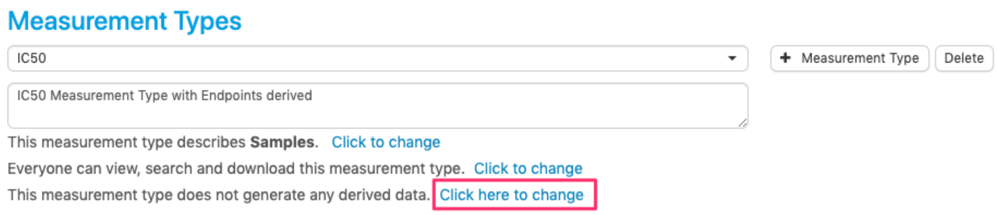


Measurement Type: Endpoints

Sample ID	Endpoint	Qualifier	Value
Sample 1	IC50	<=	3.53354
Sample 1	R2	L	54.14
Sample 2	IC50	>=	2.55264
Sample 2	R2	M	24.14

Measurement types support the specification of derived data – in the form of a map applied to the measurement type itself. This map would be applied whenever data is loaded into that measurement type, enabling you to populate two measurement types from a single file…e.g. File → IC50 → Endpoints.

To implement this for a measurement type, choose to change the setting for the derived data:



IC50

IC50 Measurement Type with Endpoints derived

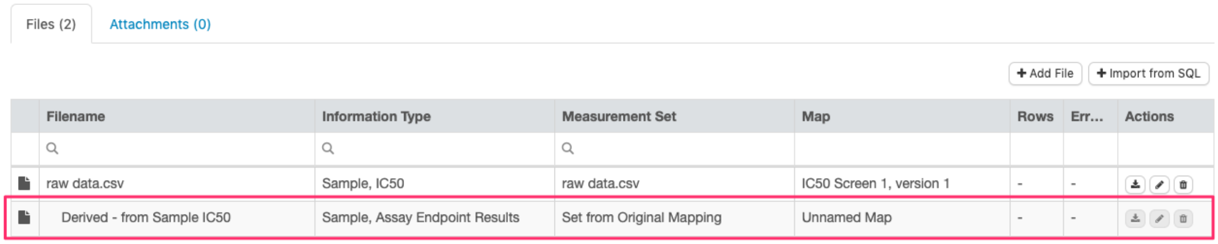
This measurement type describes **Samples**. Click to change

Everyone can view, search and download this measurement type. Click to change

This measurement type does not generate any derived data. Click here to change

The mapping screen will appear, allowing you to use the full mapping functionality to map data from the source measurement type into another (*you cannot map to the same measurement type!*)

Once a measurement type is configured to generate derived data, when used in a project, the derived measurement type will appear as an additional row alongside any files mapped to that measurement type:



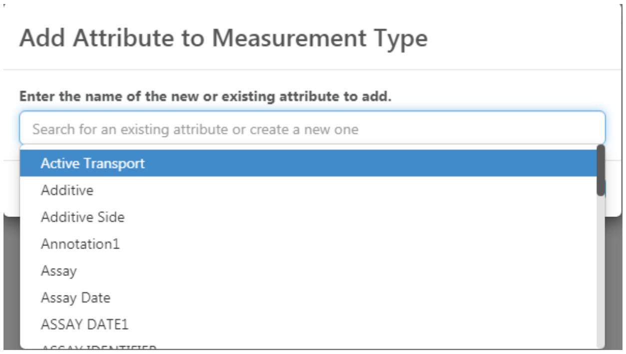
Filename	Information Type	Measurement Set	Map	Rows	Err...	Actions
raw data.csv	Sample, IC50	raw data.csv	IC50 Screen 1, version 1	-	-	
Derived - from Sample IC50	Sample, Assay Endpoint Results	Set from Original Mapping	Unnamed Map	-	-	

Note: These additional rows are displayed for information only – no actions are available here.

14.5.2.4 Measurement Type Attributes

To add attributes to measurement types:

1. From the **Measurement Types** page or in the **Create Measurement Types** page, click **+ Attribute** button. The Add Attribute to Measurement Type dialog is displayed.



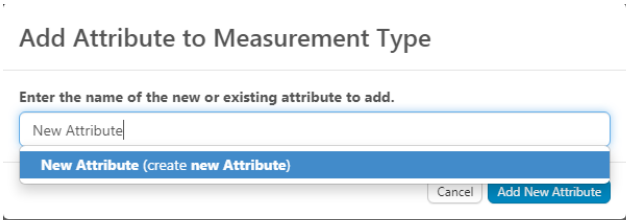
Add Attribute to Measurement Type

Enter the name of the new or existing attribute to add.

From here, you can select an existing attribute to associate with the measurement type or create a new attribute.

a) From the drop-down list box, select an existing attribute directly or type to search for an existing attribute and then click the **Add New Attribute** button to add the selected attribute to the measurement type.

b) To create a new attribute, type a new attribute name to display the Create New Attribute option, similar to the example shown below, and then click **Add New Attribute** button.



Add Attribute to Measurement Type

Enter the name of the new or existing attribute to add.

New Attribute

Note: Within Signals Data Factory, there are some symbols which should not be used when specifying names especially in the case of Measurement Types and Attributes. Refer to [Signals Data Factory Restricted Characters]().

Note: The attributes that have already been added to the measurement type will not be shown in the drop-down list box.

To edit an attribute:

1. Click the cell to edit.
2. Make the necessary modifications.
3. Click **Save**.

To delete an attribute:

1. Hover the mouse over the attribute to delete. An 🗑 icon appears in the last column for that row.

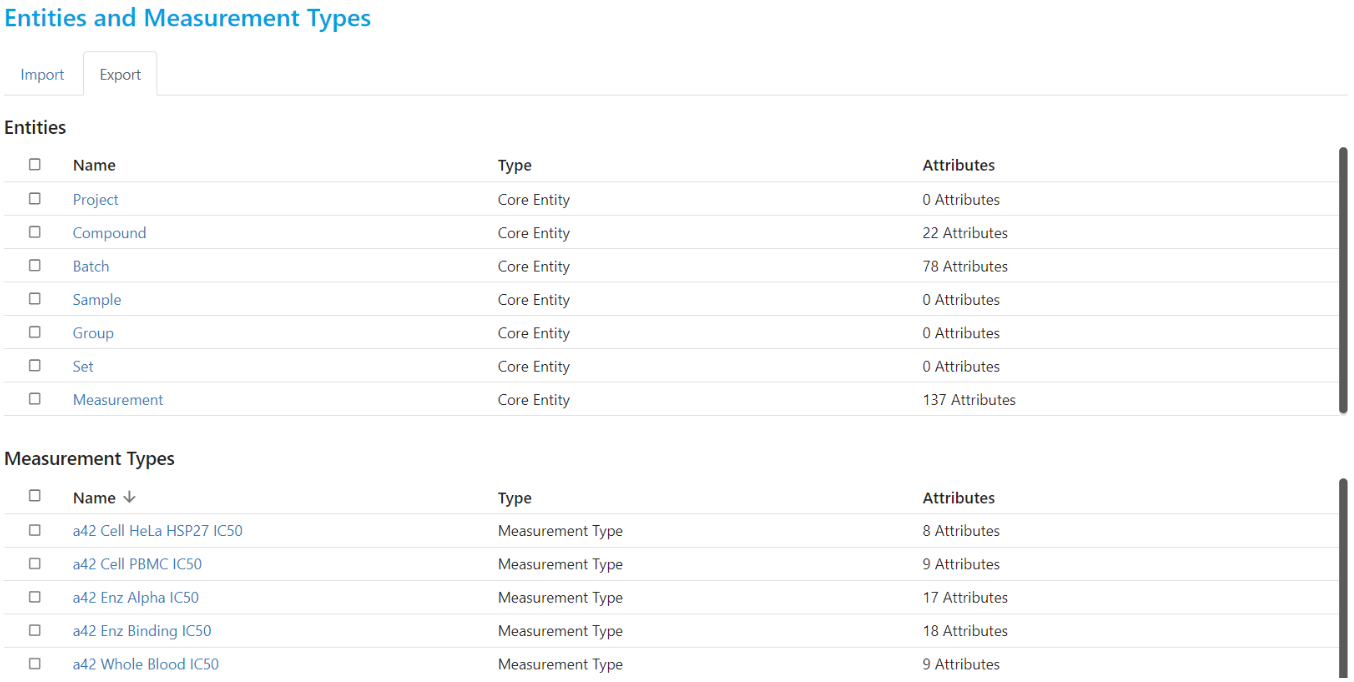
2. Click the 🗑 icon. The attribute is deleted.

14.5.3 Import/Export

There is a single unified page that allows you to import/export entities and measurement types.

1. Navigate to **Information Design > Import / Export**.

Under the **Export** tab, you can export the entire system (all entities and measurement types) or selectively choose which entities and measurement types to in include in the export.



Entities and Measurement Types

Entities

☐	Name	Type	Attributes
☐	Project	Core Entity	0 Attributes
☐	Compound	Core Entity	22 Attributes
☐	Batch	Core Entity	78 Attributes
☐	Sample	Core Entity	0 Attributes
☐	Group	Core Entity	0 Attributes
☐	Set	Core Entity	0 Attributes
☐	Measurement	Core Entity	137 Attributes

Measurement Types

☐	Name ↓	Type	Attributes
☐	a42 Cell HeLa HSP27 IC50	Measurement Type	8 Attributes
☐	a42 Cell PBMC IC50	Measurement Type	9 Attributes
☐	a42 Enz Alpha IC50	Measurement Type	17 Attributes
☐	a42 Enz Binding IC50	Measurement Type	18 Attributes
☐	a42 Whole Blood IC50	Measurement Type	9 Attributes

The number of attributes for each entity and measurement type is displayed.

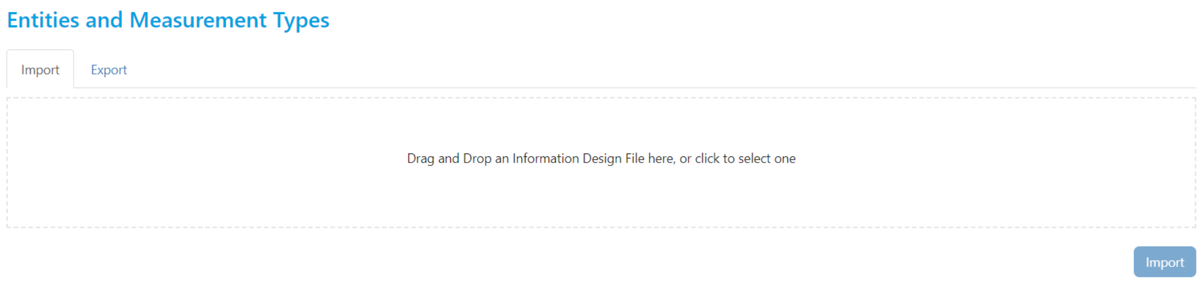
Under the Entities list, Sample and Group are not used by Signals Inventa. Measurement is the measurement attributes. You can export all attributes that are stored for measurements. When exporting the full Measurement set, it will include all measurement attributes whether they are used or not.

You can also export a measurement type which will export an information design that will create the measurement type and all the attributes that it uses.

For example in the export page shown above, of the 137 measurement attributes, 8 of them are used in the a42 Cell HeLa HSP27 IC50 measurement type.

Clicking the **Export** button will generate an information design export file (*.csv) and download it to your local system from which you can view the information that has been exported.

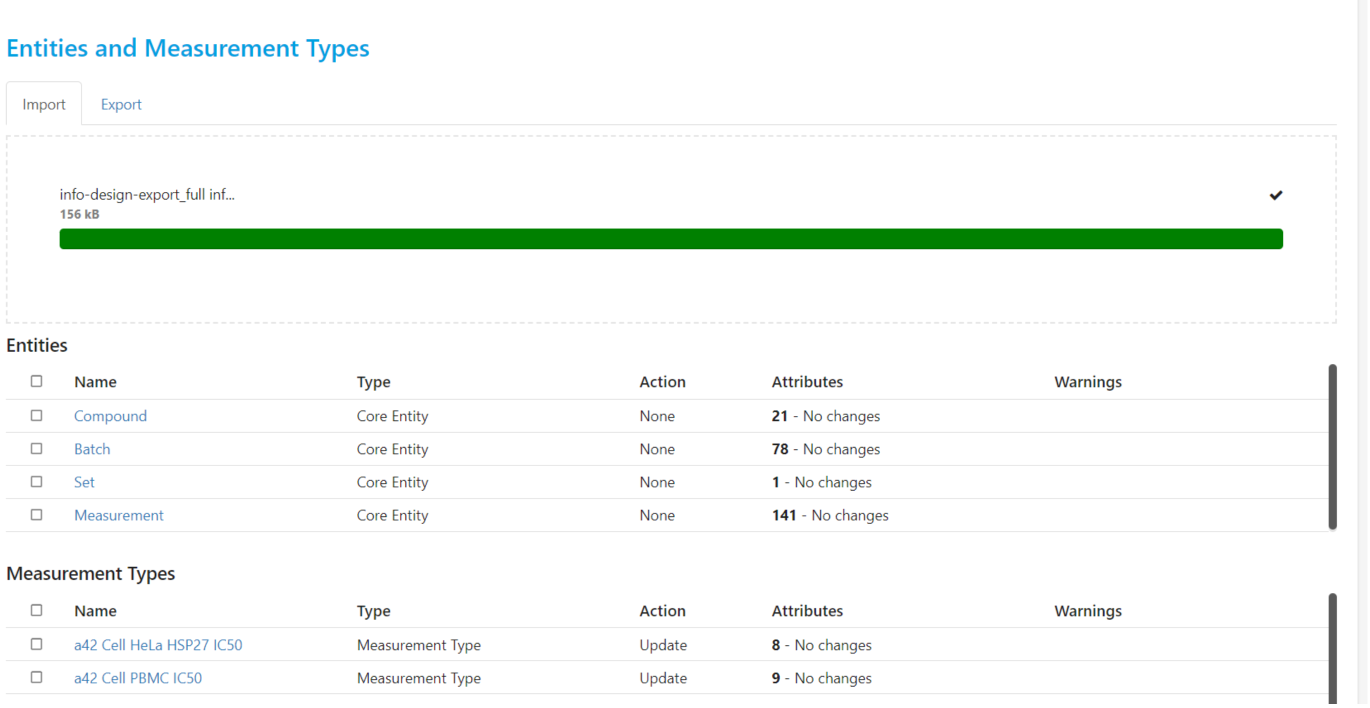
Under the **Import tab**, you can drag and drop an Information Design File (*.csv), or click to browse for the file that you have generated using the Export functionality.



Drag and Drop an Information Design File here, or click to select one

A preview is displayed showing the entities and measurement types contained in the file and their associated action, attributes and warnings.

The example shown below illustrates a full export file.



info-design-export_full inf...
156 kB

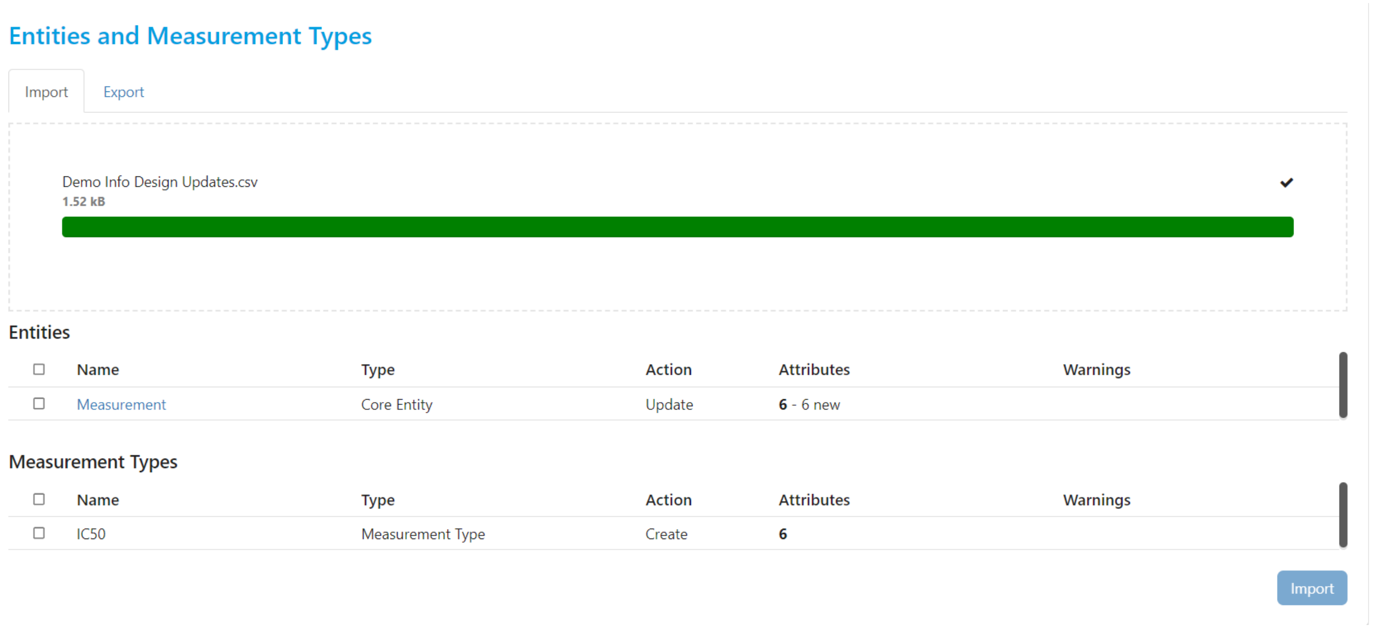
Entities

☐	Name	Type	Action	Attributes	Warnings
☐	Compound	Core Entity	None	**21** - No changes	
☐	Batch	Core Entity	None	**78** - No changes	
☐	Set	Core Entity	None	**1** - No changes	
☐	Measurement	Core Entity	None	**141** - No changes	

Measurement Types

☐	Name	Type	Action	Attributes	Warnings
☐	a42 Cell HeLa HSP27 IC50	Measurement Type	Update	**8** - No changes	
☐	a42 Cell PBMC IC50	Measurement Type	Update	**9** - No changes	

Although there are no changes to the attributes in the example shown here, the Action for the measurement type is listed as ‘Update’ because when you are importing a measurement type, you are not just associating its attributes, a measurement type has other setting associated with it. For example which entities it can link to, secondary maps, security on the measurement type could be updated for this measurement type.



Entities and Measurement Types

Demo Info Design Updates.csv
1.52 kB

Entities

☐	Name	Type	Action	Attributes	Warnings
☐	Measurement	Core Entity	Update	**6** - 6 new	

Measurement Types

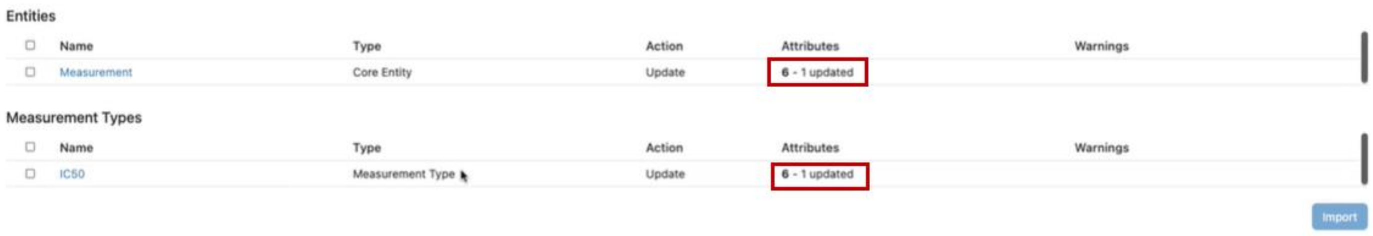
☐	Name	Type	Action	Attributes	Warnings
☐	IC50	Measurement Type	Create	**6**	

In the example shown abovre, if you choose to import this file, it will create a new measurement type (e.g. IC50) with 6 attributes.

At the same time, it will import the attributes for that measurement type. In the example above, there are 6 attributes for the new measurement type, and in this case, all 6 are new.

In the example shown below, the measurement type (e.g. IC50) is already in the system and is going to have 6 attributes, and the action will be to update one of them. You can also see there are 6 measurement attributes and one is being updated. One attribute is being changed in some way by this import, for example, the data type may be changing from text to a keyword.

It is important to verify what consequences updating an existing attribute may have as it could be affecting other measurement types as well.



Entities

☐	Name	Type	Action	Attributes	Warnings
☐	Measurement	Core Entity	Update	**6** - 1 updated	

Measurement Types

☐	Name	Type	Action	Attributes	Warnings
☐	IC50	Measurement Type	Update	**6** - 1 updated	

From here, you can select the entities and measurement types to import into your system.

Clicking the **Import** button will import the file into the system.

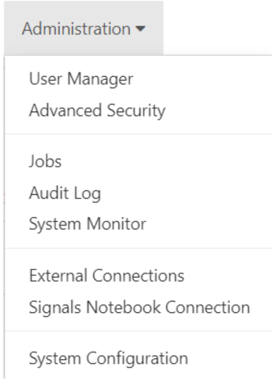
14.5.4 Inventa Configuration

Signals Data Factory also provides the features and user interface components for managing measurement types, attributes and maps. However, these are general features that support common scientific data transformation use cases. With the exception of Compound/Batch attribute management, it is strongly recommended you use the measurement type, attributes and maps management features in Signals Inventa to accomplish information design, as the features in Signals Inventa may provide you advanced capabilities such as assay endpoint mapping definition, guided measurement type creation, etc.

To access the Signals Inventa configuration for measurement types, attributes and maps, select the **Inventa Configuration** sub-menu from **Information Design** in Signals Data Factory. Once you have been redirected to the Signals Inventa configuration page, you can navigate back to Signals Data Factory by selecting the **SDF Configuration** sub-menu from **Information Design** in Signals Inventa.

14.6 Administration

Using the **Administration** dropdown menu, you can access the administrative tasks.



14.6.1 Advanced Security

(This is an optional feature, and requires a System Administrator to enable it)

In addition to the Project Security and Measurement Type Security, there is also an option to restrict users access to data at the row-level. These restrictions can apply to core entities (Compounds, Batches, Samples etc) as well as their measurements.

Note: These permissions are combined with any existing Project and Measurement type security and will not override any of those settings. For example, if you do not have permission to see a project or measurement type, then granting permissions from the Advanced Security screen module will have no effect.

By default, there are no restrictions on any entities or measurements.

Once a 'permission' for an entity or measurement is assigned to a group, it immediately becomes restricted and only users belonging to that group can see that restricted entity.

Note: Once an entity is restricted, that restriction will also apply to all child entities. For example, a user that can only see 'Signals Inventa' project would also be restricted to only seeing Compounds and Batches belonging to this project, as well as their measurements.

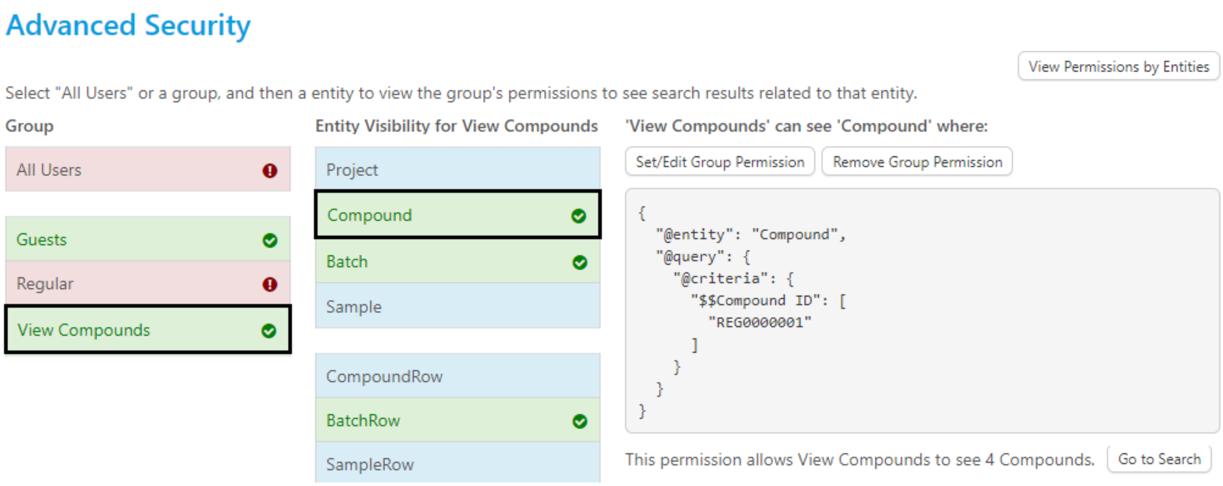
Permissions are additive so, if different permissions for the same entity are assigned to two groups, and a user is a member of both groups, they will be able to see the union of both sets of permissions.

Default permissions – i.e. permission that you wish to be granted to any user – can be assigned to the group entry named 'All Users'. (there is no requirement to create an actual 'All Users' group – this is managed internally)

Example – Assigning groups to see Compounds by a specified Compound ID:

- Starting from a position where projects are not restricted
- Create a User Groups named "View Compounds"
- Navigate to the Advanced Security page (via the Signals – Advanced Security menu)
- Select the "View Compounds" group, and the "Compound" Entity

- Click the “Set/Edit Group Permission” button and type an advanced search criteria which identities the Compounds you wish to allow the selected group to see. In this case, the following search is likely applicable:



Advanced Security

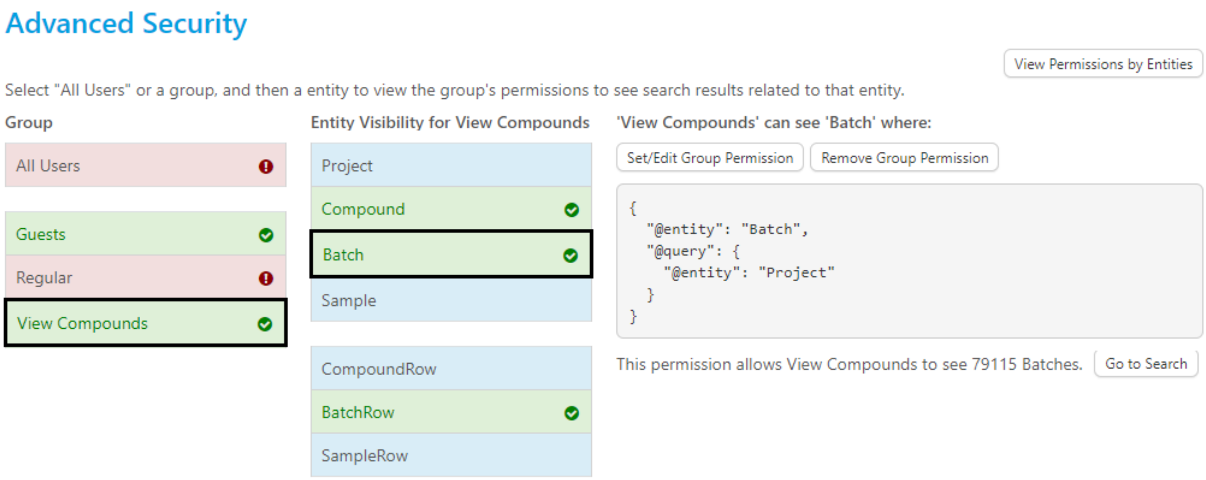
Select "All Users" or a group, and then a entity to view the group's permissions to see search results related to that entity.

'View Compounds' can see 'Compound' where:

```
{
  "@entity": "Compound",
  "@query": {
    "@criteria": {
      "$$Compound ID": [
        "REG0000001"
      ]
    }
  }
}
```

This permission allows View Compounds to see 4 Compounds.

- Select the “Batch” Entity
- Click the “Set/Edit Group Permission” button and type an advanced search criteria:



Advanced Security

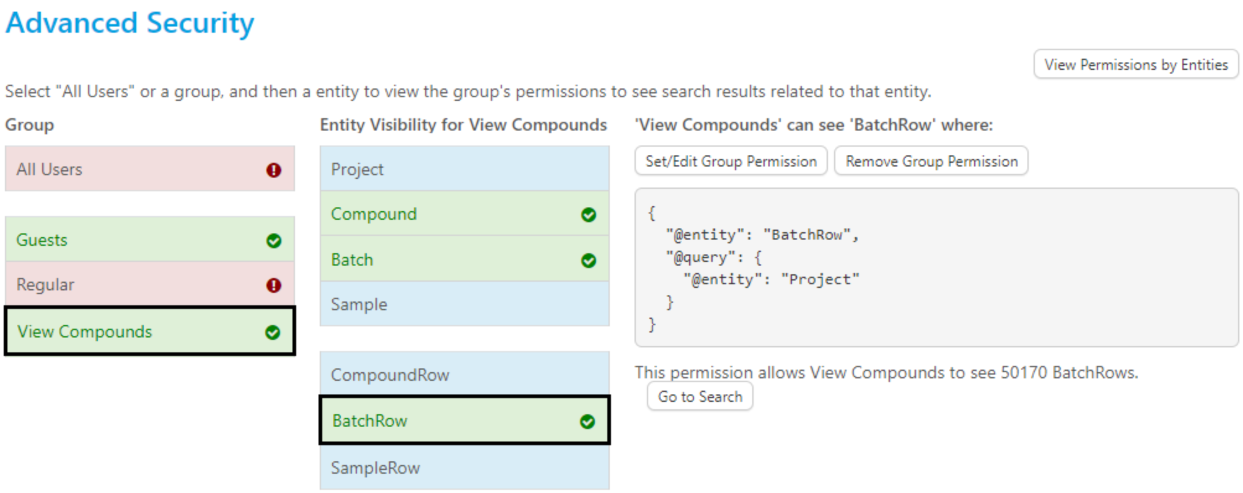
Select "All Users" or a group, and then a entity to view the group's permissions to see search results related to that entity.

'View Compounds' can see 'Batch' where:

```
{
  "@entity": "Batch",
  "@query": {
    "@entity": "Project"
  }
}
```

This permission allows View Compounds to see 79115 Batches.

- Select the “BatchRow” Entity
- Click the “Set/Edit Group Permission” button and type an advanced search criteria:



Select "All Users" or a group, and then a entity to view the group's permissions to see search results related to that entity.

```
{
  "@entity": "BatchRow",
  "@query": {
    "@entity": "Project"
  }
}
```

This permission allows View Compounds to see 50170 BatchRows.

- Once this setting has been applied, only users within the “View Compounds” group will be able to see compounds, and they will only be able to see the compound “REG0000001”.
    - Those users will also be restricted to only seeing child Batches and Measurements related to this compound.
- This can be repeated, creating a group that can see the compounds with other Compound IDs.

The above configures for Batch and BatchRow are to allow the group users see all Batch and BatchRow data with the union of the above specified Compounds when you perform searching by Global Search in Spotfire.

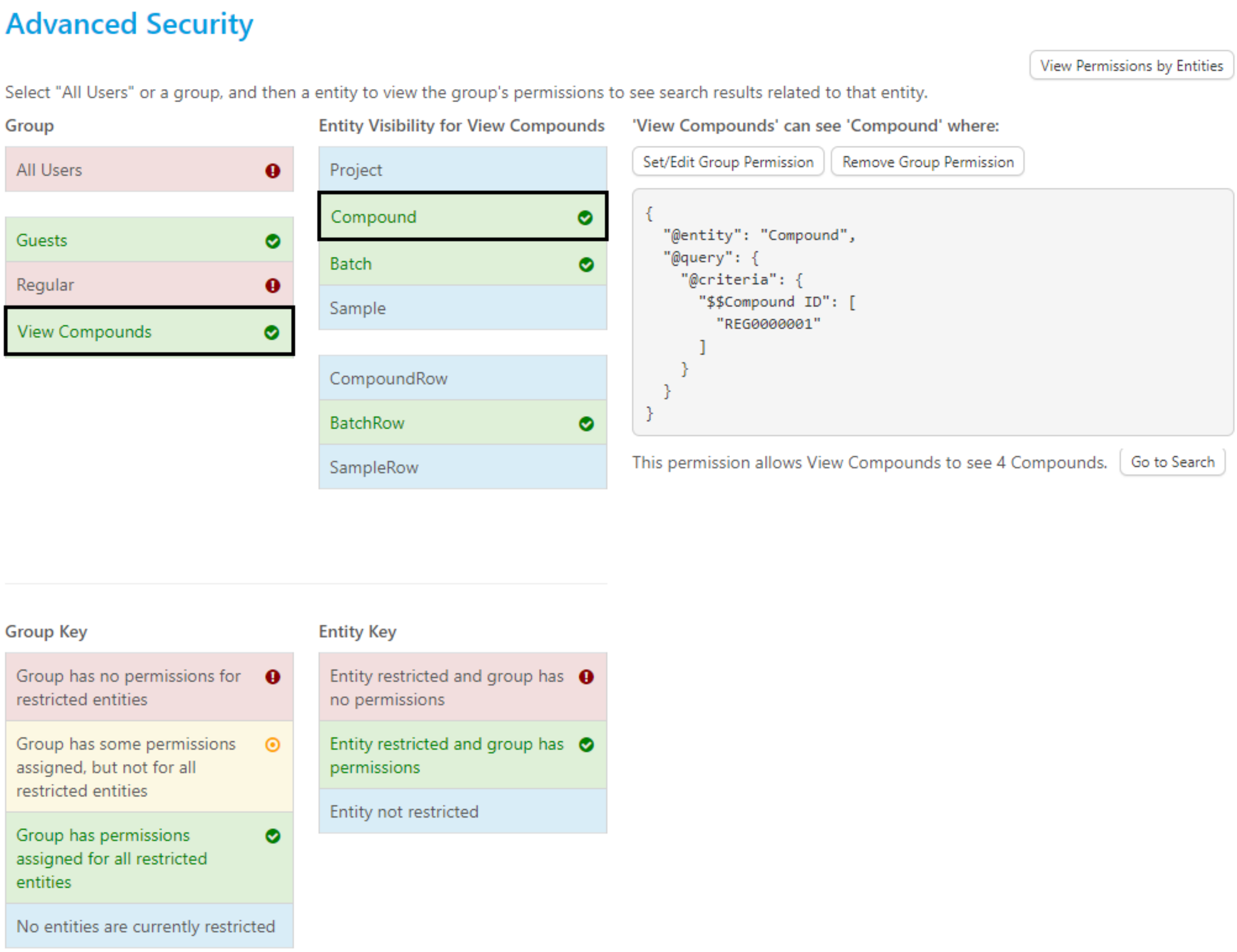
Notice that ‘All Users’ has a warning showing – this is indicating that there is an entity (Compound, Batch or BatchRow in this case) that has restrictions and which there is no default permission for all users – meaning that users must be a member of a group in order to see any Compounds, Batches or BatchRows. This is just a warning - this may be the desired configuration and is a perfectly valid setup.

On the Advanced Security page there are two view modes – View Permissions by Groups, and View Permissions by Entities. Switch between these views using the button at the top-right of the screen.

View by Groups:

In this view the groups are listed first, with indicators to whether that group has permissions assigned the currently restricted entities.

Selecting a group will display the permissions for each entity for that group, and from there it is possible to set/clear permissions.



Advanced Security

Select "All Users" or a group, and then a entity to view the group's permissions to see search results related to that entity.

Group	Entity Visibility for View Compounds
All Users !	Project
Guests ✓	Compound ✓
Regular !	Batch ✓
View Compounds ✓	Sample
	CompoundRow
	BatchRow ✓
	SampleRow

'View Compounds' can see 'Compound' where:

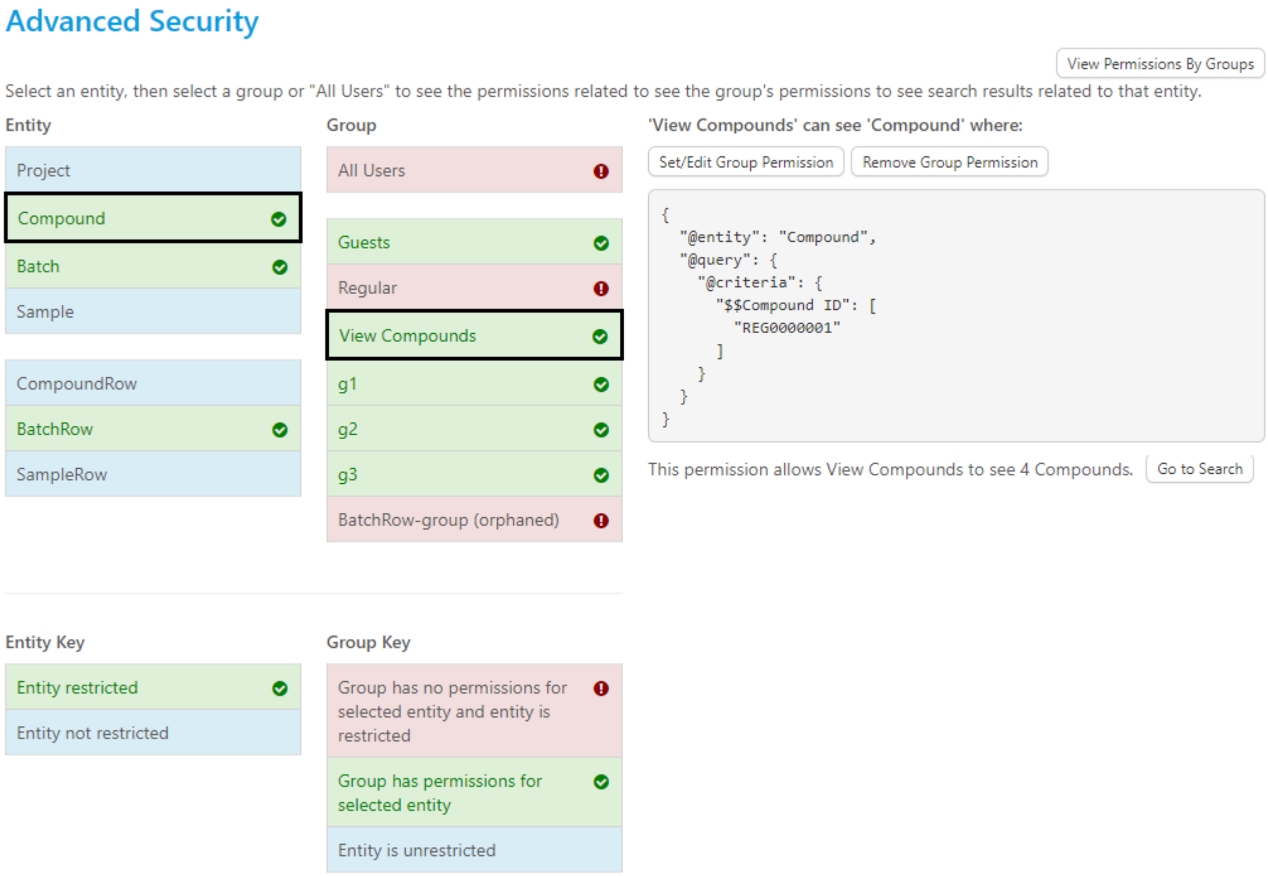
```
{
  "@entity": "Compound",
  "@query": {
    "@criteria": {
      "$$Compound ID": [
        "REG0000001"
      ]
    }
  }
}
```

This permission allows View Compounds to see 4 Compounds.

Group Key	Entity Key
Group has no permissions for restricted entities !	Entity restricted and group has no permissions !
Group has some permissions assigned, but not for all restricted entities ◉	Entity restricted and group has permissions ✓
Group has permissions assigned for all restricted entities ✓	Entity not restricted
No entities are currently restricted	

View by Entities

An alternative view is by Entity– selecting an entity will then update each group listed in the second column to indicate permissions granted to that group for the selected entity.



Advanced Security

Select an entity, then select a group or "All Users" to see the permissions related to see the group's permissions to see search results related to that entity.

'View Compounds' can see 'Compound' where:

```
{
  "@entity": "Compound",
  "@query": {
    "@criteria": {
      "$$Compound ID": [
        "REG0000001"
      ]
    }
  }
}
```

This permission allows View Compounds to see 4 Compounds.

Note: Currently, this security is not applied when accessing project data from the project details pages, or when staging exports using the export mechanism – therefore these features are restricted and/or disabled when this security feature is enabled.

Examples of Advanced Security:

Restriction examples for a group ‘ExampleGroup’

#	Description	Project Setting		MType Setting		Advanced Security			
		Groups with Write Access	Groups with Read Access	View /Search	Download	Project	Compound	Batch	BatchRow

1	ExampleGroup can access all data in the project	ExampleGroup	<default>	<default>	<default>	<default>	{
							"@entity": "Compound",
							"@query": {
							"@entity": "Project"
							}
							}
								{
								"@entity": "Batch",
								"@query": {
								"@entity": "Project"
								}
								}
									{
									"@entity": "BatchRow",
									"@query": {
									"@entity": "Project"
									}
									}

2	ExampleGroup can only access the data of the compound 'REG00046426"	ExampleGroup	<default>	<default>	<default>	<default>	{
							"@entity": "Compound",
							"@query": {
							"@criteria": {
							"$$Compound ID": [
							"REG00046426"
							]
							}
							}
							}
								{
								"@entity": "Batch",
								"@query": {
								"@entity": "Project"
								}
								}
									{
									"@entity": "BatchRow",
									"@query": {
									"@entity": "Project"
									}
									}

3	ExampleGroup can only access the data of the compounds whose 'Batch Project ID' is '234"	ExampleGroup	<default>	<default>	<default>	<default>	{
							"@entity": "Compound",
							"@query": {
							"@entity": "Project"
							}
							}
								{
								"@entity": "Batch",
								"@query": {
								"@criteria": {
								"Batch Project ID": [
								"234"
								]
								}
								}
								}
									{
									"@entity": "BatchRow",
									"@query": {
									"@entity": "Project"
									}
									}

4	ExampleGroup can only access the data that the 'Temperature' in the mtype 'SLDIntegrationTestMeasurementType' is greater or equals to 30 (only the rows in SLDIntegrationTestMeasurementType' is restricted, and all rows in Compounds, Batch and AER will be returned with no restriction).	ExampleGroup	<default>	<default>	<default>	<default>
5	ExampleGroup can only access the data of compounds whose 'Temperature' in 'SLDIntegrationTestMeasurementType' mtype equals to '21'.	ExampleGroup	<default>	<default>	<default>	<default>

4

```
{
  "@entity": "Compound",
  "@query": {
    "@entity": "Project"
  }
}
```

```
{
"@entity": "Batch",
"@query": {
"@entity": "Project"
}
}
```

```
{
  "@entity": "BatchRow",
  "@query": {
    "@or": [
      {
        "@criteria": {
          "$$Type ID": [
            "Assay Endpoint Results"
          ]
        }
      },
      {
        "@criteria": {
          "$$Type ID": [
            "SLDIntegrationTestMeasurementType"
          ],
          "Temperature": [
            {
              "@range": {
                "gte": 30
              }
            }
          ]
        }
      }
    ]
  }
}
```

5

```
{
  "@entity": "Compound",
  "@query": {
    "@entity": "Compound",
    "@query": {
      "@entity": "BatchRow",
      "@query": {
        "@and": [
          {
            "@criteria": {
              "$$Type ID": "SLDIntegrationTestMeasurementType"
            }
          },
          {
            "@criteria": {
              "Temperature": {
                "@in": [
                  "21"
                ]
              }
            }
          }
        ]
      }
    }
  }
}
```

```
{
  "@entity": "Batch",
  "@query": {
    "@entity": "Project"
  }
}
```

```
{
  "@entity": "BatchRow",
  "@query": {
    "@or": [
      {
        "@criteria": {
          "$$Type ID": [
            "Assay Endpoint Results"
          ]
        }
      },
      {
        "@criteria": {
          "$$Type ID": [
            "SLDIntegrationTestMeasurementType"
          ],
          "Temperature": [
            {
              "@range": {
                "gte": 30
              }
            }
          ]
        }
      }
    ]
  }
}
```

6	ExampleGroup can only access the data of the compound 'REG00046426" whose 'Batch Project ID' is '234"	ExampleGroup	<default>	<default>	<default>	<default>	{
							"@entity": "Compound",
							"@query": {
							"@criteria": {
							"$$Compound ID": [
							"REG00046426"
							]
							}
							}
							}
								{
								"@entity": "Batch",
								"@query": {
								"@criteria": {
								"Batch Project ID": [
								"234"
								]
								}
								}
								}
									{
									"@entity": "BatchRow",
									"@query": {
									"@entity": "Project"
									}
									}

7	ExampleGroup can only access the data of the compound 'REG00046426' whose 'Temperature' in the mtype 'SLDIntegraionTestMeasurementType' is greater or equals to 30.	ExampleGroup	<default>	<default>	<default>	<default>	{
							"@entity": "Compound",
							"@query": {
							"@criteria": {
							"$$Compound ID": [
							"REG00046426"
							]
							}
							}
							}
								{
								"@entity": "Batch",
								"@query": {
								"@entity": "Project"
								}
								}
									{
									"@entity": "BatchRow",
									"@query": {
									"@or": [
									{
									"@criteria": {
									"$$Type ID": [
									"Assay Endpoint Results"
									]
									}
									},
									{
									"@criteria": {
									"$$Type ID": [
									"SLDIntegrationTestMeasurementType"
									],
									"Temperature": [
									{
									"@range": {
									"gte": 30
									}
									}
									]
									}
									}
									]
									}
									}

8	ExampleGroup can only access the data of the compounds whose 'Batch Project ID' is '234" and 'Temperature' in the mtype 'SLDIntegraionTestMeasurementType' is greater or equals to 30.	ExampleGroup	<default>	<default>	<default>	<default>

```
{
  "@entity":
"Compound",
  "@query": {
    "@entity": "Project"
  }
}
```

```
{
"@entity": "Batch",
"@query": {
"@criteria": {
"Batch Project ID": [
"234"
]
}
}
}
```

```
{
  "@entity":
"BatchRow",
  "@query": {
    "@or": [
      {
        "@criteria": {
          "$$Type ID": [
            "Assay
Endpoint Results"
          ]
        }
      },
      {
        "@criteria": {
          "$$Type ID": [

"SLDIntegrationTestMe
asurementType"
          ],
          "Temperature": [
            {
              "@range": {
                "gte": 30
              }
            }
          ]
        }
      }
    ]
  }
}
```

9	ExampleGroup can only access the data of the compound 'REG00046426' whose 'Batch Project ID' is '234" and 'Temperature' in the mtype 'SLDIntegraionTestMeasurementType' is greater or equals to 30.	ExampleGroup	<default>	<default>	<default>	<default>

```
{
"@entity":
"Compound",
"@query": {
"@criteria": {
"$$Compound ID": [
"REG00046426"
]
}
}
}
```

```
{
"@entity": "Batch",
"@query": {
"@criteria": {
"Batch Project ID": [
"234"
]
}
}
}
```

```
{
  "@entity":
"BatchRow",
  "@query": {
    "@or": [
      {
        "@criteria": {
          "$$Type ID": [
            "Assay
Endpoint Results"
          ]
        }
      },
      {
        "@criteria": {
          "$$Type ID": [

"SLDIntegrationTestMe
asurementType"
          ],
          "Temperature": [
            {
              "@range": {
                "gte": 30
              }
            }
          ]
        }
      }
    ]
  }
}
```

10	ExampleGroup can only access the data that any fields match '54.1523031' OR '3.532165686'	ExampleGroup	<default>	<default>	<default>	<default>	{
							"@entity": "Compound",
							"@query": {
							"@entity": "Project"
							}
							}
								{
								"@entity": "Batch",
								"@query": {
								"@entity": "Project"
								}
								}
									{
									"@entity": "BatchRow",
									"@query": {
									"@queryString": {
									"query": "54.1523031 OR 3.532165686"
									}
									}
									}

11	ExampleGroup can only access the compounds with the 'exact' structure query criteria	ExampleGroup	<default>	<default>	<default>	<default>	{
							"@entity": "Compound",
							"@query": {
							"@criteria": {
							"Chemical Structure": {
							"@chemSearch": {
							"chemicalStructure": "CN1N(C2=CC=CC=C2)C(C(NC(C(N(C)C)C)=O)=C1C)=O",
							"chemicalStructureType": "chemical/smiles",
							"searchType": "exact"
							}
							}
							}
							}
							}
								{
								"@entity": "Batch",
								"@query": {
								"@entity": "Project"
								}
								}
									{
									"@entity": "BatchRow",
									"@query": {
									"@entity": "Project"
									}
									}

12	ExampleGroup can only access the compounds with the 'substructure' structure query criteria	ExampleGroup	<default>	<default>	<default>	<default>	{
							"@entity": "Compound",
							"@query": {
							"@criteria": {
							"Chemical Structure": {
							"@chemSearch": {
							"chemicalStructure": "[N]C1=CC=CC=C1",
							"chemicalStructureType": "chemical/smiles",
							"searchType": "substructure",
							"tautomericSearch": true,
							"tetrahedralstereo": "either",
							"doublebondstereo": true,
							"hitanychargehetero": true,
							"hitanychargecarbon": true
							}
							}
							}
							}
							}
								{
								"@entity": "Batch",
								"@query": {
								"@entity": "Project"
								}
								}
									{
									"@entity": "BatchRow",
									"@query": {
									"@entity": "Project"
									}
									}

13	ExampleGroup can only access the compounds with the 'full' structure query criteria	ExampleGroup	<default>	<default>	<default>	<default>	{
							"@entity": "Compound",
							"@query": {
							"@criteria": {
							"Chemical Structure": {
							"@chemSearch": {
							"chemicalStructure": "CN1N(C2=CC=CC=C2)C(C(NC(C(N(C)C)C)=O)=C1C)=O",
							"chemicalStructureType": "chemical/smiles",
							"searchType": "full",
							"tautomericSearch": true
							}
							}
							}
							}
							}
								{
								"@entity": "Batch",
								"@query": {
								"@entity": "Project"
								}
								}
									{
									"@entity": "BatchRow",
									"@query": {
									"@entity": "Project"
									}
									}

14	ExampleGroup can only access the compounds with the 'similar' structure query criteria	ExampleGroup	<default>	<default>	<default>	<default>	{
							"@entity": "Compound",
							"@query": {
							"@criteria": {
							"Chemical Structure": {
							"@chemSearch": {
							"chemicalStructure": "CN1N(C2=CC=CC=C2)C(C(NC(C(N(C)C)C)=O)=C1C)=O",
							"chemicalStructureType": "chemical/smiles",
							"searchType": "similar",
							"substructureSearch": false,
							"similarityThreshold": 90
							}
							}
							}
							}
							}
								{
								"@entity": "Batch",
								"@query": {
								"@entity": "Project"
								}
								}
									{
									"@entity": "BatchRow",
									"@query": {
									"@entity": "Project"
									}
									}

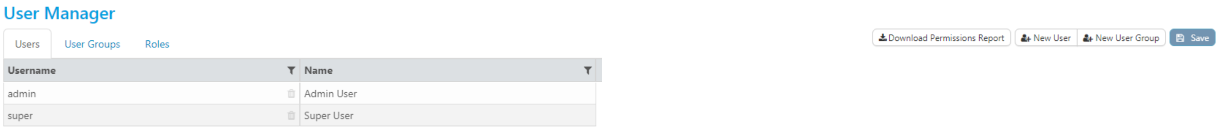
4.6.2 Manage Users

Administrators can create new Users and Groups and assign roles to each.

To manage users:

1. Log in to Signals Data Factory as an Administrative User.
2. Navigate to **Administration > User Manager**.

The User Manager screen appears. The Users tab is displayed by defaults displaying a list of existing users.

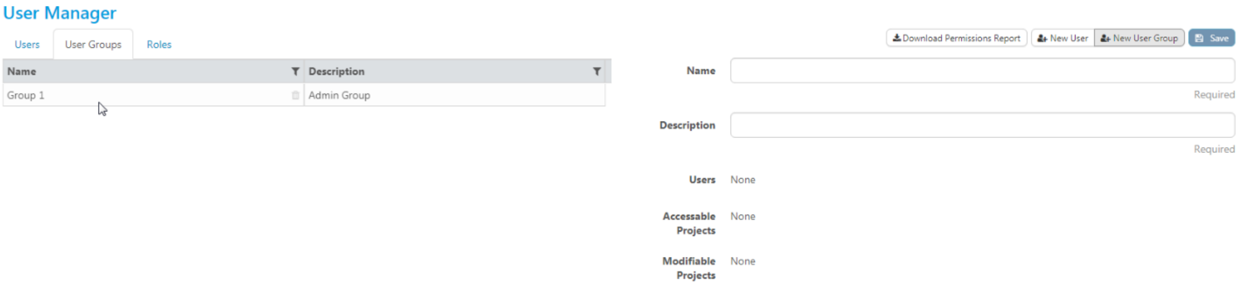


Username	Name
admin	Admin User
super	Super User

Note: Click the **Download Permissions Report** button to download a permissions report allowing you to verify access rights of all users and groups for the application.

To create a new user group:

1. From the User Groups tab, click **New User Group**.



Name	Description
Group 1	Admin Group

Name

Description

Users None

Accessable Projects None

Modifiable Projects None

2. Enter a Name and Description for the new group.
3. Click **Save**.

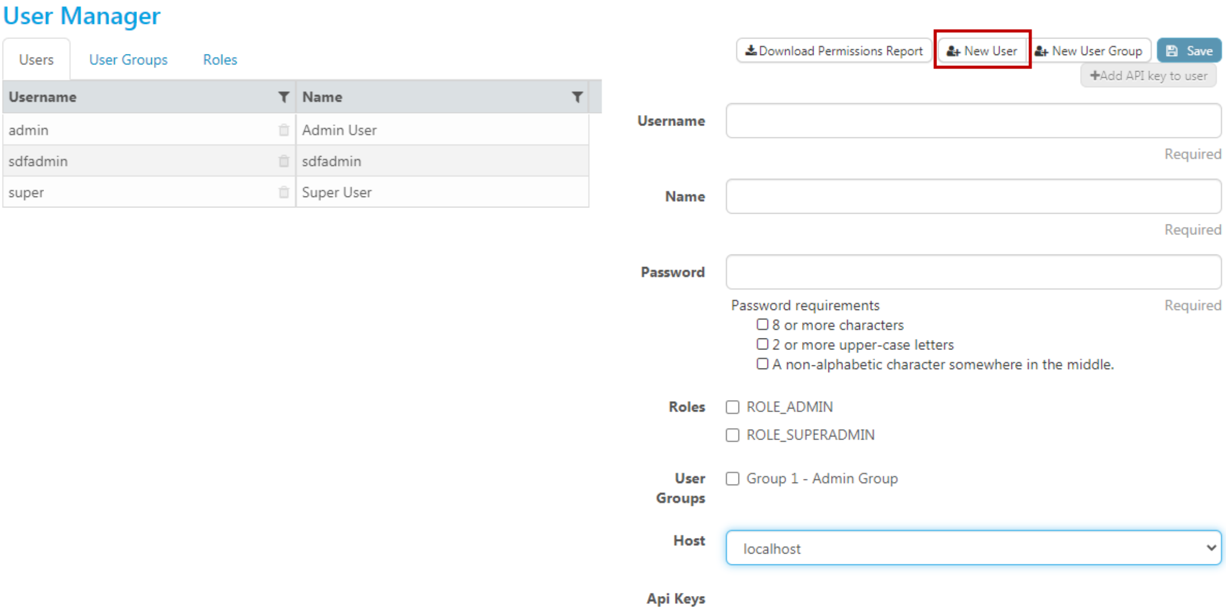
Note: The Administrative User must sign out of Signals Data Factory for changes to user roles or groups to take effect.

To delete a group:

1. Hover the mouse over the user to delete. An 🗑 icon appears in the Name column for that row.
2. Click the 🗑 icon. The user is deleted.

To create a new user:

1. Click **New User**.



Username	Name
admin	Admin User
sdfadmin	sdfadmin
super	Super User

Username

Name

Password

Password requirements
☐ 8 or more characters
☐ 2 or more upper-case letters
☐ A non-alphabetic character somewhere in the middle.

Roles ☐ ROLE_ADMIN
☐ ROLE_SUPERADMIN

User Groups ☐ Group 1 - Admin Group

Host localhost

Api Keys

2. Enter user details as required.
3. Assign user to Roles and User Groups (if applicable).
4. From the Host drop down list, select a host URL to associate with the user.
5. Click **Save**.

Note: It is not possible to create new roles, as the Roles tab displays only the System defined roles such as ROLE_ADMIN, ROLE_USER, AND ROLE_SUPERADMIN.

Note: The Administrative User must sign out of Signals Data Factory for changes to user roles or groups to take effect.

To delete a user:

1. Hover the mouse over the user to delete. An 🗑 icon appears in the Username column for that row.
2. Click the 🗑 icon. The user is deleted.

14.6.2.1 API Keys

Signals Data Factory supports the use of API keys for third party integrations.

To create an API key for a given user, select the user and click the **Add API Key to User** button.

Active API keys will be listed beneath the User Groups list and can be de-activated by deleting them using the trash icon.

14.6.3 Managing Jobs

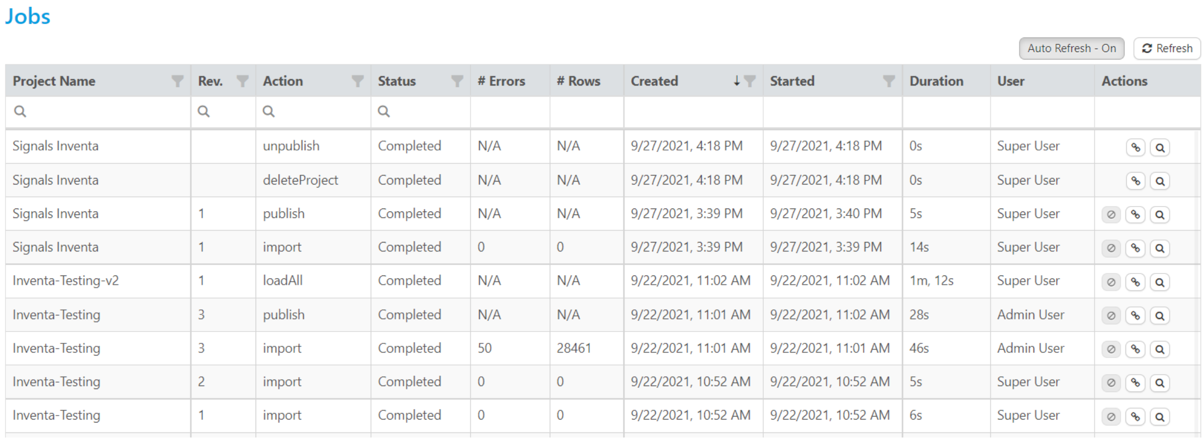
Here you can verify all jobs running on the system and manage them as required. You can also navigate directly to the respective project page for a job. You can also view the Job Execution Log for each job.

You can toggle the Jobs page to Auto-Refresh.

To view the job details:

1. Navigate to **Administration > Jobs**.

From the Jobs page, you can view/analyse the last five days of project data.



Project Name	Rev.	Action	Status	# Errors	# Rows	Created	Started	Duration	User	Actions
Signals Inventa		unpublish	Completed	N/A	N/A	9/27/2021, 4:18 PM	9/27/2021, 4:18 PM	0s	Super User	
Signals Inventa		deleteProject	Completed	N/A	N/A	9/27/2021, 4:18 PM	9/27/2021, 4:18 PM	0s	Super User	
Signals Inventa	1	publish	Completed	N/A	N/A	9/27/2021, 3:39 PM	9/27/2021, 3:40 PM	5s	Super User	
Signals Inventa	1	import	Completed	0	0	9/27/2021, 3:39 PM	9/27/2021, 3:39 PM	14s	Super User	
Inventa-Testing-v2	1	loadAll	Completed	N/A	N/A	9/22/2021, 11:02 AM	9/22/2021, 11:02 AM	1m, 12s	Super User	
Inventa-Testing	3	publish	Completed	N/A	N/A	9/22/2021, 11:01 AM	9/22/2021, 11:02 AM	28s	Admin User	
Inventa-Testing	3	import	Completed	50	28461	9/22/2021, 11:01 AM	9/22/2021, 11:01 AM	46s	Admin User	
Inventa-Testing	2	import	Completed	0	0	9/22/2021, 10:52 AM	9/22/2021, 10:52 AM	5s	Super User	
Inventa-Testing	1	import	Completed	0	0	9/22/2021, 10:52 AM	9/22/2021, 10:52 AM	6s	Super User	

2. Select a job and click **Go to Project** or **Go to Job Details** to view additional details for the project/job.

14.6.4 Audit Log

Here you can view the history of actions in Signals Data Factory including Projects, Information Design settings, User Management, and export/download operations.

You can also view the history of a selected project or measurement type (and associated attributes).

You have the option to Download the current view.

To open the audit log:

1. Navigate to **Administration > Audit Log**.
2. Click on any audit log for additional information.

	Date	User	Actions
✓	2/28/2020, 10:59 AM	super	user.users.update
✓	2/28/2020, 10:58 AM	super	user.groups.create
✓	2/28/2020, 10:56 AM	super	user.users.create
✓	2/28/2020, 10:27 AM	super	user.users.login
✓	2/27/2020, 3:47 PM	super	user.users.login
✓	2/27/2020, 3:15 PM	super	information.ontologies.create
✓	2/27/2020, 3:05 PM	super	user.users.login
✓	2/27/2020, 11:41 AM	super	information.attributes.delete
✓	2/27/2020, 11:41 AM	super	user.users.login
✓	2/27/2020, 11:04 AM	super	user.users.login
✓	2/27/2020, 10:37 AM	super	user.users.login
✓	2/26/2020, 9:21 PM	super	user.users.login

'user.groups.create' by super

02/28/2020, 10:58 AM

```
{
  "groups": [
    {
      "groupName": "Group 1",
      "groupDescription": "Admin Group"
    }
  ]
}
```

There are 3 elements to an audit log entry: target, result, and parameters:

- Target - details of the object, if it is being updated (in the state before the update). It will also include details of any other related objects that are affected by the change. For example, updating an attribute will also list all measurement types that include the attribute at the time of the update.
- Result: details of an updated item; or of a new item, if the action is 'create'.
- Parameters: details of all parameters provided in the API call that invoked the operation.

3. Filter the audit logs based on Projects or Measurement Types using the dropdown list box and entering the project or measurement type, by selecting them as follows and then enter the name of the project or measurement type.

Note: There are links to filter the audit log directly from the Project Detail or Measurement Type pages.

4. Click the **Download Current View** button to download the current audit log page details to your system.

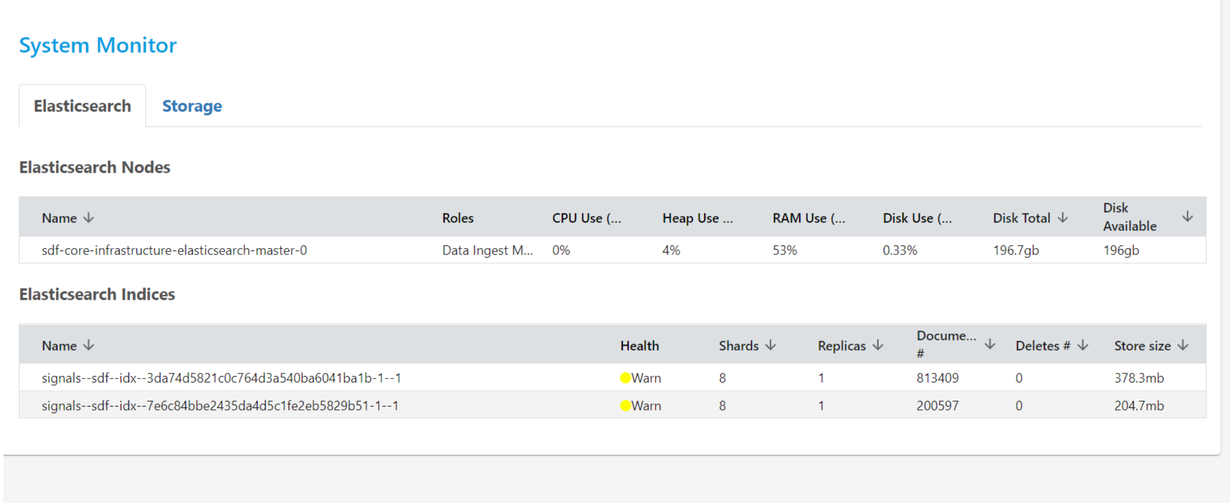
14.6.5 System Monitor

The System Monitor page allows you to monitor the status of the Elastic Search cluster and the general storage.

To open the System Monitor page:

1. Navigate to **Administration > System Monitor.**

Elastic Search



Elasticsearch Nodes

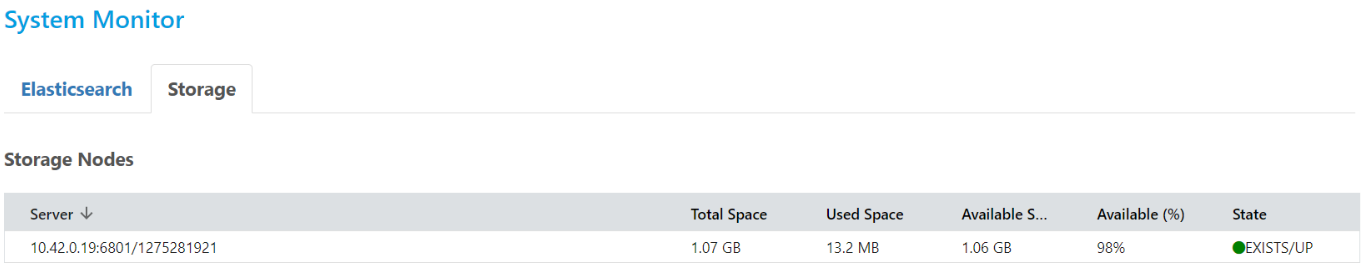
Name ↓	Roles	CPU Use (...	Heap Use ...	RAM Use (...	Disk Use (...	Disk Total ↓	Disk Available ↓
sdf-core-infrastructure-elasticsearch-master-0	Data Ingest M...	0%	4%	53%	0.33%	196.7gb	196gb

Elasticsearch Indices

Name ↓	Health	Shards ↓	Replicas ↓	Docume... # ↓	Deletes # ↓	Store size ↓
signals--sdf--idx--3da74d5821c0c764d3a540ba6041ba1b-1--1	● Warn	8	1	813409	0	378.3mb
signals--sdf--idx--7e6c84bbe2435da4d5c1fe2eb5829b51-1--1	● Warn	8	1	200597	0	204.7mb

Storage

This page allows you to ensure that you are not going to run out of disk space. This is the SETH general data storage and is indepent of the Elasticsearch storage.



Storage Nodes

Server ↓	Total Space	Used Space	Available S...	Available (%)	State
10.42.0.19:6801/1275281921	1.07 GB	13.2 MB	1.06 GB	98%	● EXISTS/UP

14.6.6 External Connections

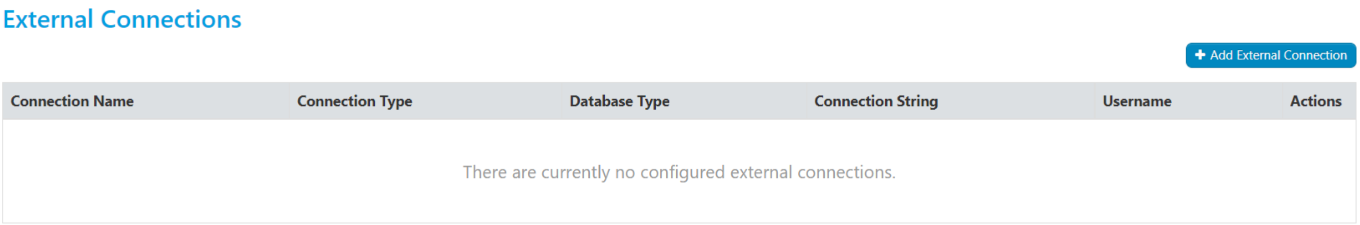
Signals Data Factory supports connections to external data sources – currently SQL data source is supported, which can be used to connect to other databases.

To load data from an external connection, an administrator must first configure the external connection.

Note: The configured external connections can be used with the Import from SQL feature on the Projects page.

To configure external connection:

1. Navigate to **Administration > External Connections.** The **Add External Connection** page is displayed.

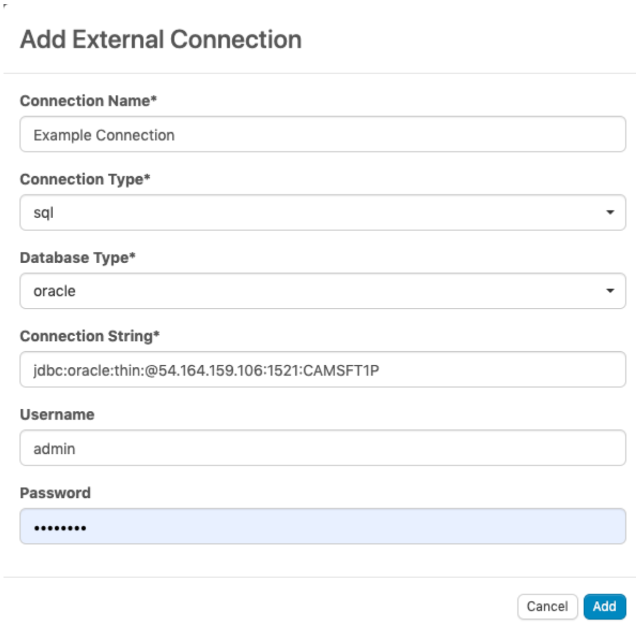


Connection Name	Connection Type	Database Type	Connection String	Username	Actions
There are currently no configured external connections.					

2. Click **Add External Connection** button.

When adding a connection, the following information is required:

- the **connection type** (currently only SQL is available)
- the **database type**
    - Oracle
    - MySQL
    - MSSQL
    - Redshift (also supports Redshift Spectrum)
    - Impala
    - Postgres
    - Snowflake
- the connection string
- username and password credentials



Connection Name*: Example Connection
Connection Type*: sql
Database Type*: oracle
Connection String*: jdbc:oracle:thin:@54.164.159.106:1521:CAMSFT1P
Username: admin
Password: ••••••••

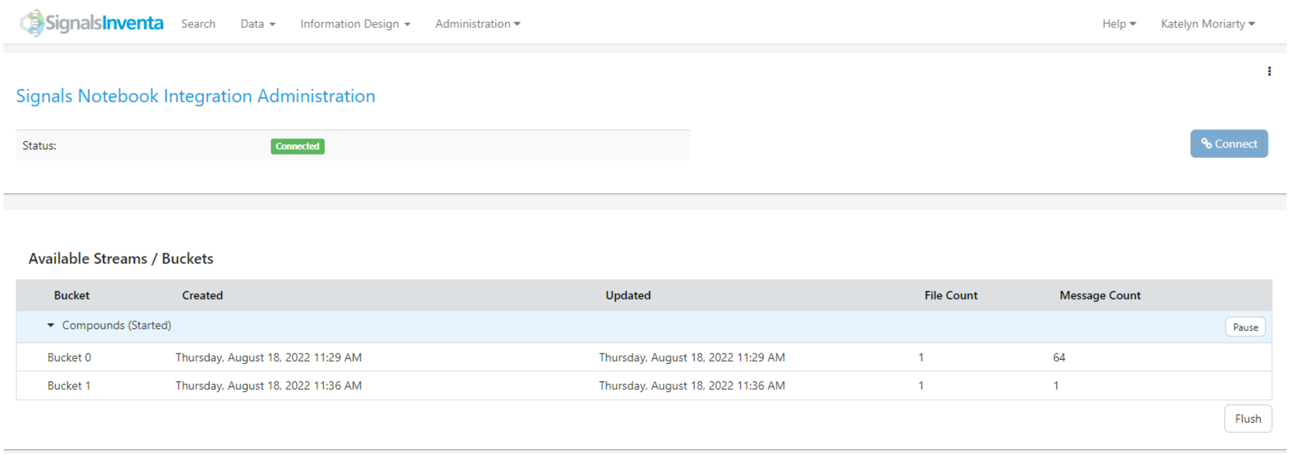
Once configured, project administrators will be able to import using this connection on the project details page.

14.6.7 Signals Notebook Connection

Compounds in Revvity Signals Notebook can be published to Signals Data Factory via the material synchronization feature so that these assets are then available in Signals Inventa's Global Search.

Once enabled in Signals Notebook, a **Streams** tab is added to each project in Signals Data Factory allowing the user to manage the subscription to the stream at the project level.

From Signals Data Factory, select **Administration > Signals Notebook Connection** from the top toolbar.



Signals Notebook Integration Administration

Status: Connected

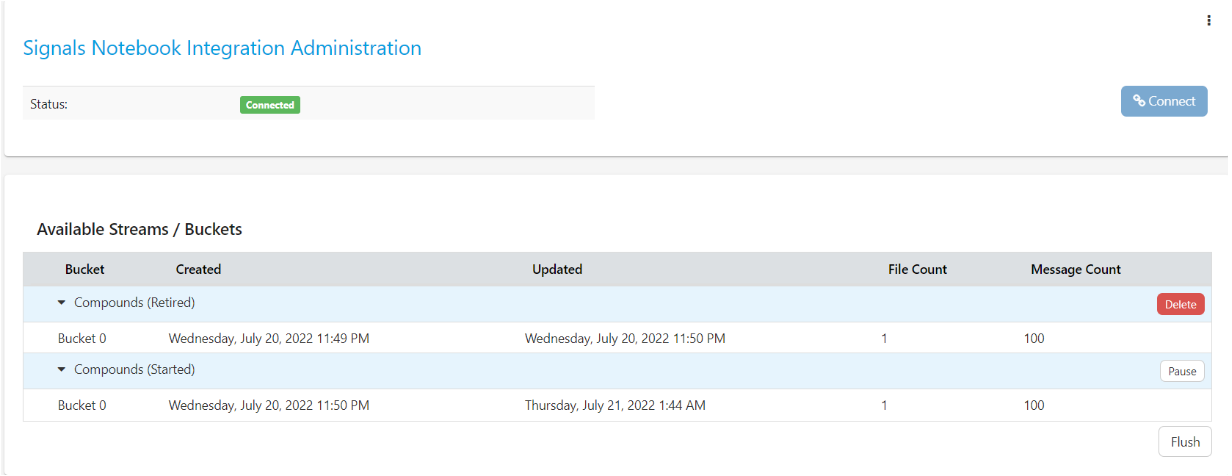
Available Streams / Buckets

Bucket	Created	Updated	File Count	Message Count
Compounds (Started)				
Bucket 0	Thursday, August 18, 2022 11:29 AM	Thursday, August 18, 2022 11:29 AM	1	64
Bucket 1	Thursday, August 18, 2022 11:36 AM	Thursday, August 18, 2022 11:36 AM	1	1

The available streams (buckets) from Signals Notebook are listed. The following controls are also available:

- **Pause**: stops the monitoring of the system by temporarily disrupting the stream
- **Resume:** restarts a paused stream
- **Delete:** removes all buckets in the stream (can only be applied when the stream is retired and there are no subscribed projects)
- **Flush**: forces a refresh and sync

Refer to Appendix E: Signals Notebook Integration for more information.



Signals Notebook Integration Administration

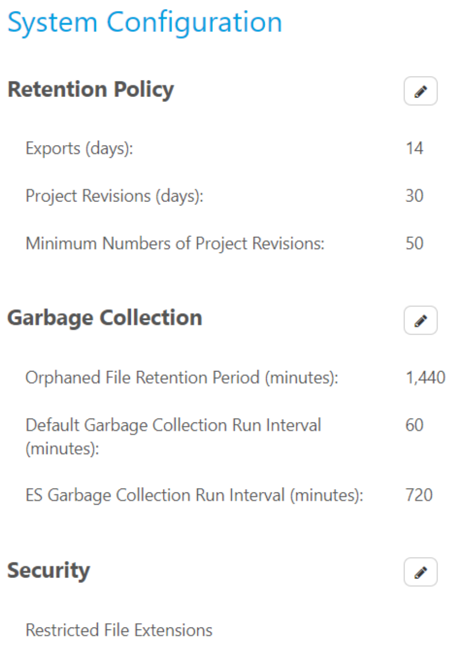
Status: Connected

Available Streams / Buckets

Bucket	Created	Updated	File Count	Message Count
Compounds (Retired)				
Bucket 0	Wednesday, July 20, 2022 11:49 PM	Wednesday, July 20, 2022 11:50 PM	1	100
Compounds (Started)				
Bucket 0	Wednesday, July 20, 2022 11:50 PM	Thursday, July 21, 2022 1:44 AM	1	100

14.6.8 System Configuration

The System Configuration page displays current system settings for Retention Policy and Garbage Collection with the ability to modify the settings. Changes will take effect immediately and it is not necessary to restart your system in order for changes to take effect.



System Configuration

Retention Policy

Exports (days):	14
Project Revisions (days):	30
Minimum Numbers of Project Revisions:	50

Garbage Collection

Orphaned File Retention Period (minutes):	1,440
Default Garbage Collection Run Interval (minutes):	60
ES Garbage Collection Run Interval (minutes):	720

Security

Restricted File Extensions

A user with the ROLE_ADMIN role will be able to the menu to access this page and will be able to update the settings. Any other user will not see the menu to access the page.

Retention Policy

The retention policy determines the number of days exports and project revisions are stored in the system before they are deleted.

Export (days):
- The period to time in days that an export is retained in the storage system

Project Revisions
- The period to time in days that a project revision is retained in the storage system

Minimum Number of Project Revisions:
- The minimum number of project revisions to retain before deleting revisions from the system

In the example above, a project revision will be deleted provided it is over 30 days, and there are at least 50 subsequent revisions in the system.

Garbage Collection

At a designated interval the trawler will go through the system storage and check all files. If a file is orphaned a tag is added which sets a target deletion date. This date is set according to the retention policy. If a file is orphaned and the date has passed it will be deleted.

A file is considered **not**-orphaned if
- it is referenced by any dataset in an active (i.e. not deleted) revision
- it is the output of an import job for a revision
- it is referenced by an ontology
- it is part of an export

Orphaned File Retention Period (minutes):
- The period after being identified as an orphan that the file is retained in the system storage

Default Garbage Collection Run Interval (minutes):
- The interval at which the garbage collection process is run

ES Garbage Collection Run Interval (minutes):
- The interval at which garbage collection is run for the search index

Security

Restricted File Extensions
- Comma separated list of file extensions restricted from being uploaded. Wildcards are not permitted.

14.7 Signals Data Factory Restricted Characters

Measurement Type Name	Attribute Name
|| double pipe	**||** double pipe
` back tick	**`** back tick
**** back slash	**** back slash
# number sign	**#** number sign
: colon	**.** period
/ forward slash	**\r\n** new line
~ tilde	**“** double quote
& ampersand	**^** caret
+ plus	**$$** double dollar sign (at the beginning)
***** star	
? question mark	
[opensquare bracket	
] closesquare bracket	
{ open brace	
} close brace	
_ underscore	

15 Appendix C: Transformation Steps and Templates for Custom Aggregates

A custom aggregation consists of one or multiple transformation steps, each of which is described as a JSON object (a JSON snippet that is included in a pair of braces). A custom aggregation is actually defined by a JSON object array that contains multiple JSON objects.

For example, the following JSON document describes a custom aggregation that has two transformation steps:

```
[
  {
    "Expression": "(Avg([Result Number]) OVER ([Result Name],[%IdentityColumn%])) & ' ' & (First([Endpoint
Unit]) OVER ([Result Name],[%IdentityColumn%])) & ' +/- ' & (StdDev([Result Number]) OVER ([Result
Name],[%IdentityColumn%])) & ' (' & (Count() OVER ([Result Name],[%IdentityColumn%])) & ')'",
    "ResultColumnName": "Temp Result",
    "Actions": null,
    "name": "siaAddCalculatedColumnTransformation_New",
    "typeId": "signals.transformations.addCalculatedColumn"
  },
  {
    "CategoryColumns": [
      …
    ],
    "Actions": null,
    "name": "siaPivotTransformation_New",
    "typeId": "signals.transformations.pivot"
  }
]
```

In the above example, the first step is to add a calculated column, the calculation expression is defined in the “Expression” element, and the resulting column will be named as “Temp Result”. In the second step, it does a pivot operation and the generated columns are then added to the SAR table.

Signals Inventa provides two kinds of JSON objects that users can use for building their custom aggregations: Transformation Steps and Templates. Transformation Steps are the steps that are already implemented in Spotfire. Providing Transformation Steps in Signals Inventa allows the users to describe the custom aggregations in a text-based JSON format. Templates are custom aggregations made up of several Transformation Steps, they are provided out-of-the-box: Users can create one custom aggregation by using a template and then make slight changes to meet their needs. Users can also define the custom aggregations by using the Transformation Steps from scratch so as to address more complex data process scenarios.

For each of the transformation step, its JSON object could have the following elements:

- **name**: The name of the current step, users can modify the name when necessary
- **typeId**: The transformation step type identifier. Do not change the value of this property, it is used by the custom aggregation execution engine
- **Actions**: A list of actions to be executed before or after a column is going to be/has been processed. Actions are described in its own section below

Transformation Steps

Signals Inventa offers the following Transformation Steps. Most of these steps have the same name and function as the data transformations offered in Spotfire:

- Exclude columns
- Replace value
- Replace specific value
- Unpivot
- Change data types
- Change column names
- Calculate new column
- Filter rows
- Pivot
- Calculate and replace column

The following table lists the parameters (JSON elements) for each transformation step.

Transformation Step	Parameter	Description	Example
Exclude columns	ColumnsToExclude	An array of JSON elements that describes the name and data type of the columns to exclude	

```
{
  "ColumnsToExclude": [
   {
      "Name": "Salt Name",
      "DataType": "String"
   },
   {
      "Name": "Salt MW",
      "DataType": "Real"
   },
   {
      "Name": "Assay Date",
      "DataType": "DateTime"
   },
   {
      "Name": "QATest-Image-1",
      "DataType": "Binary"
   }
```

```
  ],

  "Actions": null,

  "name":
"siaExcludeColumnsTransformation_New",

  "typeId":
"signals.transformations.excludeColumns"

}
```

Replace value	Column	A JSON object that represents the data column whose value should be replaced	
	NewValue	The new value to replace	
	OriginValue	The original value to be replaced	

```
{

    "Column": {

      "Name": "Temperature",

      "DataType": "Real"

    },

    "NewValue": "1",

    "OriginValue": "77",

    "Actions": null,

    "name":
"siaReplaceValueTransformation_New",

    "typeId":
"signals.transformations.replaceValue"

}
```

Replace specific value	Column	A JSON object that represents the data column whose value should be replaced	
	NewValue	The new value to replace	
	OriginValue	The original value to be replaced	
	RowIdentifyingColumns	An array of JSON elements that describes the data columns whose values will be used for identifying the rows to be replaced	
	RowIdentifyingColumnValues	An array of JSON values that	

```
{

  "Column": {

      "Name": "Temperature",

      "DataType": "Real"

  },

  "NewValue": 1,

  "OriginValue": 66,

  "RowIdentifyingColumns": [

    {

      "Name": "Lit Ref",

      "DataType": "String"

    }

  ],
```

		identifies the rows	
	WarnWhenReplacingMultipleValues	A Boolean value which indicates whether a warning should be prompted when multiple values are replaced. Default value is **false**	

```
  "RowIdentifyingColumnValues": [
      "TH1318:K10"
  ],
  "WarnWhenReplacingMultipleValues": false,
  "Actions": null,
  "name":
"siaReplaceSpecificValueTransformation_New",
  "typeId":
"signals.transformations.replaceSpecificValue"
}
```

Unpivot	CategoryName	The name of the column that summarizes the information provided in the columns that you have selected to transform. For instance, "Year" could be used when sales figures for several different years are to be combined to a single column	
	DataType	The data type of the category column name if several are possible	
	IdentityColumns	The identity columns that should be transferred to the unpivoted data set without any transformation	
	RemoveNull	A Boolean value which indicates whether the null values should be removed. The default value is **false**	
	ResultName	The name of the value column	

```
{
  "CategoryName": "Category",
  "DataType": "String",
  "IdentityColumns": [
    {
      "Name": "Compound ID",
      "DataType": "String"
    }
  ],
  "RemoveNull": true,
  "ResultName": "Value",
  "ResultType": "String",
  "ValueColumns": [
    {
      "Name": "Assay Date",
      "DataType": "DateTime"
    },
    {
      "Name": "Salt Name",
      "DataType": "String"
    },
    {
      "Name": "Temperature",
```

	ResultType	The data type of the value column	
	ValueColumns	An array of JSON elements that represents the column values to be combined into a single column	

```
      "DataType": "Real"
    }
  ],
  "Actions": null,
  "name": "siaUnpivotTransformation_New",
  "typeId": "signals.transformations.unpivot"
}
```

Change data types	Columns	An array of JSON elements whose data type needs to be changed	
	NewDataType	The new data type for the specified columns	

```
{
  "Columns": [
    {
      "Name": "Salt Name",
      "DataType": "String"
    },
    {
      "Name": "Salt MW",
      "DataType": "Real"
    }
  ],
  "NewDataType": "String",
  "Actions": null,
  "name":
"siaChangeDataTypeTransformation_New",
  "typeId":
"signals.transformations.changeDataType"
}
```

Change column names	ColumnNameExpression	An expression which defines the name to which the column name should be changed	
	ColumnsToRename	An array of JSON elements that specifies the columns whose names are going to be changed	

```
{
  "ColumnNameExpression": "Upper([%C])",
  "ColumnsToRename": [
    {
      "Name": "Salt Name",
      "DataType": "String"
    },
    {
      "Name": "Salt MW",
```

```
      "DataType": "Real"
    }
  ],
  "Actions": null,
  "name": "siaChangeNameTransformation_New",
  "typeId":
"signals.transformations.changeName"
}
```

Calculate new column	Expression	The expression that is used for calculating the new column
	ResultColumnName	The name of the resulting column

```
{
  "Expression": "[Salt MW]*2",
  "ResultColumnName": "SALT NAME * 2",
  "Actions": null,
  "name":
"siaAddCalculatedColumnTransformation_New",
  "typeId":
"signals.transformations.addCalculatedColumn"
}
```

Filter rows	Expression	The expression which defines the rule of the row filtering

```
{
  "Expression": "[Result Number]=1700",
  "Actions": null,
  "name": "siaFilterRowsTransformation_New",
  "typeId":
"signals.transformations.filterRows"
}
```

Pivot	CategoryColumns	Each unique value in the chosen category column or hierarchy produces a new column for each aggregation method in the generated data table. Selecting more than one column means that the new data table will have a separate column for each unique combination of

```
{
  "CategoryColumns": [
    {
      "Name": "Result Text",
      "DataType": "String"
    },
  {
      "Name": "Temperature",
      "DataType": "Real"
    },
  {
```

		values in the chosen columns
	CategorySeparator	A string that represents the category separator
	IdentityColumns	An array of JSON elements that represents the identity columns. Each unique value in the chosen identity column or hierarchy produces a row in the generated table. If you choose more than one column, the new table will have a separate row for each unique combination of values in the chosen columns
	ResultNamingExpression	Specifies how the pivoted columns should be named
	TransferColumns	An array of JSON elements that specifies the transfer columns
	TransferNamingExpression	Specifies how the transfer columns should be named
	ValueColumns	An array of JSON elements that specifies the value columns

```
      "Name": "Assay Date",
      "DataType": "DateTime"
    }
  ],
  "CategorySeparator": "$$",
  "IdentityColumns": [
    {
      "Name": "Compound ID",
      "DataType": "String"
    }
  ],
  "ResultNamingExpression": "%M(%V) for %C",
  "TransferColumns": null,
  "TransferNamingExpression": null,
  "ValueColumns": [
    {
      "Aggregation": "Concatenate",
      "Column": {
        "Name": "Result Text",
        "DataType": "String"
      }
    }
  ],
  "Actions": null,
  "name": "siaPivotTransformation_New",
  "typeId": "signals.transformations.pivot"
}
```

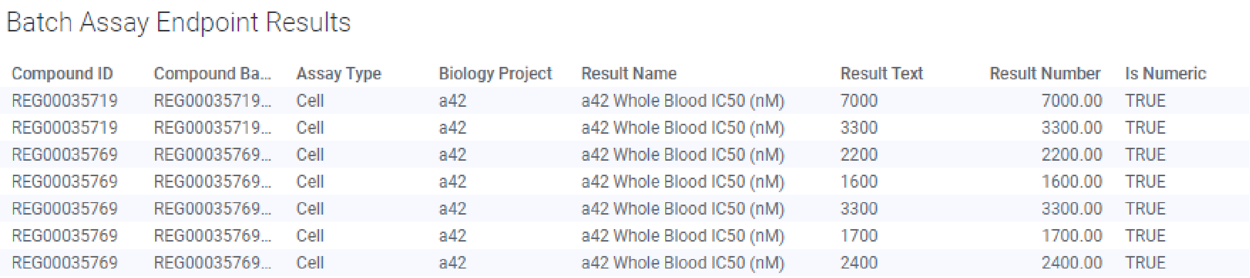
Calculate and replace column	ColumnToReplace	The JSON object which represents the column to be replaced
	Expression	The calculation expression for generating the new value

```
{
  "ColumnToReplace": {
    "Name": "Salt Name",
    "DataType": "String"
  },
```

	ResultColumnName	Specifies the result column name	`"Expression": "[Temperature]+2",`
			`"ResultColumnName": "aaa",`
			`"Actions": null,`
			`"name": "siaReplaceColumnTransformation_New",`
			`"typeId": "signals.transformations.replaceColumn"`
			`}`

Example - Concatenate Quoted Result Values

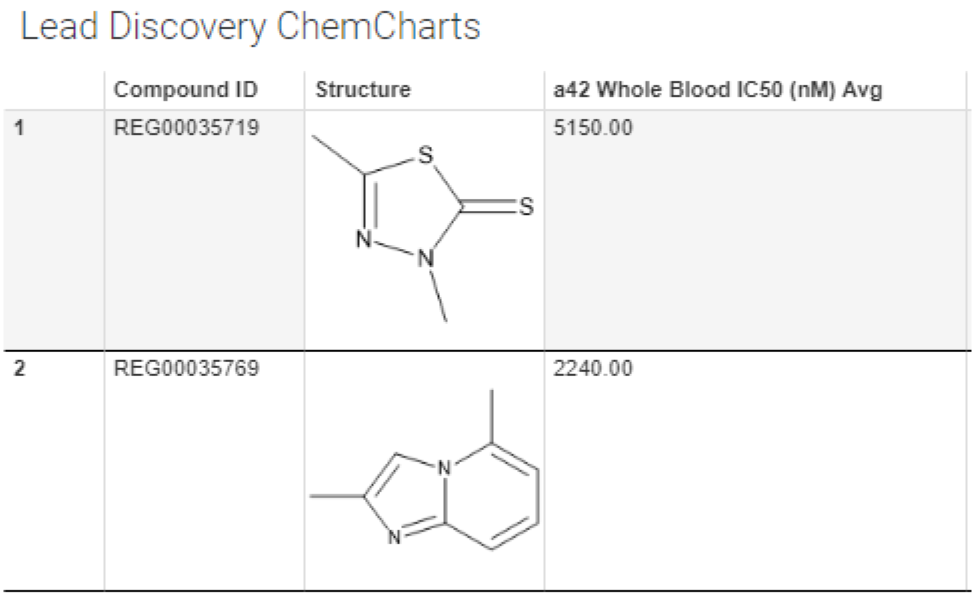
Suppose the Batch Assay Endpoint Results table has the following rows:



Batch Assay Endpoint Results

Compound ID	Compound Ba...	Assay Type	Biology Project	Result Name	Result Text	Result Number	Is Numeric
REG00035719	REG00035719...	Cell	a42	a42 Whole Blood IC50 (nM)	7000	7000.00	TRUE
REG00035719	REG00035719...	Cell	a42	a42 Whole Blood IC50 (nM)	3300	3300.00	TRUE
REG00035769	REG00035769...	Cell	a42	a42 Whole Blood IC50 (nM)	2200	2200.00	TRUE
REG00035769	REG00035769...	Cell	a42	a42 Whole Blood IC50 (nM)	1600	1600.00	TRUE
REG00035769	REG00035769...	Cell	a42	a42 Whole Blood IC50 (nM)	3300	3300.00	TRUE
REG00035769	REG00035769...	Cell	a42	a42 Whole Blood IC50 (nM)	1700	1700.00	TRUE
REG00035769	REG00035769...	Cell	a42	a42 Whole Blood IC50 (nM)	2400	2400.00	TRUE

After the SAR table has been generated, by default, the result value will be aggregated by the Avg method:



Lead Discovery ChemCharts

	Compound ID	Structure	a42 Whole Blood IC50 (nM) Avg
1	REG00035719		5150.00
2	REG00035769		2240.00

Follow the steps below to create a custom aggregation which doubles the result value:

1. From the **Configuration** tab in the SAR app, click the **Manage Custom Aggregations** button.

2. In the Advanced Aggregation Setting dialog, click Create new button to create a new custom aggregation.

3. For the **Name** field, input *Concatenate Quoted Results.*

4. Optionally input the **Description** field to give the custom aggregation a descriptive text.

5. In the **Transformation Steps** drop-down, choose **Calculate new column**, then click **Add** button. This will add a JSON object to the JSON array in the JSON editor.

6. Edit the added JSON object in the JSON editor:

    a) Modify the value of "`Expression`" element to **`Concatenate('\"', Substitute([Result Text],'\"','\\\\\"'), '\"')`**

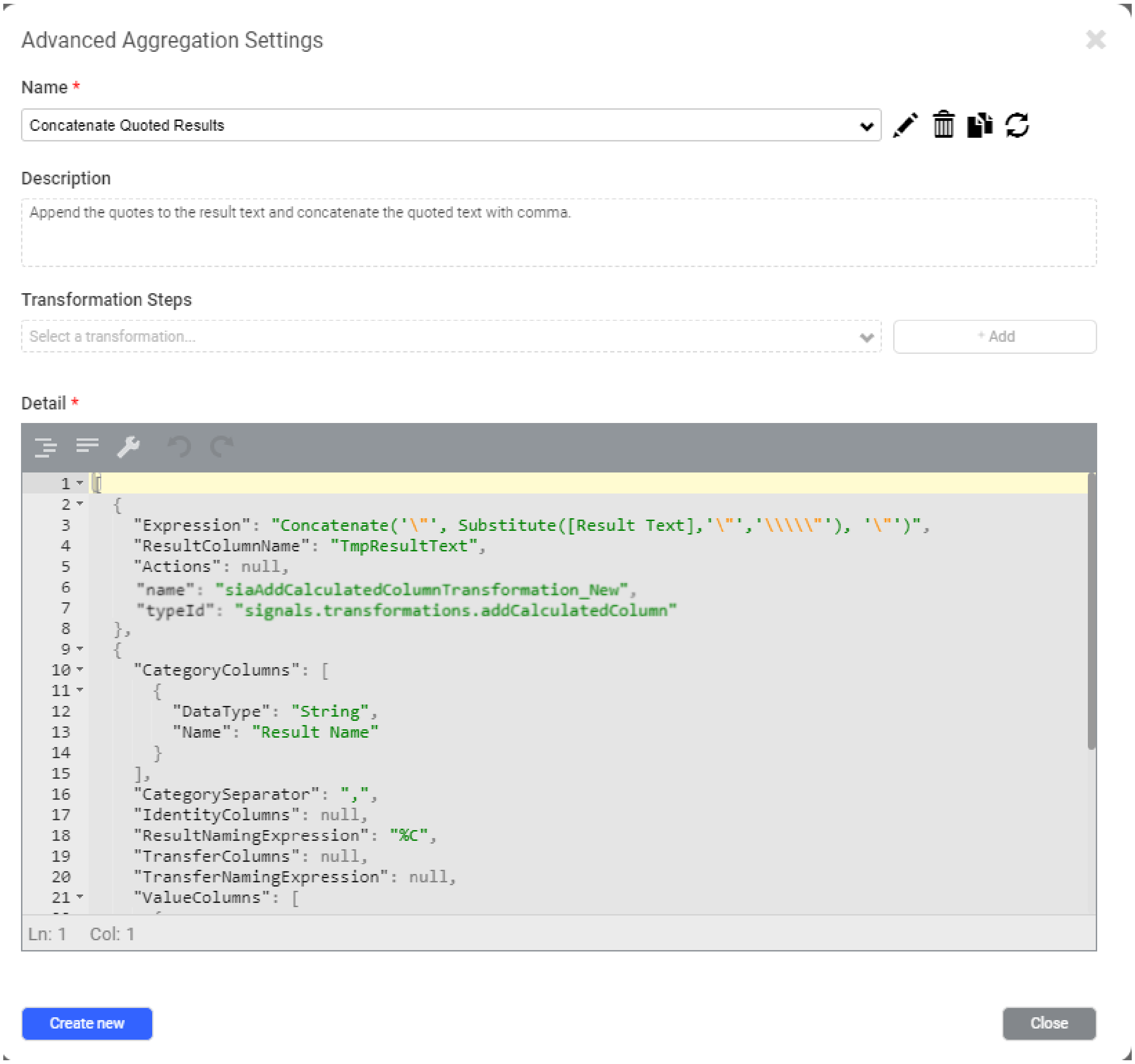
    b) Modify the value of "ResultColumnName" element to **`TmpResultText`**

7. In the **Transformation Steps** drop-down, choose **Pivot**, then click **Add** button. This will add another JSON object to the JSON array in the JSON editor.

8. Edit the added JSON object in the JSON editor, the modified JSON object should be similar to the following:

```
{
    "CategoryColumns": [
      {
        "DataType": "String",
        "Name": "Result Name"
      }
    ],
    "CategorySeparator": ",",
    "IdentityColumns": null,
    "ResultNamingExpression": "%C",
    "TransferColumns": null,
    "TransferNamingExpression": null,
    "ValueColumns": [
      {
        "Aggregation": "Concatenate",
        "Column": {
          "DataType": "String",
          "Name": "TmpResultText"
        }
      }
    ],
    "Actions": null,
    "name": "siaPivotTransformation_New",
    "typeId": "signals.transformations.pivot"
  }
```

9. Click the **Save** (💾) button to save the custom aggregation. At this point, your **Advanced Aggregation Settings** dialog would be similar to the example shown below:



Advanced Aggregation Settings

Name *

Concatenate Quoted Results

Description

Append the quotes to the result text and concatenate the quoted text with comma.

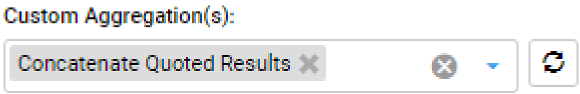
Transformation Steps

Detail *

```
[
  {
    "Expression": "Concatenate('\"', Substitute([Result Text],'\"','\\\\\"'), '\"')",
    "ResultColumnName": "TmpResultText",
    "Actions": null,
    "name": "siaAddCalculatedColumnTransformation_New",
    "typeId": "signals.transformations.addCalculatedColumn"
  },
  {
    "CategoryColumns": [
      {
        "DataType": "String",
        "Name": "Result Name"
      }
    ],
    "CategorySeparator": ",",
    "IdentityColumns": null,
    "ResultNamingExpression": "%C",
    "TransferColumns": null,
    "TransferNamingExpression": null,
    "ValueColumns": [
```

10. Click **Close** button to close the dialog.

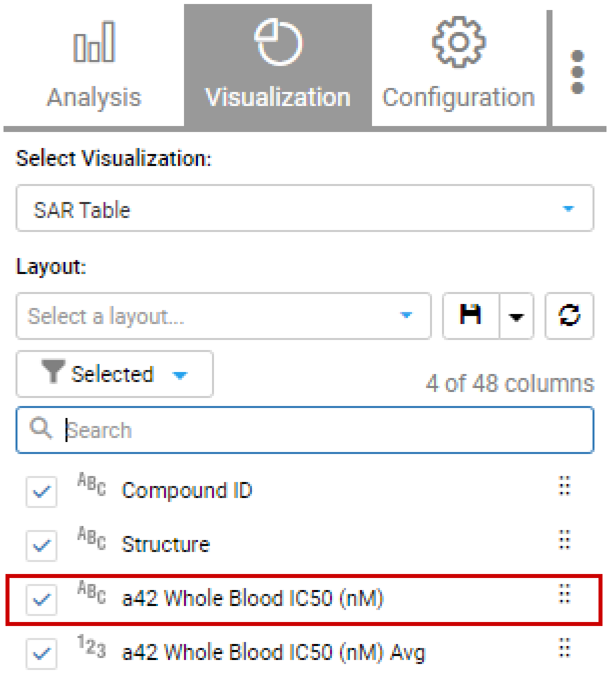
11. In the **Custom Aggregation(s)** drop-down box, choose *Concatenate Quoted Results*, and click the **OK** button.



Custom Aggregation(s):

Concatenate Quoted Results

12. After the SAR table refreshes, you will see an additional column whose name is the name of the result in the visualization layout:



Select Visualization: SAR Table

Layout: Select a layout...

Selected

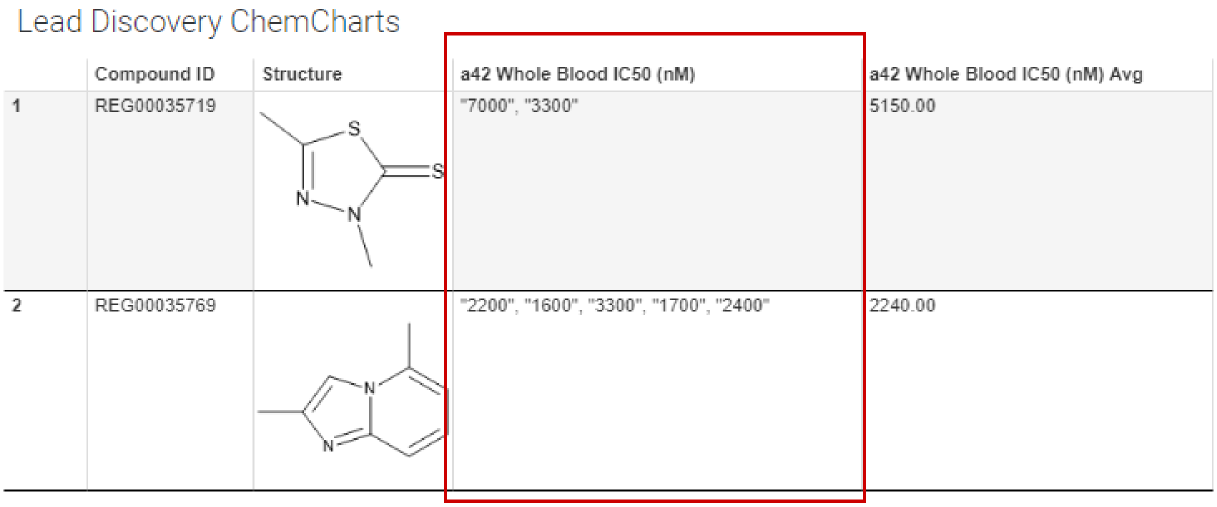
4 of 48 columns

Search

☑ Compound ID
☑ Structure
☑ a42 Whole Blood IC50 (nM)
☑ a42 Whole Blood IC50 (nM) Avg

Note: The column is named after the result name because in the Pivot transformation step, we set the **ResultNamingExpression** to “%C”, which means it will take the pivoted column name as the name of the result column.

13. Check the checkbox on this column, it will be displayed in the SAR table:



Lead Discovery ChemCharts

	Compound ID	Structure	a42 Whole Blood IC50 (nM)	a42 Whole Blood IC50 (nM) Avg
1	REG00035719		"7000", "3300"	5150.00
2	REG00035769		"2200", "1600", "3300", "1700", "2400"	2240.00

Actions

For each of the Built-in Transformation Steps, users can specify a series of actions that are applied before or after the step has been executed. Currently Signals Inventa supports the action of replacing the values of the specified columns with a ChemCharts SmartCell configuration, so that the values could be rendered by the ChemCharts SmartCell renderer.

Append the following JSON schema to the Actions JSON array to achieve the SmartCell rendering:

```
{
  "ApplyNumericShadowColumnProperty": true,
  "NumericShadowColumnPattern": "%C Avg",
  "ReplaceOriginColumn": true,
  "SmartCellTemplate": {
    "version": 0,
    "views": {
      "default": [
        {
          "type": "list",
          "values": [
            "%value%"
          ],
          "anchor": {
            "horizontal": "center",
            "vertical": "center"
          },
          "font": {
            "italic": false,
            "size": 14
          }
        }
      ]
    }
  },
  "ColumnMatchExpression": null,
  "ResultColumnName": null,
  "Type": "SiaReplaceSmartCellAction"
}
```

The explanation of the JSON elements in this schema is as follows:

- **ApplyNumericShadowColumnProperty**: If this value is set to **true**, the NumericShadow column property will be added to the resulting column, with the value of the column name that matches the pattern specified on the **NumericShadowColumnPattern** element
- **NumericShadowColumnPattern**: The pattern that defines how the Numeric Shadow column should be determined. Use “%C” as the wildcard that stands for the name of the original column based on which the pivoted column is generated
- **ReplaceOriginColumn**: The Boolean value which indicates whether the SmartCell action should replace the original column. True to replace the original column, set it to false to add a new column
- **SmartCellTemplate**: A SmartCell template string that describes how the content of the value should be rendered. For the detailed explanation about the SmartCell template, please refer to **Revvity Lead Discovery Premium 3.5 Smart Cell Guide**. Note you can use the %value% placeholder to indicate the place where the column value should be put in the template
- **ColumnMatchExpression**: A regular expression that defines the columns that match this pattern should be processed by the current action
- **ResultColumnName**: The name of the result column

Example - Rendering Concatenate Quoted Results with SmartCell

Follow the steps below to render the values generated by the Concatenate Quoted Results custom aggregation with the SmartCell renderer:

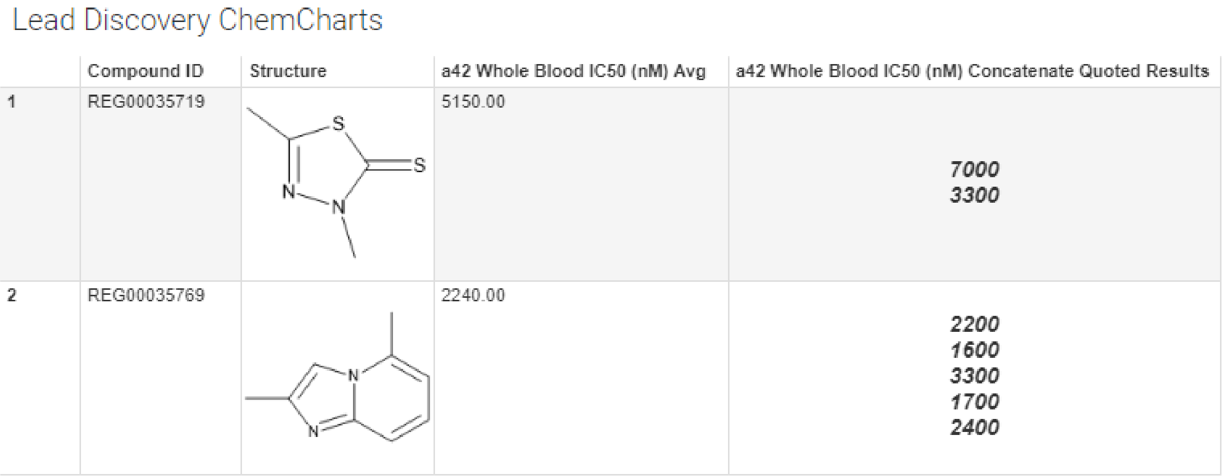
1. Under the **Configuration** tab of the SAR app, click **Manage Custom Aggregations** button.
2. In the **Advanced Aggregation Settings** dialog, choose **Concatenate Quoted Results** custom aggregation that we created previously.
3. Click the **Edit** (✎) button to edit this custom aggregation.
4. In the JSON editor, scroll down to the second JSON object (which is the Pivot transformation step), modify its Actions element as follows:

```
 "Actions": [
  {
    "ApplyNumericShadowColumnProperty": true,
    "NumericShadowColumnPattern": "%C Avg",
    "ReplaceOriginColumn": true,
    "SmartCellTemplate": {
      "version": 0,
      "views": {
        "default": [
          {
            "type": "list",
            "values": [
              "%value%"
            ],
            "anchor": {
              "horizontal": "center",
              "vertical": "center"
            },
            "font": {
              "italic": true,
              "bold": true,
              "size": 14
            }
          }
        ]
      }
    },
    "ColumnMatchExpression": null,
    "ResultColumnName": null,
    "Type": "SiaReplaceSmartCellAction"
  }
]
```

5. Click **Save** (💾) button to save the changes.
6. If the **Concatenate Quoted Results** has already been selected in the **Custom Aggregation(s)** drop-down, the SAR table will be refreshed automatically when the custom aggregation is saved. If it is not selected, select it from the **Custom Aggregation(s)** drop-down:

Custom Aggregation(s):
Concatenate Quoted Results

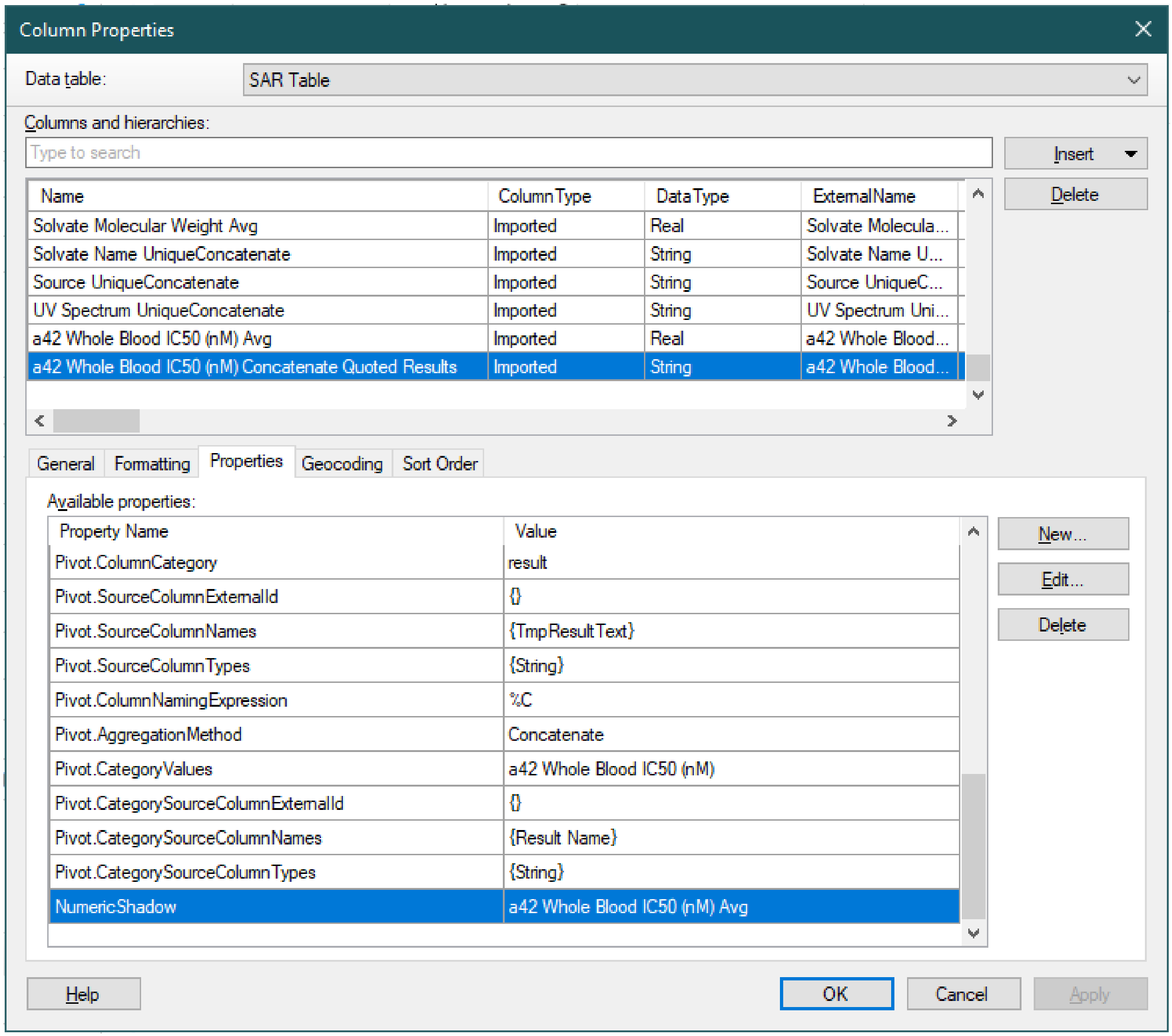
7. After the SAR table refreshes, the resulting column will be displayed, similar to the example shown below:



Lead Discovery ChemCharts

	Compound ID	Structure	a42 Whole Blood IC50 (nM) Avg	a42 Whole Blood IC50 (nM) Concatenate Quoted Results
1	REG00035719		5150.00	***7000*** ***3300***
2	REG00035769		2240.00	***2200*** ***1600*** ***3300*** ***1700*** ***2400***

8. In Spotfire Analyst Client, from **Data** menu, click **Column properties**
9. Check the column property of the resulting column on SAR Table, the NumericShadow property has been set correctly:



Data table: SAR Table

Name	Column Type	Data Type	External Name
Solvate Molecular Weight Avg	Imported	Real	Solvate Molecula...
Solvate Name UniqueConcatenate	Imported	String	Solvate Name U...
Source UniqueConcatenate	Imported	String	Source UniqueC...
UV Spectrum UniqueConcatenate	Imported	String	UV Spectrum Uni...
a42 Whole Blood IC50 (nM) Avg	Imported	Real	a42 Whole Blood...
a42 Whole Blood IC50 (nM) Concatenate Quoted Results	Imported	String	a42 Whole Blood...

Property Name	Value
Pivot.ColumnCategory	result
Pivot.SourceColumnExternalId	{}
Pivot.SourceColumnNames	{TmpResultText}
Pivot.SourceColumnTypes	{String}
Pivot.ColumnNamingExpression	%C
Pivot.AggregationMethod	Concatenate
Pivot.CategoryValues	a42 Whole Blood IC50 (nM)
Pivot.CategorySourceColumnExternalId	{}
Pivot.CategorySourceColumnNames	{Result Name}
Pivot.CategorySourceColumnTypes	{String}
NumericShadow	a42 Whole Blood IC50 (nM) Avg

Important Note: SmartCell action only works in Lead Discovery ChemCharts. Spotfire Table Plot visualization doesn’t support SmartCell rendering.

Out-of-the-Box Templates

By default, the SAR Analysis app comes with four pre-defined templates that helps you to create your aggregations on the fly:

- Avg +- StdDev
- Avg +- StdDev (Count)
- Avg +- StdDev (Count)[MultiAnchor]
- Avg +- StdDev (Range, Count)
- All-In-One

To create a custom aggregation based on the template:

1. Under the **Configuration** tab of the SAR app, click **Manage Custom Aggregations** button.
2. On the Advanced Aggregation Settings dialog, click Create new button.
3. In the Name field, input the name of the new custom aggregation.
4. In the Description field, optionally input the description.
5. In the Transformation Steps drop-down box, choose the template you want to use, templates have the “(Template)” suffix on their names, then click Add button, this will add the template JSON to the Detail JSON editor.
6. Click Save (💾) button to save the custom aggregation.

To use the custom aggregation created based on a template, in the **Custom Aggregation(s)** drop-down box, choose the custom aggregation that you just created.

Avg +- StdDev

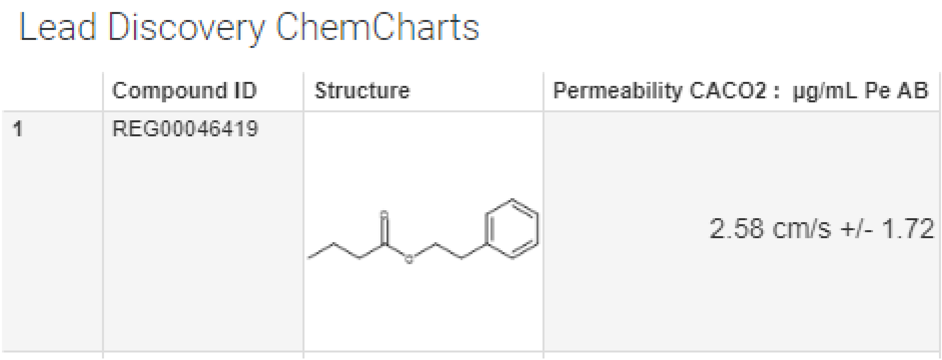
This custom aggregation aggregates the result value by both Avg and StdDev methods and combines the aggregated result with +/- sign.

For example, the measurement result for compound REG00046419 in the Batch Assay Endpoint Result table:

Batch Assay Endpoint Results

Compound ID ▲	Compound Batch ID	Assay Type	Biology Project	Assay	Result Name	Is Numeric	Result Text	Result Number
REG00046406	REG00046406-02	ADMET	Permeability	Permeability C...	Permeability CACO2 : µg/mL Pe AB Avg (cm/s)	TRUE	5.72	5.72
REG00046419	REG00046419-02	ADMET	Permeability	Permeability C...	Permeability CACO2 : µg/mL Pe AB Avg (cm/s)	TRUE	1.36	1.36
REG00046419	REG00046419-03	ADMET	Permeability	Permeability C...	Permeability CACO2 : µg/mL Pe AB Avg (cm/s)	TRUE	3.79	3.79
REG00046426	REG00046426-02	ADMET	Permeability	Permeability C...	Permeability CACO2 : µg/mL Pe AB Avg (cm/s)	TRUE	2.64	2.64
REG00046429	REG00046429-03	ADMET	Permeability	Permeability C...	Permeability CACO2 : µg/mL Pe AB Avg (cm/s)	TRUE	2.44	2.44

will result in the following ***Avg +- StdDev*** result:



Lead Discovery ChemCharts

	Compound ID	Structure	Permeability CACO2 : µg/mL Pe AB
1	REG00046419		2.58 cm/s +/- 1.72

Avg +- StdDev (Count)

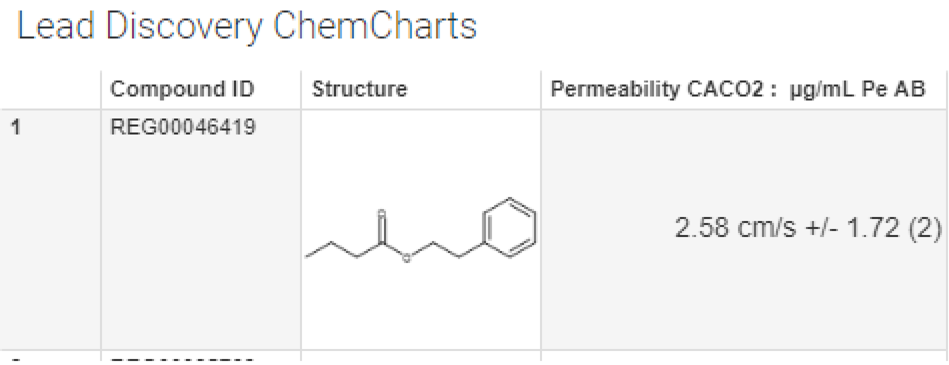
This custom aggregation aggregates the result value by both Avg and StdDev methods and combines the aggregated result with +/- sign, followed by the number of results being aggregated.

For example, the measurement result for compound REG00046419 in the Batch Assay Endpoint Result table:

Batch Assay Endpoint Results

Compound ID	Compound Batch ID	Assay Type	Biology Project	Assay	Result Name	Is Numeric	Result Text	Result Number
REG00046406	REG00046406-02	ADMET	Permeability	Permeability C...	Permeability CACO2 : µg/mL Pe AB Avg (cm/s)	TRUE	5.72	5.72
REG00046419	REG00046419-02	ADMET	Permeability	Permeability C...	Permeability CACO2 : µg/mL Pe AB Avg (cm/s)	TRUE	1.36	1.36
REG00046419	REG00046419-03	ADMET	Permeability	Permeability C...	Permeability CACO2 : µg/mL Pe AB Avg (cm/s)	TRUE	3.79	3.79
REG00046426	REG00046426-02	ADMET	Permeability	Permeability C...	Permeability CACO2 : µg/mL Pe AB Avg (cm/s)	TRUE	2.64	2.64
REG00046429	REG00046429-03	ADMET	Permeability	Permeability C...	Permeability CACO2 : µg/mL Pe AB Avg (cm/s)	TRUE	2.44	2.44

will result in the following ***Avg+- StdDev (Count)*** result:



Lead Discovery ChemCharts

	Compound ID	Structure	Permeability CACO2 : µg/mL Pe AB
1	REG00046419		2.58 cm/s +/- 1.72 (2)

Avg +- StdDev (Count)[MultiAnchor]

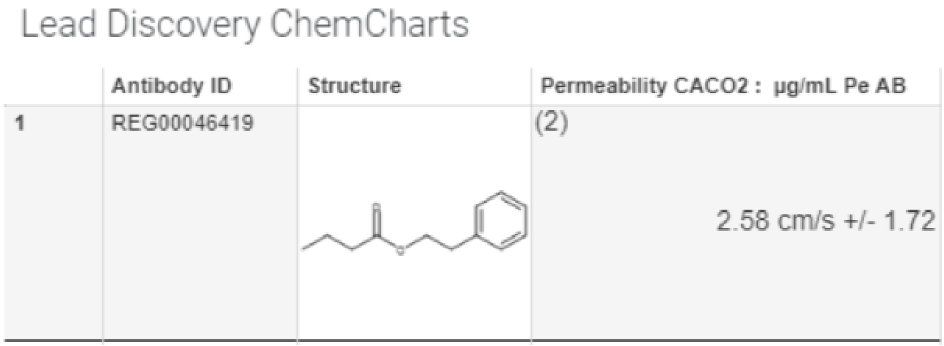
This custom aggregation behaves similarly to Avg +- StdDev (Count), however, it will put the result into different part with different location.

For example, the measurement result for compound REG00046419 in the Batch Assay Endpoint Result table:

Batch Assay Endpoint Results

Compound ID	Compound Batch ID	Assay Type	Biology Project	Assay	Result Name	Is Numeric	Result Text	Result Number
REG00046406	REG00046406-02	ADMET	Permeability	Permeability C...	Permeability CACO2 : µg/mL Pe AB Avg (cm/s)	TRUE	5.72	5.72
REG00046419	REG00046419-02	ADMET	Permeability	Permeability C...	Permeability CACO2 : µg/mL Pe AB Avg (cm/s)	TRUE	1.36	1.36
REG00046419	REG00046419-03	ADMET	Permeability	Permeability C...	Permeability CACO2 : µg/mL Pe AB Avg (cm/s)	TRUE	3.79	3.79
REG00046426	REG00046426-02	ADMET	Permeability	Permeability C...	Permeability CACO2 : µg/mL Pe AB Avg (cm/s)	TRUE	2.64	2.64
REG00046429	REG00046429-03	ADMET	Permeability	Permeability C...	Permeability CACO2 : µg/mL Pe AB Avg (cm/s)	TRUE	2.44	2.44

will result in the following ***Avg+- StdDev (Count) [MultiAnchor]*** result:



Lead Discovery ChemCharts

	Antibody ID	Structure	Permeability CACO2 : µg/mL Pe AB
1	REG00046419		(2) 2.58 cm/s +/- 1.72

Avg +- StdDev (Range, Count)

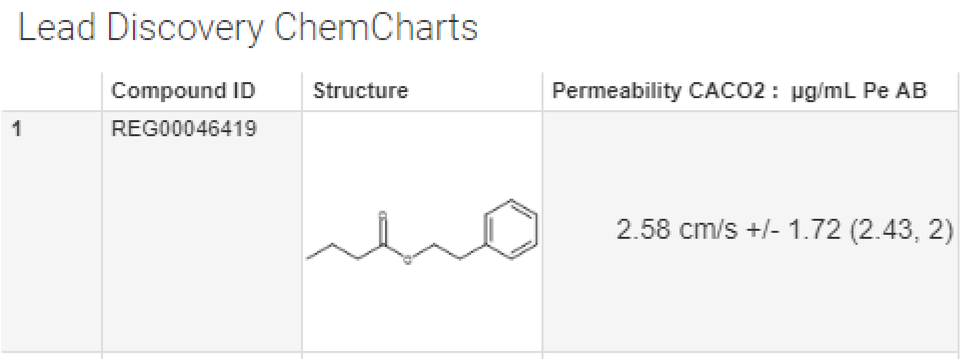
This custom aggregation aggregates the result value by both Avg and StdDev methods and combines the aggregated result with +/- sign, followed by both the range and number of results being aggregated.

For example, the measurement result for compound REG00046419 in the Batch Assay Endpoint Result table:

Batch Assay Endpoint Results

Compound ID ▲	Compound Batch ID	Assay Type	Biology Project	Assay	Result Name	Is Numeric	Result Text	Result Number
REG00046406	REG00046406-02	ADMET	Permeability	Permeability C...	Permeability CACO2 : µg/mL Pe AB Avg (cm/s)	TRUE	5.72	5.72
REG00046419	REG00046419-02	ADMET	Permeability	Permeability C...	Permeability CACO2 : µg/mL Pe AB Avg (cm/s)	TRUE	1.36	1.36
REG00046419	REG00046419-03	ADMET	Permeability	Permeability C...	Permeability CACO2 : µg/mL Pe AB Avg (cm/s)	TRUE	3.79	3.79
REG00046426	REG00046426-02	ADMET	Permeability	Permeability C...	Permeability CACO2 : µg/mL Pe AB Avg (cm/s)	TRUE	2.64	2.64
REG00046429	REG00046429-03	ADMET	Permeability	Permeability C...	Permeability CACO2 : µg/mL Pe AB Avg (cm/s)	TRUE	2.44	2.44

will result in the following ***Avg+- StdDev (Range, Count)*** result:



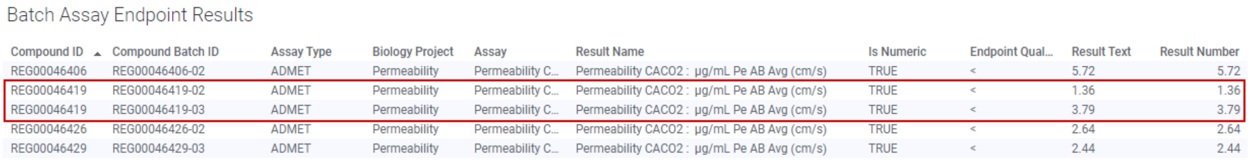
Lead Discovery ChemCharts

	Compound ID	Structure	Permeability CACO2 : µg/mL Pe AB
1	REG00046419		2.58 cm/s +/- 1.72 (2.43, 2)

All-In-One

This custom aggregation concatenates the result value with the endpoint qualifier and aggregates the concatenated strings with the new-line separator.

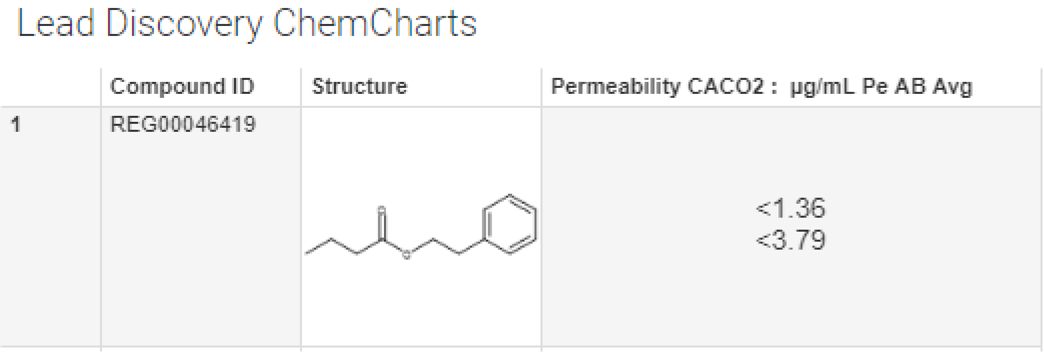
For example, the measurement result for compound REG00046419 in the Batch Assay Endpoint Result table:



Batch Assay Endpoint Results

Compound ID ▲	Compound Batch ID	Assay Type	Biology Project	Assay	Result Name	Is Numeric	Endpoint Qual...	Result Text	Result Number
REG00046406	REG00046406-02	ADMET	Permeability	Permeability C...	Permeability CACO2 : µg/mL Pe AB Avg (cm/s)	TRUE	<	5.72	5.72
REG00046419	REG00046419-02	ADMET	Permeability	Permeability C...	Permeability CACO2 : µg/mL Pe AB Avg (cm/s)	TRUE	<	1.36	1.36
REG00046419	REG00046419-03	ADMET	Permeability	Permeability C...	Permeability CACO2 : µg/mL Pe AB Avg (cm/s)	TRUE	<	3.79	3.79
REG00046426	REG00046426-02	ADMET	Permeability	Permeability C...	Permeability CACO2 : µg/mL Pe AB Avg (cm/s)	TRUE	<	2.64	2.64
REG00046429	REG00046429-03	ADMET	Permeability	Permeability C...	Permeability CACO2 : µg/mL Pe AB Avg (cm/s)	TRUE	<	2.44	2.44

will result in the following **All-In-One** result:



Lead Discovery ChemCharts

	Compound ID	Structure	Permeability CACO2 : µg/mL Pe AB Avg
1	REG00046419		<1.36 <3.79

16 Appendix D: Tips for Importing Images into Spotfire

Thumbnails, curve images, and other images can be encoded differently depending on the file source. Often curve images from Signals VitroVivo and other programs are represented as ‘Strings’. In order to be interpreted as an image, the format much be converted from string to binary. The “Base64Decode()” option from the ‘Calculate New Column’ dialog can be used to convert strings into binary options. When mapping/publishing measurement types where the expected format is an ‘image’, users must select a binary column.

Additional Notes:

- Thumbnails are static images and cannot be edited directly
- There's not a way to automatically take a base64-encoded string and interpret it as binary upon import into Spotfire (users must do the manual data transformation)
- Base64-encoding strings can be quite long, so it's preferable files with strings are saved as delimited file type (csv, tsv). Excel (xlsx, xls) is not recommended since the max string length for excel is 32,767 characters. If the base64-encoded string is >32767 characters, the string will be truncated and images won't display properly. You can check to see if this is an issue by using the excel LEN() function to count the number of characters in a string.
- JPEG and PNG are supported image types.
- Formats like BMP and TIFF are not normally displayable within a web browser and thus not in Spotfire.

17 Appendix E: Signals Notebook Integration

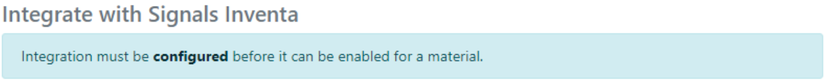
17.1 Signals Notebook Material Synchronization

Compounds in Revvity Signals Notebook can be published to Signals Data Factory via the material synchronization feature so that these assets are then available in Signals Inventa's Global Search.

Once enabled, a **Streams** tab is added to each project in Signals Data Factory allowing the user to manage the subscription to the stream at the project level.

17.1.1 Enabling Signals Notebook Material Synchronization

1. From Signals Notebook, select your username in the top right-hand corner **> System Configuration**. Administrative privileges are required to select this option.
2. Login at the prompt.
3. Select the **Materials** icon from the top toolbar, then the **configured** link to open **Signals Inventa Integration**.

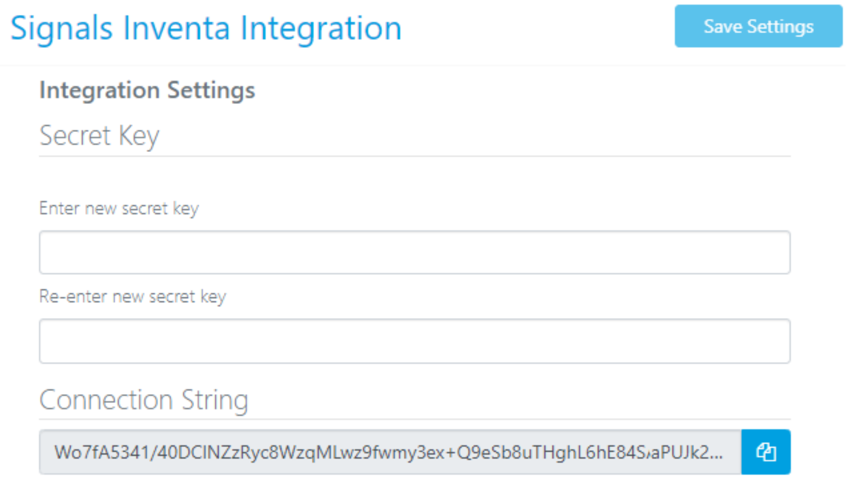


Integrate with Signals Inventa

Integration must be **configured** before it can be enabled for a material.

Note: This menu may also be accessed from the **System Settings** icon from the top tool bar **> Other > Signals Inventa Integration.**

4. Enter a **Secret Key** into the textboxes provided and select **Save Settings**, then copy the provided connection string.



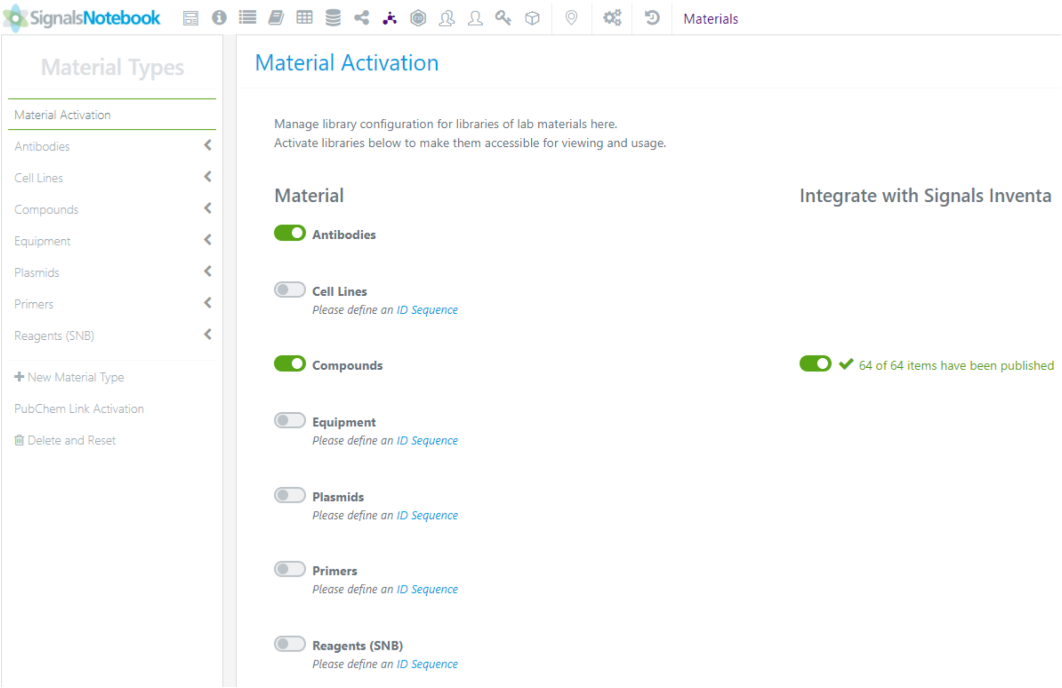
Wo7fA5341/40DCINZzRyc8WzqMLwz9fwmy3ex+Q9eSb8uTHghL6hE84S/aPUJk2...

5. From Signals Data Factory, select **Administration > Signals Notebook Connection** from the top toolbar.
6. Select **Connect** and paste the connection string and **Secret Key** into the appropriate textboxes.

7. Select **Connect** to establish the connection.

Note: If the **Secret Key** is updated in Signals Notebook, it must also be updated from this page by selecting the ⋮ button in the upper-right-hand corner **> Update Secret Key.**

8. Return to Signals Notebook, from the **Materials** page, toggle on the **Integrate with Signals Inventa** toggle to begin the publishing process.



Material Activation

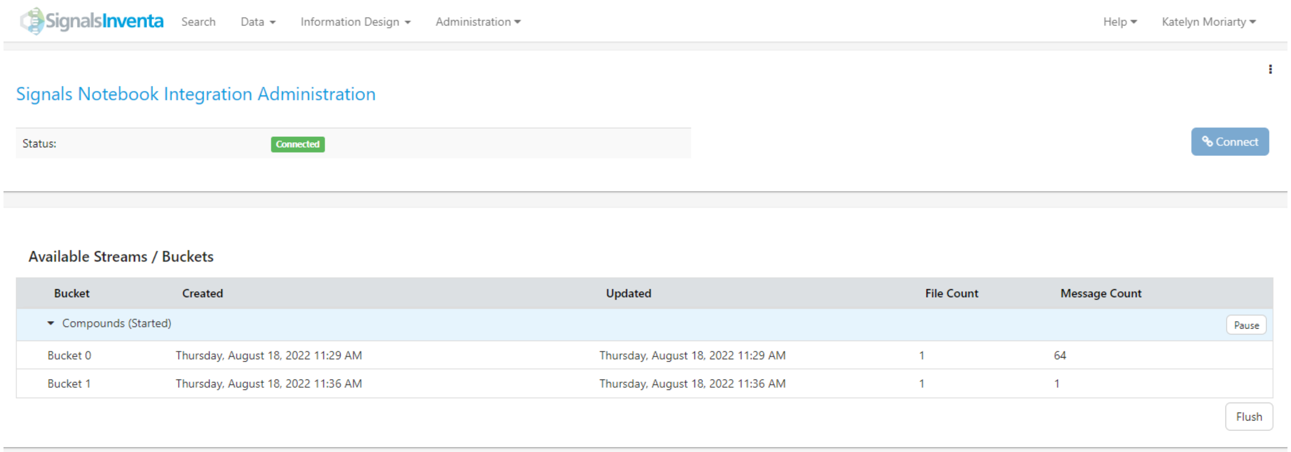
Manage library configuration for libraries of lab materials here.
Activate libraries below to make them accessible for viewing and usage.

Material	Integrate with Signals Inventa
● Antibodies	
○ Cell Lines *Please define an ID Sequence*	
● Compounds	● ✓ 64 of 64 items have been published
○ Equipment *Please define an ID Sequence*	
○ Plasmids *Please define an ID Sequence*	
○ Primers *Please define an ID Sequence*	
○ Reagents (SNB) *Please define an ID Sequence*	

Note: At this time, only the **Compounds** material can be toggled on.

9. Return to Signals Data Factory, from the **Signals Notebook Connection** page, note the available streams (buckets) now listed. The following controls are also available:

- **Pause**: stops the monitoring of the system by temporarily disrupting the stream
- **Resume:** restarts a paused stream
- **Delete:** removes all buckets in the stream (can only be applied when the stream is retired and there are no subscribed projects)
- **Flush**: forces a refresh and sync



Signals Notebook Integration Administration

Status: Connected

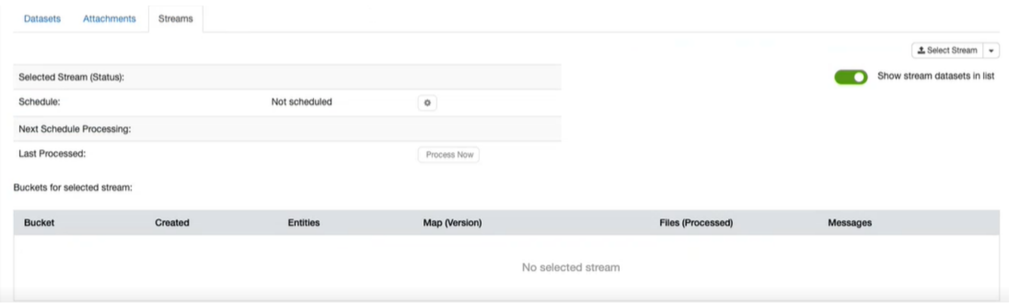
Available Streams / Buckets

Bucket	Created	Updated	File Count	Message Count
▾ Compounds (Started)				
Bucket 0	Thursday, August 18, 2022 11:29 AM	Thursday, August 18, 2022 11:29 AM	1	64
Bucket 1	Thursday, August 18, 2022 11:36 AM	Thursday, August 18, 2022 11:36 AM	1	1

Note: New buckets are only added if the shape of the data changes (i.e. a new column is added) so that the user may map the new data appropriately.

17.1.2 Selecting and Mapping a Stream in Signals Data Factory

1. Open the desired project in Signals Data Factory.
2. From the **Streams** tab, select Select Stream ▾.



Selected Stream (Status):

Schedule: Not scheduled

Next Schedule Processing:

Last Processed:

Buckets for selected stream:

Bucket	Created	Entities	Map (Version)	Files (Processed)	Messages
No selected stream					

3. Select the desired steam entry and then the **Select stream** button.

Select a stream

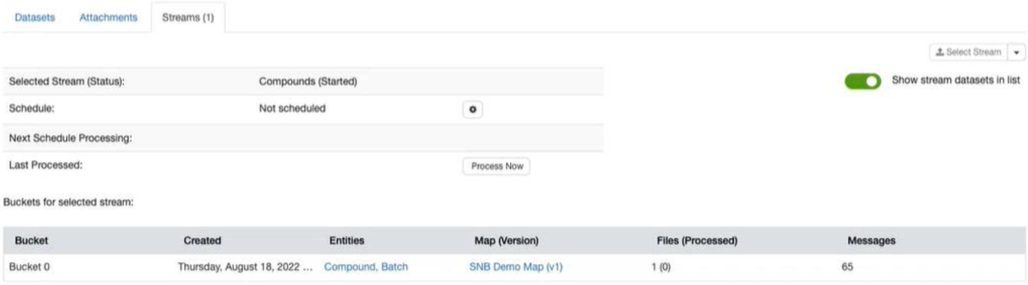
Status	Name	Start Date	Message Count	Files Count
Started	Compounds	Thursday, August 18, 2022 3:57 PM	65	1

4. From the **Streams** tab, select **<click to map>** under the **Map (Version)** header. Refer to [Mapping](#) section in Appendix B:Signals Data Factory for more details on how map data. The 'assetID' must be mapped to **Compound**, and batchID' to **Batch**. Alternatively, the user can select a pre-existing map via **Load Map**.

Note: The user cannot map materials to a measurement type and this feature is therefore disabled.

5. Select **Update Bucket** to return to the **Streams** tab.

6. Selecting **Process Now** will save the file and messages as a dataset, apply the specified map, and load the data. This button can be selected at any time to update the data from Signals Notebook to Signals Data Factory.



Selected Stream (Status): Compounds (Started)
Schedule: Not scheduled
Next Schedule Processing:
Last Processed:

Buckets for selected stream:

Bucket	Created	Entities	Map (Version)	Files (Processed)	Messages
Bucket 0	Thursday, August 18, 2022 ...	Compound, Batch	SNB Demo Map (v1)	1 (0)	65

Note: When a new field is added in Signals Notebook, a new bucket is created once processed. By default, it will use the previous bucket's map. The user may optionally map the new field via the **Streams** tab to update the map, if desired. The most recent map is applied to all records and only the most recent bucket's map can be edited.

Buckets for selected stream:

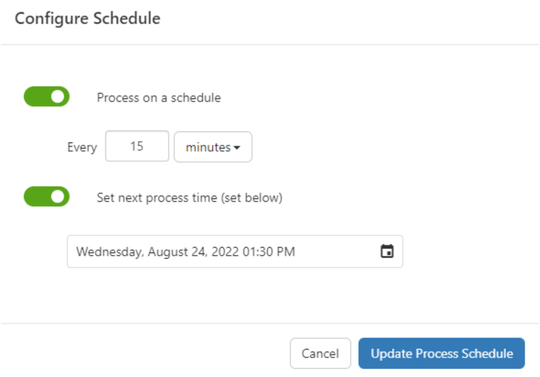
Bucket	Created	Entities	Map (Version)	Files (Processed)	Messages
Bucket 1	Thursday, August 18, 2022 ...	< as bucket 0 >	< as bucket 0 >	1 (1)	1
Bucket 0	Thursday, August 18, 2022 ...	Compound, Batch	SNB Demo Map (v1)	5 (5)	76

7. The dataset will now appear in the **Datasets** tab. These entries can be hidden by disabling the **Show stream dataset in list** toggle in the **Streams** tab.

Note: Even if an entity or compound is deleted from Signals Notebook, a record will exist in Signals Data Factory. This can be viewed using an **New Search (beta)** feature with the tag "*$$$isDeleted": true*.

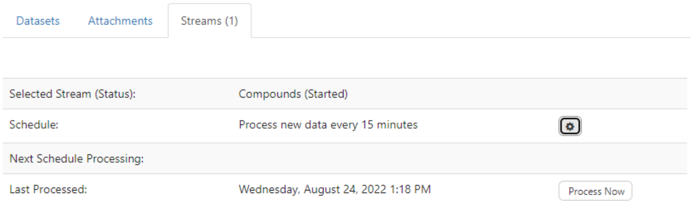
17.1.3 Configuring a Process Schedule

1. From the **Streams** tab, select the ⚙ icon to launch the **Configure Schedule** menu. Specify a numerical value for how often the system should check for changes and the desired unit of time (minutes, hours, days). Optionally select the date and time to begin the process schedule and select **Update Process Schedule**.



Process on a schedule
Every 15 minutes
Set next process time (set below)
Wednesday, August 24, 2022 01:30 PM

2. The **Streams** tab will now display the process schedule.

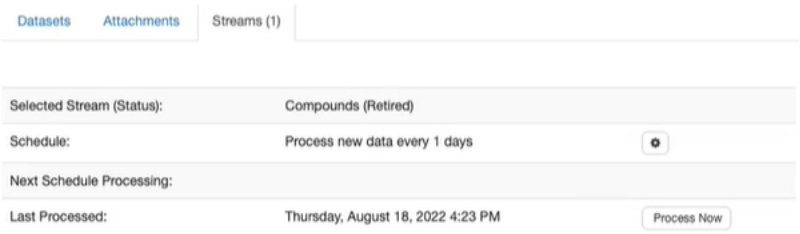


Selected Stream (Status):	Compounds (Started)
Schedule:	Process new data every 15 minutes
Next Schedule Processing:	
Last Processed:	Wednesday, August 24, 2022 1:18 PM

17.1.4 Retiring and Restarting a Stream

1. If the user wishes to resend all stream data, they can turn off the **Integrate with Signals Inventa** toggle from the **Materials** page of Signals Notebook. A message warning the user that the stream will be deactivated is shown, select **Deactivate**.

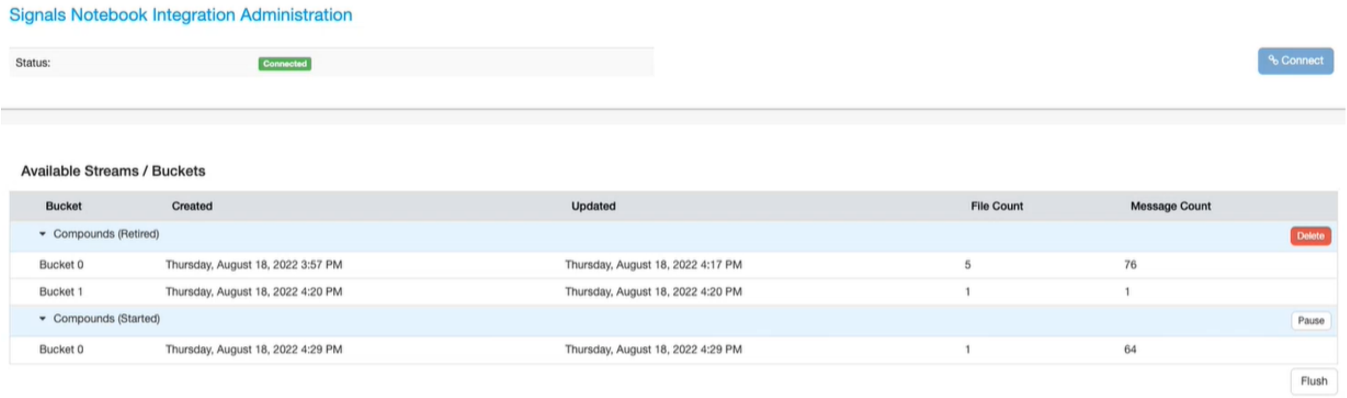
2. The **Selected Stream (Status)** will update in SDF to indicate it has been **Retired**.



Selected Stream (Status):	Compounds (Retired)
Schedule:	Process new data every 1 days
Next Schedule Processing:	
Last Processed:	Thursday, August 18, 2022 4:23 PM

3. Turn on the **Integrate with Signals Inventa** toggle from the **Materials** page of Signals Notebook to begin a new stream.

4. From the **Administration > Signals Notebook Connection** page in Signals Data Factory, the original stream will show as **Retired** and the new stream will show as **Started**. Select **Flush** to begin receiving messages.



Signals Notebook Integration Administration

Status: Connected

Available Streams / Buckets

Bucket	Created	Updated	File Count	Message Count
▾ Compounds (Retired)				
Bucket 0	Thursday, August 18, 2022 3:57 PM	Thursday, August 18, 2022 4:17 PM	5	76
Bucket 1	Thursday, August 18, 2022 4:20 PM	Thursday, August 18, 2022 4:20 PM	1	1
▾ Compounds (Started)				
Bucket 0	Thursday, August 18, 2022 4:29 PM	Thursday, August 18, 2022 4:29 PM	1	64

5. From the **Streams** tab, select the arrow next to the Select Stream ▾ button > **Delete stream**.

6. Select the Select Stream ▾ button again and select the **Started** stream **> Select stream.**

Select a stream

Status	Name	Start Date	Message Count	Files Count
Started	Compounds	Thursday, August 18, 2022 4:29 PM	64	1
Retired	Compounds	Thursday, August 18, 2022 3:57 PM	77	6

7. Select **<click to map>** under the **Map (Version)** header and map as previously described. Select **Process Now** to save the file and messages as a dataset, apply the specified map, and load the data.

8. From the **Administration > Signals Notebook Connection** page in Signals Data Factory, the retired stream can now be deleted via the **Delete** button.

18 Glossary

Measurement

A Measurement is a collection of values.

Measurement Attribute

A Measurement Attribute is the definition of the values. A single conceptual column information that can be collected when data is published to Signals Data Factory through Signals Inventa. Measurement Attributes represent the abstract or conceptual definition of that information (e.g. "Assay Date", "IC50", "Assay Scientist") rather than the data itself. A Measurement Type will be a set of Measurement Attributes that together capture all the information about a particular type of result, annotation, or experiment that would be helpful to scientists that access those data later. A good analogy is that Measurement Attributes are like the columns of an Excel spreadsheet or a coma delimited tabular file.

Measurement Type

A Measurement Type represents the conceptual definition of some data that you would like to capture and publish through Signals Inventa. For example, a particular assay protocol that generates IC50 results could be represented with a Measurement Type. Measurement Types are composed of a collection of Measurement Attributes that together capture all the information about a particular measurement. A good analogy is that Measurement Types are like an Excel spreadsheet that is used to report assay or experimental results to other scientists.

Measurement Type Map

A Measurement Type Map is a set of information that relates the columns of a spread sheet or a csv table of results to the Measurement Type and Measurement Attributes that capture and publish those results through Signals Inventa. This map is generally built once for relating given spreadsheet to a Measurement Type and then can be reused whenever new similar spreadsheets are published to the system.

Endpoint

An Endpoint is a multi-valued attribute that includes the key measured value together with additional information that puts the measured value in context. For example, the IC50 endpoint attribute includes the numerical IC50 measured value, a textual representation of that value, its units, the name of the measured quantity, the type of the measured quantity, and optionally a qualifier for the measured value. Defining the measured value with such consistent and detailed result attributes allows for the unification of endpoints from disparate assay protocols so that they can be searched and retrieved for analysis.

Endpoint Publication Map

A special map that is created by a Data Administrator to relate a Measurement Type, and importantly the Endpoints of the Measurement Type, to the overall Signals Inventa data index. This map is defined once and only once for each Measurement Type and includes information about how each Endpoint should be represented in the index - this drives data discovery and access.

Publication

A term for making data available to an index.

Data Set

A set of measurements that are collected together and labelled for future reference.

When data is published to Signals Inventa you can create Data Set to organize the data into manageable groupings. As part of the act of publishing data you can elect to create a new data set, update, or overwrite an existing Data Set.