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|  |

| Related Artifacts | |
| --- | --- |
| Ref. | Name |
|  |  |
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|  |  |
| --- | --- |
| Abbreviations and Acronyms | |
| **ELN** | Electronic Lab Notebook |
| **rxn** | Reaction file |

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# Introduction

Indigo ELN, the open-source Chemistry Electronic Lab Notebook, provides scientists with a proven way to create, store, retrieve, and share electronic records of chemistry and biology-related information in the way of meeting legal, regulatory, technical, and scientific requirements. The key entities - project, notebook, experiment and component allow users to organize scientific data among the group of scientists. Flexible sharing feature allows users to provide various types of access level to created entities. The user with administrative roles is able to create an experiment template using a set of pre-defined components. Other users create experiments based on existing templates. A current set of pre-defined components allows scientists to fully describe any chemical experiment, starting from selection of the starting compounds and their quantitative relations, ending with creation and description of specific products and their properties, or the concept from the proposed synthesis of the hypothetical reactants or hypothetical products. List of the components can be extended to describe any type of an experiment. Through the use of Indigo ELN, the user can upgrade an existing ELN with a proven and tested open-source platform, and to do it free of charge.

An electronic laboratory notebook is a system to:

* Create,
* Store,
* Retrieve, and
* Share

electronic records in the way of meeting all legal, regulatory, technical, and scientific requirements, while maintaining the responsibility of a scientist for care and maintenance of laboratory records.

An important feature of this application is flexibility and ability to easily adjust for custom needs in terms of user’s access policy, integration with existing databases, and registration with electronic signature services. Also application propose mechanism of templates to create different types of experiments without the need to change the code.

This document describes the process of using Indigo ELN.

# Program Overview

## Logical and Database Entities

The database entities match logical entities of the application. The following entities build a hierarchy:



The following table describes the database entities.

|  |  |
| --- | --- |
| Name | Description |
| Project | Entity that contains a list of Notebooks and some information describing **Project** |
| Notebook | Entity that contains a list of Experiments and some information describing **Notebook** |
| Experiment | Entity that contains a list of Components and some information such as **Template** or **Experiment Number** |
| Component | Predefined set of tables, buttons and fields to allow user record and handle different kind of experimental data |
| Template | Template is a list of components that Administrators compose with the help of the Template Editor. A template is used only at the moment of Experiment creation. If a Template changes, it does not affect Experiments created on the basis of this Template. |
| Permission | Access level to certain entities inside application |
| Authority | User privileges allowed on application level |
| User | Unique identity corresponding to a user of the application. Users have a number of authorities inside the application and can be given permissions to access chosen entities |

## User Management

Indigo ELN supports a User-Role-Authority model on application level and ACL (Access Control List) for an entity (Project, Notebook, or Experiment) that contains the User Permissions for a user." It means that administrator can manage possible user actions on application level. User can share entity with different permissions level.

Each User is given a Role or a set of Roles which contain a set of Authorities.

User privileges are formed from a distinct set of authorities from all user's roles.

Authorities set global privileges for a specified User while User Permissions define User access level for certain Entity (see Section 2.3.2 User Permissions).

Each User has a unique login. Each Role has a unique name.

The following is the full set of user authorities:

|  |  |
| --- | --- |
| Authority | Authority Description |
| User editor | Read / create / update users |
| Role editor | Read / create / update / remove roles |
| Content editor | Read / create / update entity in spite of absence in ACL for this entity or some restrictions by ACL for this entity. Allows to see all entities in the system. “All Project” section is present in navigation tree |
| Template editor | Read / create / update / remove template |
| Project reader | Read Project |
| Project creator | Read/ create/update Project |
| Notebook reader | Read Notebook |
| Notebook creator | Read / create/update Notebook |
| Experiment reader | Read Experiment |
| Experiment creator | Read / create/update Experiment |
| Dictionary editor | Read / create / update / remove dictionaries |
| Search within the system | Allow to user execute search of entities by set of criteria, including Structure and Reaction search |

1. The application sets the “Entity reader” authority automatically when you select the “Entity creator” authority. The “Entity creator” authority removal does not affect “Entity reader” authority selection.

The application sets the “Notebook reader” authority automatically when you select the “Experiment creator “authority.

To create/edit a Role, see Section 5.2 Roles.

### User Permissions

The following table describes and explains types of Permissions available for the entities in the program.

Please note: In case of sharing entity such as Project and Notebook given Permission will be applied to sub-entities. In case of Experiment entity sharing corresponding Notebook and Project also will be shared with minimal permission Viewer.

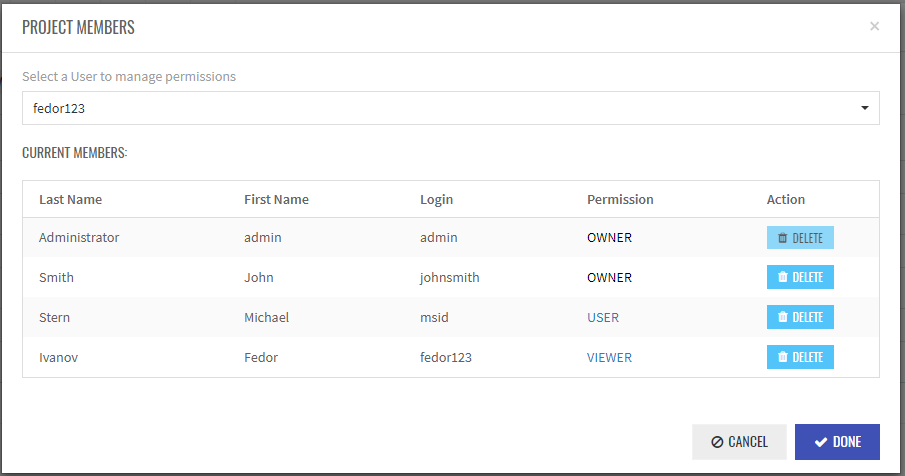
This Permission type determines possible actions on the entity level for the user with whom this entity was shared:

|  |  |
| --- | --- |
| User Permission | Available Actions |
| Viewer | * Read entity * Read sub-entity (if they present) |
| User | * Read entity * Read sub-entity * Create sub-entity |
| Owner | * Read entity * Read sub-entity * Create sub-entity * Update entity and sub-entity |

Once User is added to Entity Members list and he/she has given Permission to that Entity, this User appears at Current Members Table of this Entity and its sub-entities (if present). System sets default Permission level VIEWER, when user just added to member list. This default values can be changed.

User to whom is shared can be deleted from Entity Member list by any user with the OWNER Permission.

1. Entity or sub-entity author is set as an OWNER automatically and cannot be deleted from the member list. Author of the entity where sub-entity was created by other user is added to this sub-entity automatically and cannot be deleted.
2. Once entity access is granted, what actions with the entity is allowed will be determined also by system authorities set in the Role given to this particular User



Clarification of available actions on shared Entities:

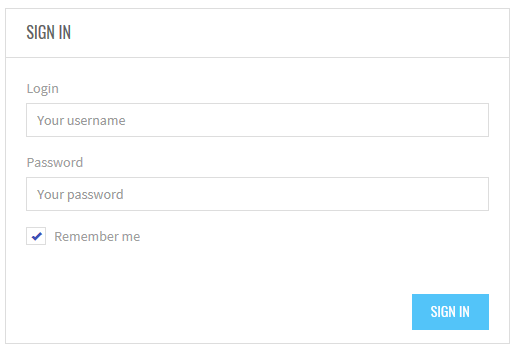
|  |  |
| --- | --- |
| Permission Description | Available Actions |
| Read entity/sub-entity | Read entity/sub-entity |
| Create sub-entity | Create sub-entity (child entity): User can create Notebooks within Projects or Experiments within Notebooks. |
| Update entity | Update entity: User can update Projects, Experiments or Notebooks |

1. Only **Read entity** and **Update entity** are available for the **Experiment**, because it doesn’t have sub-entities and consists of components which are predefined by the chosen Template.

To create a user, refer to the Section 5.1 Users.

# User Interface Basics

## Signing In

The “Sign In” page contains 2 fields:

To sign in to the system:

Enter the user name to the **Login** field. No capitals are allowed in the **Login** field. Capital letters are transferred to low case automatically

1. Each session is active for 30 minutes since you have made the last action. The alert will appear 5 minutes before switching to the login page.

Enter the password in the **Password** field. Password must be at least 6 characters long, contain at least 1 uppercase letter and 1 digit. It cannot contain spaces.

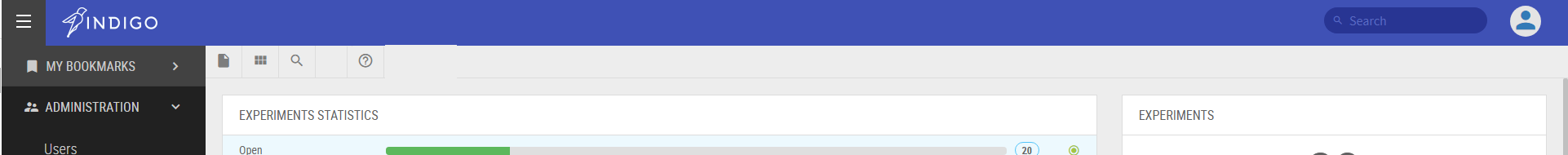
Click the **Remember me** checkbox to save the login and the password in the system. Clicking the Login field invokes the list of previously saved users.

Click “Sign in” button.

The application opens at the Home Page.

## Start Page

### Overview

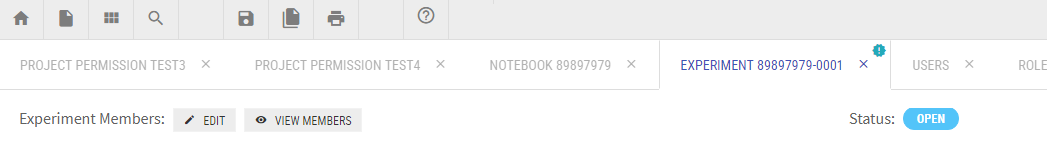
After signing in to the application, the Home Page with user dashboard opens:

The Home Page contains the following elements:

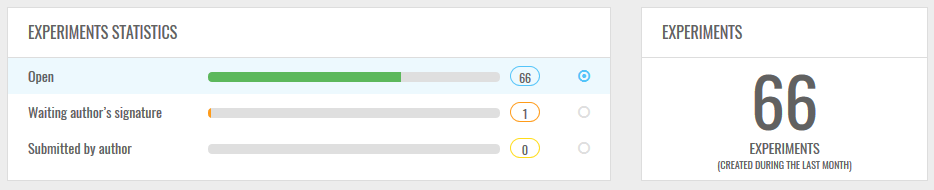
* **Title bar** (**INDIGO**) which includes **Search** field:



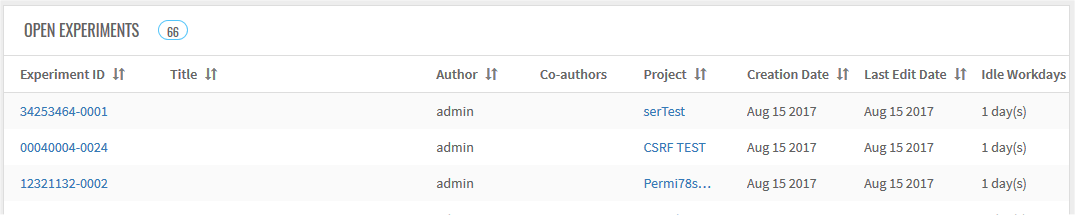
* **Toolbar** (**Menu Ribbon**) consist of icons representing most useful application commands:



**Note**: If several entities were already opened, they appear as tabs below the ribbon, until closed:

* **Navigation Tree** may contain three sections: “My Bookmarks”, “All Projects”, “Administration” (see 3.2.3 Navigation Tree)  
  **Note**: The view of the **Navigation Tree** depends on the Role of the current user (see Section 2.3.1 Roles). For example, the “**All Projects”** menu is available only for users with the “Content editor” authority in the Role.
* **Experiments Statistics** and **Experiments** panes represent statistical information about Experiments created and submitted for Signature Service by current user  
    
    
  Radio buttons to the right side of the items in the **Experiments Statistics** pane allow to choose different experiment queues to be displayed in the bottom Table

**Open Experiments** a table of experiments with “Open” status. This queue is displayed by default



Hovering above Experiment ID link evokes a structure/reaction sketch, in case the Reaction scheme component exists in the current template and is not empty.

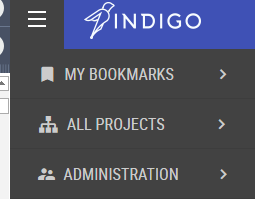
### Toolbar (Menu Ribbon) Icons

**Note**: representation of the Toolbar changes depending on opened Entity and may contain additional buttons. List of all possible buttons displayed below

|  |  |
| --- | --- |
| Icon | Description/Action |
|  | Navigates back to the Home Page |
|  | Opens a drop-down list with commands to create new entities (Project, Notebook, Experiment) |
|  | Opens a drop-down list of opened entities preceded by commands to close entities |
|  | Opens the Search page to specify search criteria and execute search in internal database |
|  | Saves a current entity to the database |
|  | Makes a replica of the current experiment’s components:   * Reaction or Concept Details, * Reaction schema, * Stoichiometry Table, * Experiment Description   In case they exist in the current template.  In case these metrics are empty, the replica will contain the same empty components. |
|  | Print is available also for Project and Notebook – they do not have components |

### Navigation Tree

Navigation Tree may contain maximum three options:



* **“My Bookmarks”** menu contains a tree of projects available for a particular user to edit and review;
* **“All Projects”** menu contains all projects, notebooks and experiments in the system;
* **“Administration”** tab can contains sections “Users”, “Roles”, “Templates”, “Dictionaries” that enables user to manage the system; this section is available for the users with administrative authorities in the Role. See Section 5 “Administration menu” to view all available actions.

Representation of “Navigation Tree” sections strongly depends on authorities provided for a particular User. For instance, the “All Projects” menu is available only for users with the “Content editor” authority.

# Working with Entities

## Manage Projects

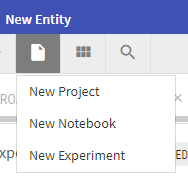
### Create a New Project

The user is able to create new projects using the corresponding button on the ribbon. The Authority “Project creator” is needed to create and edit Projects

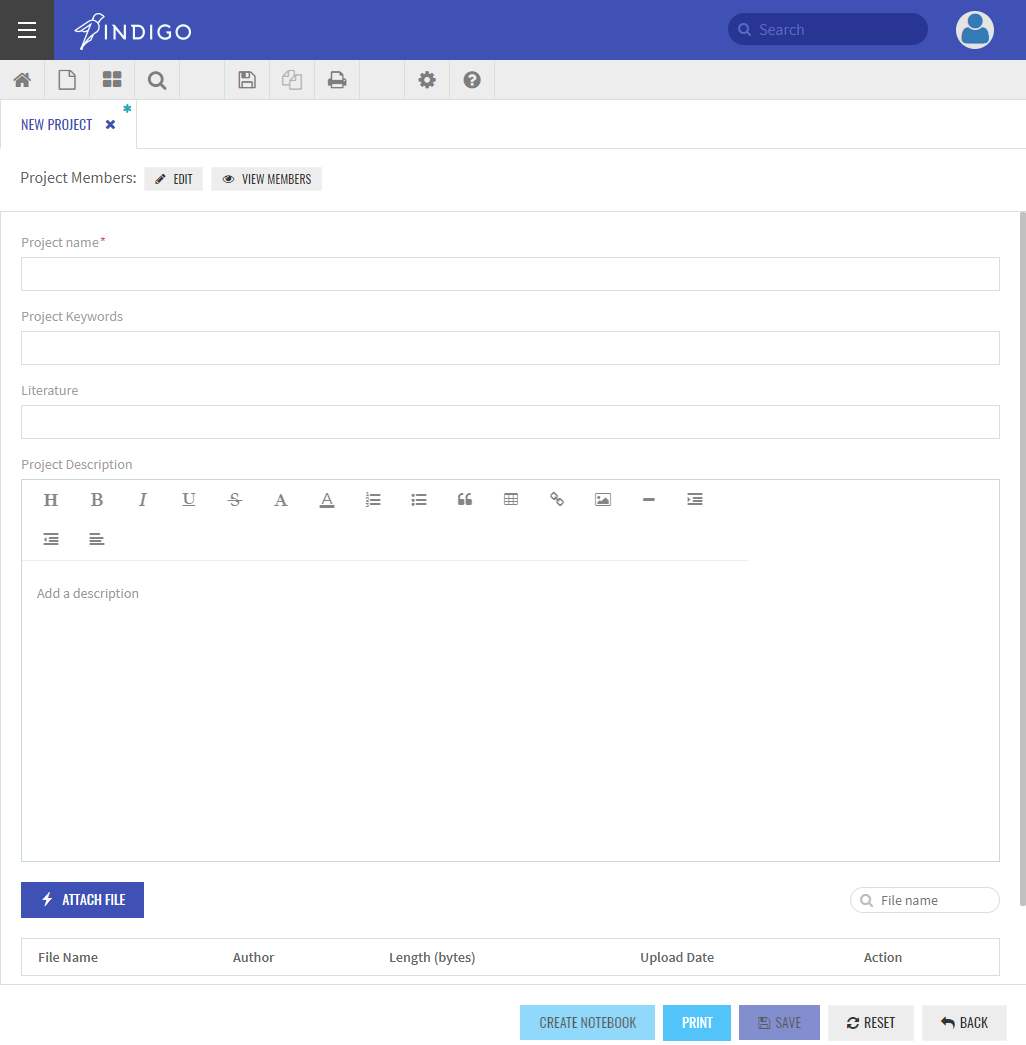
To create a new project:

Click “**New Entity” icon** on the toolbar.

Select **New Project** from the drop-down list.



The “New Project” tab opens displaying set of fields available for Project description



Fill in the following fields:

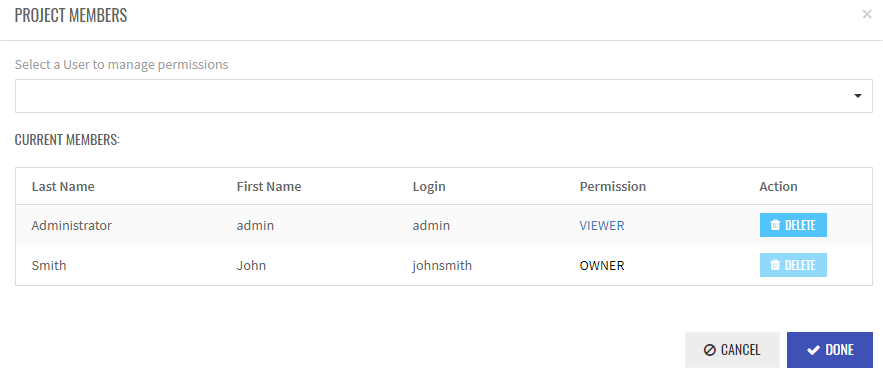
* Project Name (mandatory field)
* Project Keywords
* Literature
* Project Description

**Note**: The “**Save”** button is not active if you didn’t fill in the “Project name” field.

To share the project with other users, click **Edit** button in Project Members section:



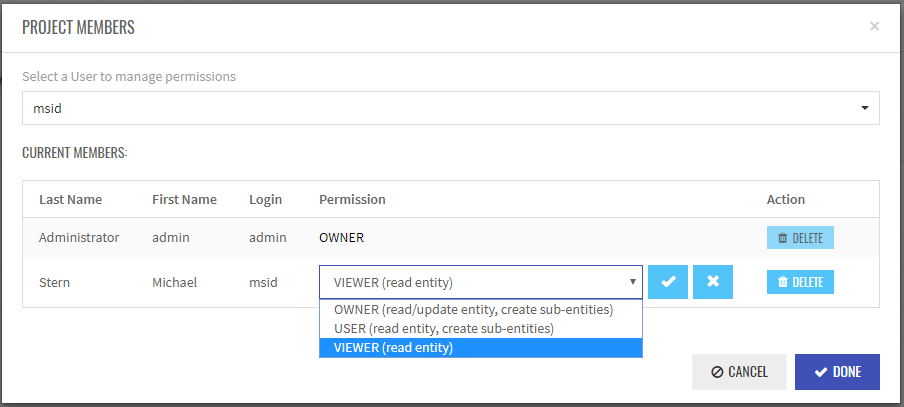
“Project Members” pop up opens:



Select users in the “Select a User to manage permissions” drop-down list, then click “**Done”**. You can select only users that exist in the drop-down list. Start to type user’s name in the text box, or select the user from the list. The new member appears in the “Current Members” Table below.

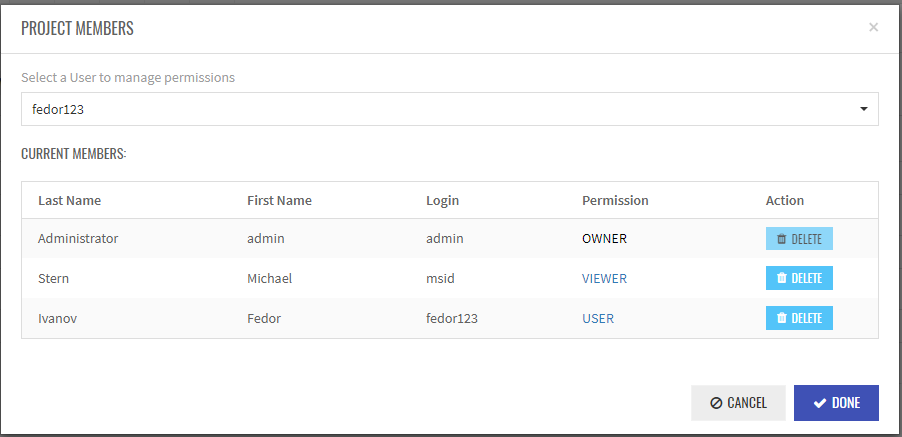
To remove user from the “Current member” table click “**Delete”**.

1. The creator of the project is added to the list automatically with the **Owner** permission by default. You cannot delete this user or edit his permissions.

Click a link in the Permission column to change permissions of the user if needed:

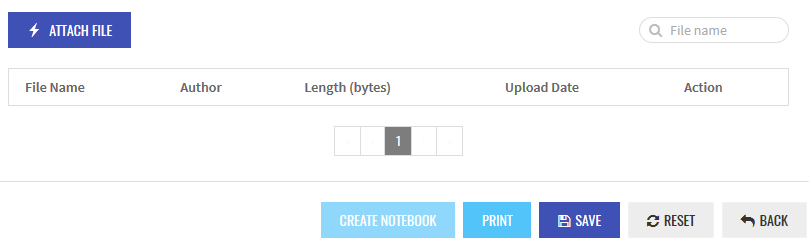
To confirm changes, click “Check Mark” icon, then press “Done” button at the bottom of “Project Members” popup. All permissions will apply to the selected users as soon as you click “**Save” button** on the entity page.

**Note**: The same interface exists for Notebooks and Experiments.

To view the list of current members of the project, click “View Members” button at the “Project Members” Panel. A popup containing “Current Members” Table opens 

Click “**Save” button on the bottom of the page** to save the New Project.

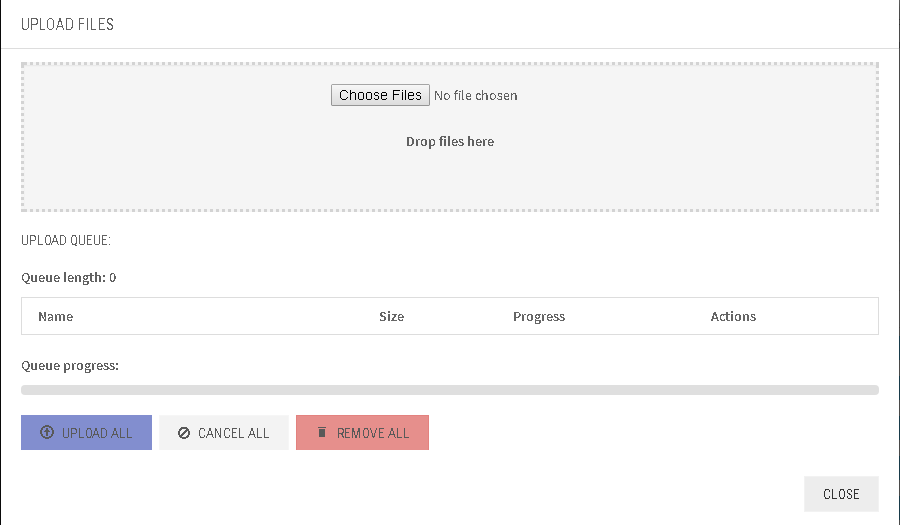
In the Project tab, click “**Attach File” button** to attach files to the project.

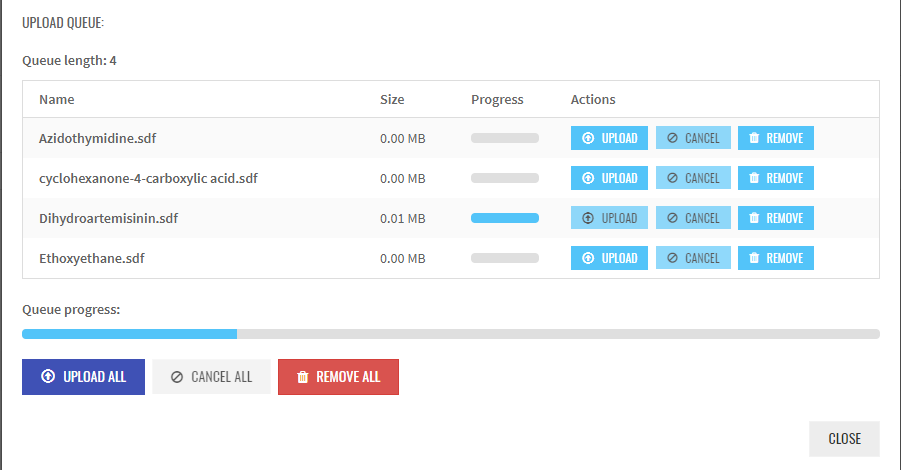


The “Upload Files” pop up opens.

1. In case you did not save a project, the alert appears:



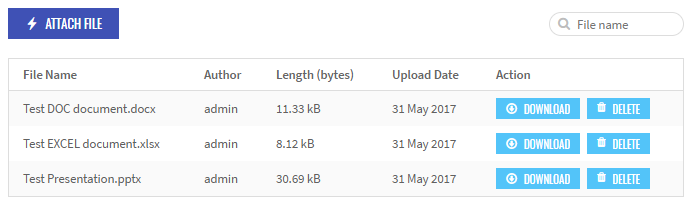


Click **Browse** or drop files to the selected area. The uploaded files appear in the Upload Queue.

Click “**Upload”**, “**Cancel”**,or “**Remove” button** to upload, cancel or remove one selected file.

Click “**Upload All”**, “**Cancel All”**, or “**Remove All” button** to upload, cancel, or remove all files from the queue.

Close the window.

New files appear in the table below the “**Attach File”** button after uploading files.  


You can select either the “**Download”** or “**Delete”** buttons to perform corresponding actions.

Click “**Create Notebook” button** to create a sub-entity. See 4.2 “Manage Notebooks” section to find information about this entity.

### Edit Project

To edit a project:

1. Click the project name in the projects tree in the Navigation Tree. The project’s tab opens.
2. Edit the desired fields.
3. Click “Save” button to save changes.
4. Click “Print” button to send the project to a \*.pdf file. If checkbox “Print attached PDF” is checked in “Print Settings” popup it will result in all attached to the Project PDF files to be added to the PDF file of the Project

Click “Create Notebook” button to create a New Notebook. See Section 4.2 “Manage Notebooks” to find an information about this entity.

1. There is no possibility to delete an existing project.

## Manage Notebooks

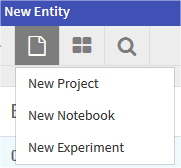
### Create New Notebook

The user is able to create new notebooks using the “New entity” icon on the toolbar or by clicking the “**Create Notebook”** button on the bottom of opened project page. The Authority “Notebook creator” is needed to create and edit Projects

If there are no projects in the projects tree yet, the user should create a project first.

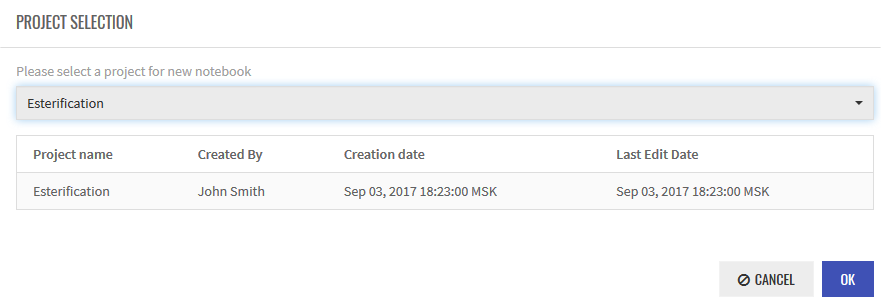
To create a new notebook:

1. Click “**New Entity” button** on the toolbar.
2. Select “**New Notebook”** from the drop-down list.

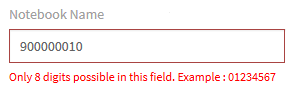


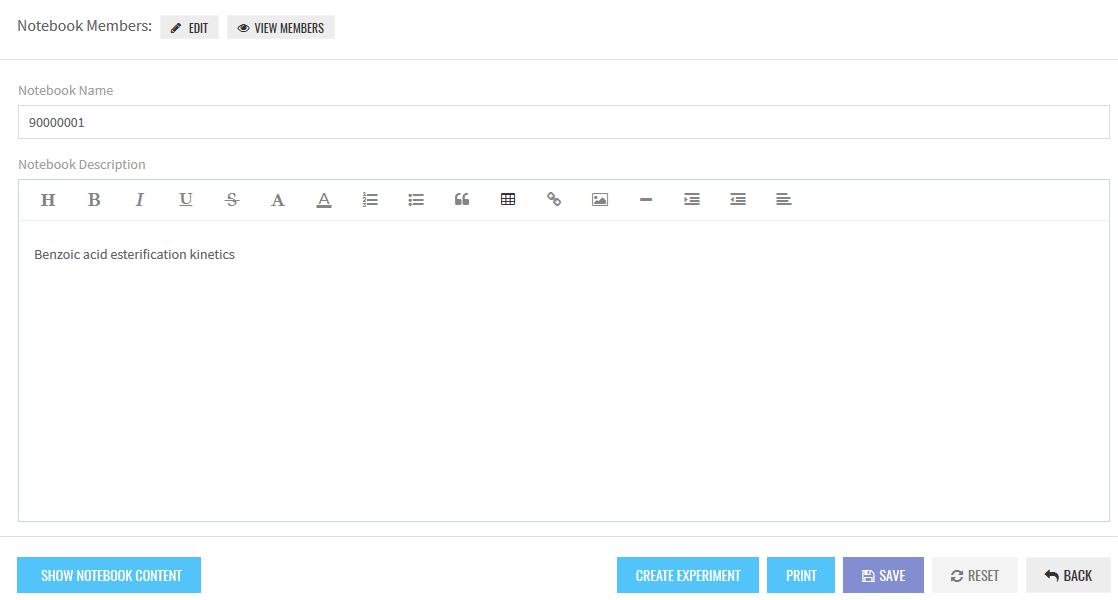
You must assign a new notebook to an existing project. The “Project Selection” popup opens.

1. Select a project from the drop-down list. The information on the project appears in the table below.



1. Click “**OK”**. The “New Notebook” tab opens.
2. Fill fields on Notebook page. Type the notebook name in the text field.
3. The notebook name should be a unique 8-digits number.

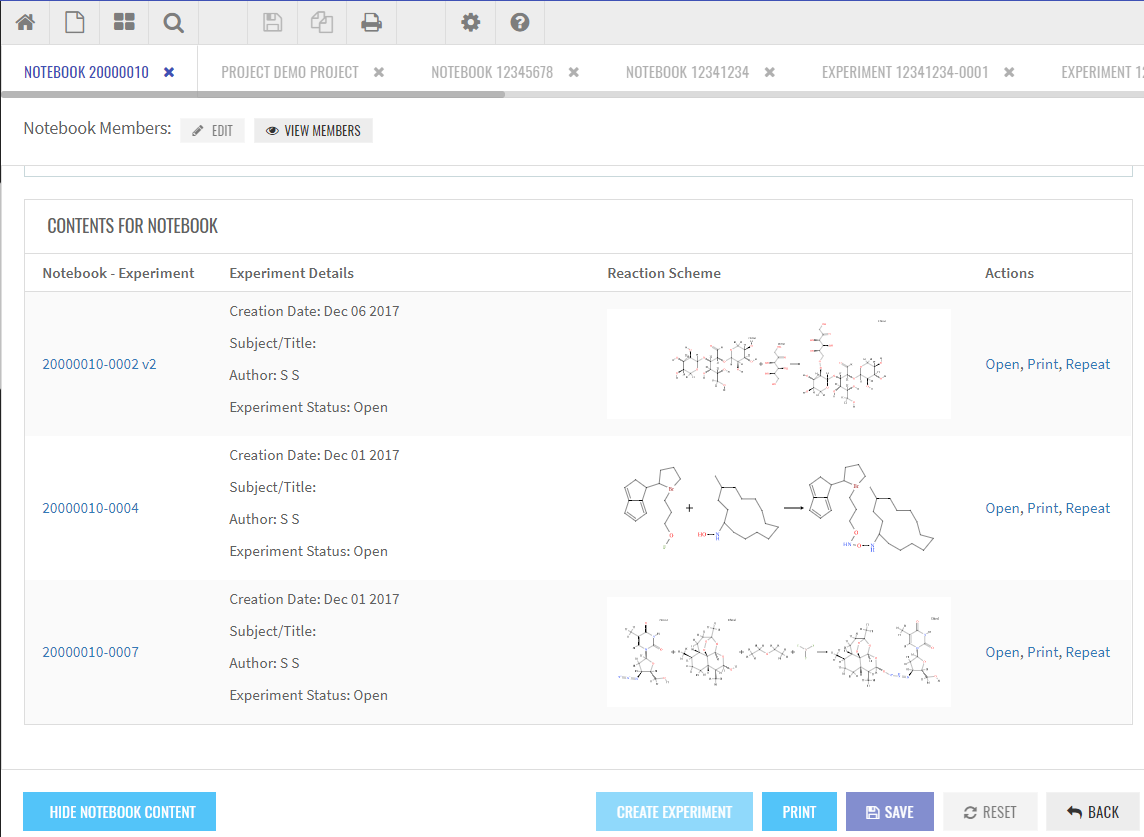


Type the notebook description in the text field.

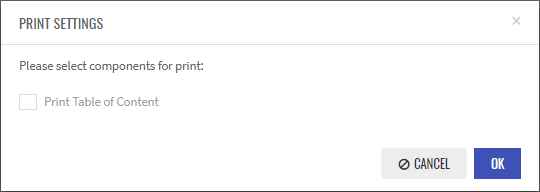
1. Click “**Save”** button to save the new Notebook.

Click “**Create Experiment” button** to create a new sub-entity. See Section 4.3 to find information about this entity.

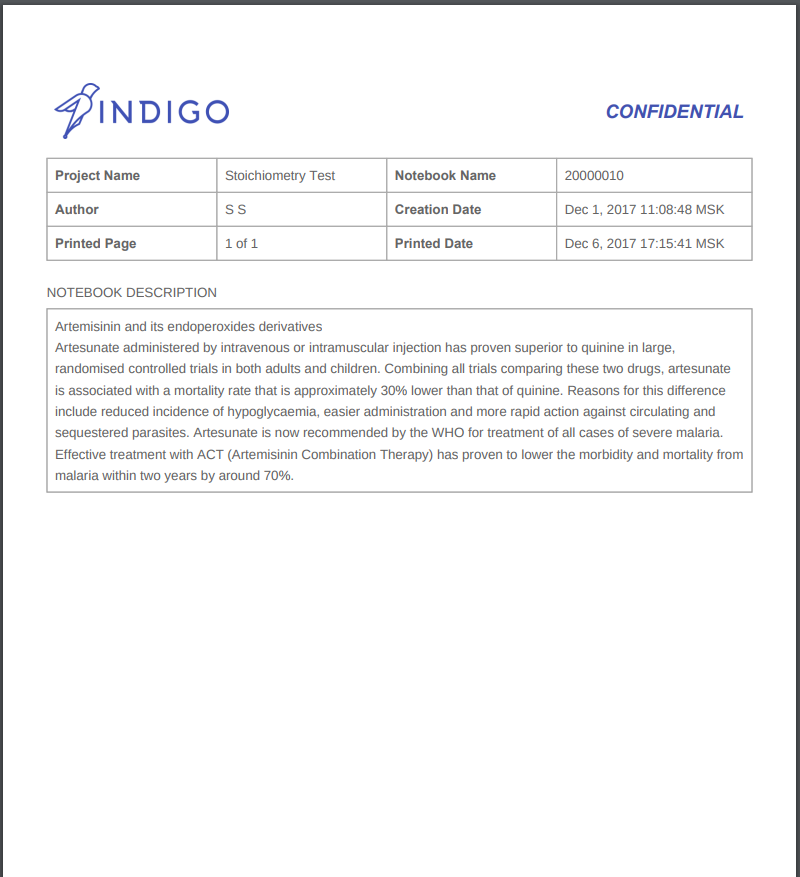
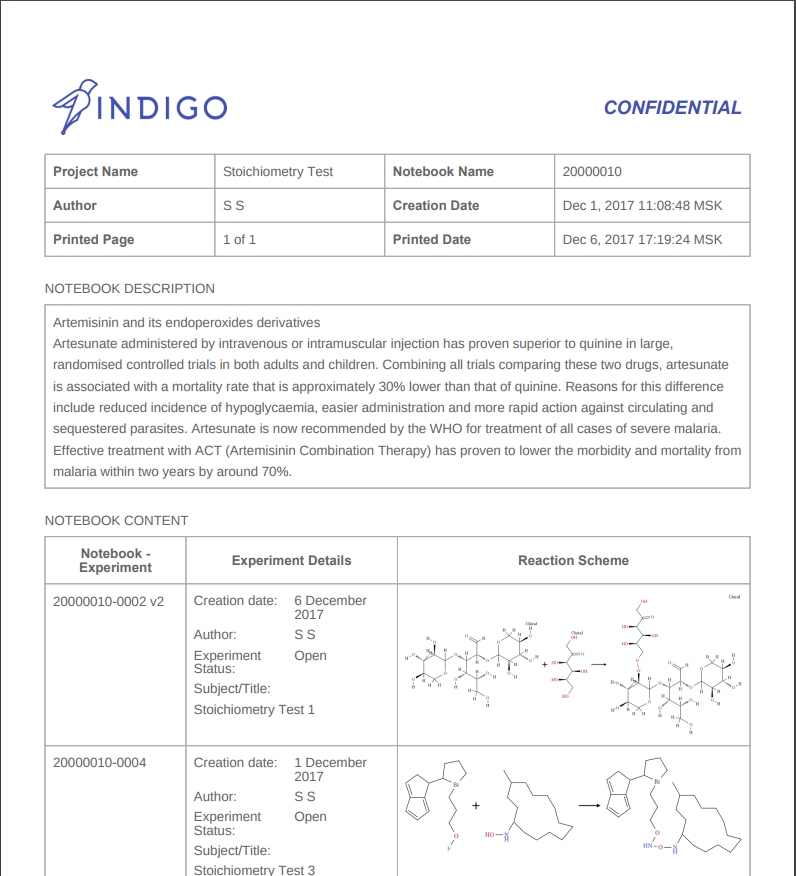
Click “**Show Notebook Content” button** to view the “Contents for Notebook” Table.



1. Click “**Print”**. The “Print Settings” pop up opens.



Mark if you want to print a “Table of Content”. Otherwise the document will contain notebook general information and description only.

1. Click “OK” button.

### Edit Notebook

To edit a notebook:

1. Click the notebook name in the projects tree of the Navigation Tree.
2. Edit the required fields.
3. There is no ability to edit notebook’s name in case there is at least one Experiment containing a Batch was created or there is at least one experiment in Non Open status
4. Click “**Save” button** to save changes.
5. Click “**Create Experiment” button on the bottom of the Notebook page** to create an experiment. See Section 4.3 Manage Experiments to find information about this entity.
6. There is no ability to delete an existing notebook.

## Manage Experiments

### Create a New Experiment

The Authority “Experiment creator” is needed to create and edit Experiments. There are several ways to Create a New Experiment:

Press “New Entity” icon in the Toolbar

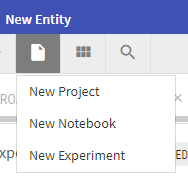
Press “Create Experiment” button on the bottom of Notebook Page

Press “Action” button on the bottom of Experiment page and select “Repeat Experiment” option (see 4.3.3 “Experiment Workflow”)

1. If there are no projects or no notebooks in the projects tree yet, the user should create a project first and then a notebook for this project.

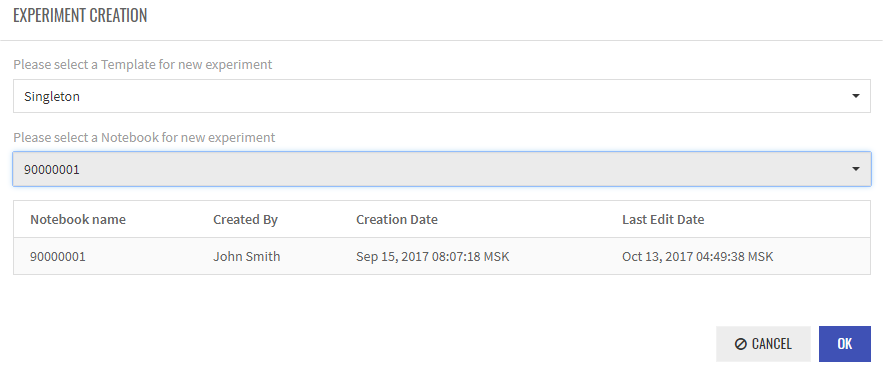
To create a new experiment:

1. Click **New Entity** on the toolbar.
2. Select **New Experiment** from the drop-down list.

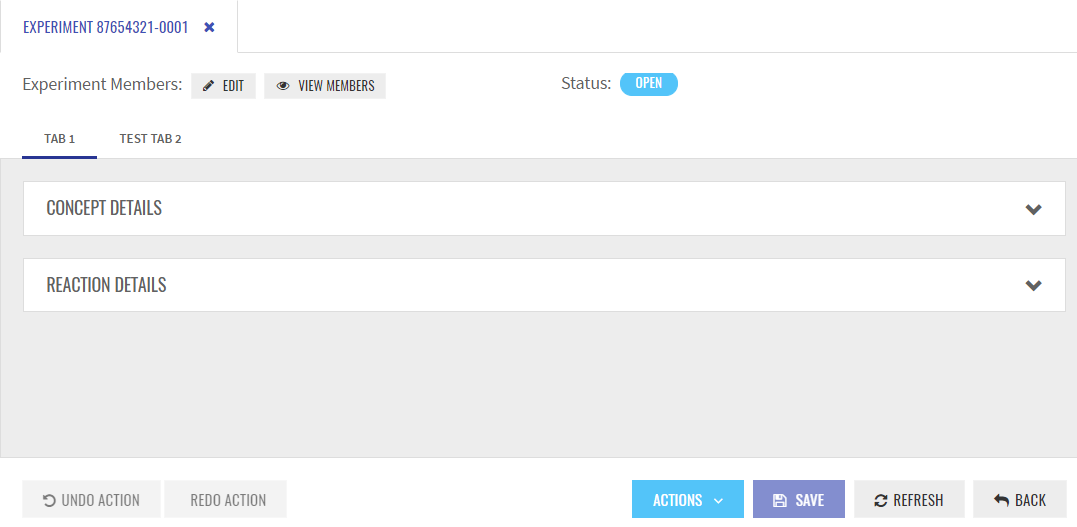


The “Experiment Creation” popup opens.

1. Select a template from the drop-down list. See Section 5.3 for the information about experiment templates.
2. Select a notebook for the new experiment. The information about the notebook appears in the table below.



1. Click “**OK”**. The new experiment opens in a tab containing components of the template.



1. The experiment name is composed of the name of the notebook and the serial number of the experiment: ‘notebook\_name-experiment\_serial\_number’. This name is displayed on table name.

Set of components in Experiment corresponds to the selected template.

1. Fill in the necessary fields of the experiment components.
2. Click **Save**.

### Edit an Experiment

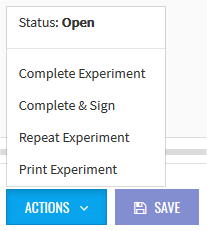
To edit an experiment:

1. Click the experiment name in the projects tree. The experiment tab opens.
2. Edit the necessary fields.
3. Click “Save” button.
4. Click “**Actions” button** to manage the experiment status. See Section 4.3.3 to see information about available experiment statuses.
5. There is no ability to delete an experiment.

Experiment Workflow

Experiment can be in several statuses: Open, Completed, Submitted and Archived. Each Experiment status allows to execute defined set of Actions.

**Note**: Status Submitted, and Archived are available if application is integrated with Signature Service



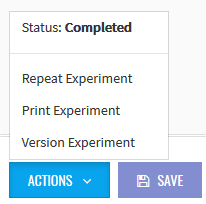
The following actions are available in “Action“ menu:

* Complete Experiment

When you click Complete Experiment, the confirmation window opens. Click “Submit”. The experiment status changes to the Completed. The experiment is non-editable. This option is used to finish an Experiment and to prohibit its further editing.

Click “Complete Experiment”, press “Submit” to confirm.

This Experiment can be Repeated, Versioned and Printed.

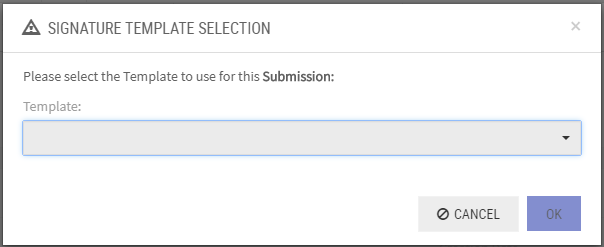


* Complete & Sign

If application is integrated with Signature service experiment can be completed and signature stamp set to the pdf report. This document will be saved and available for review in Indigo ELN To sign the document:

Click “**Complete & Sign”** in the “Actions” button drop-down list. The confirmation window opens.

Click “**Submit”**.

The Signature Template Selection window opens. Select the signature template from the drop-down list.

The experiment status changes to “Submitted”. The experiment is not editable, No further changes can be done to the Experiment. This Experiment can be Repeated, Versioned and Printed.

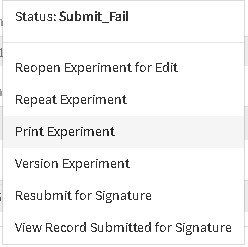
The Sign process contains a few steps. All steps are dome in Signature service but each new steps results in new experiment status, Indigo ELN shows these statuses:

Submitted

Signing

Submit\_Fail

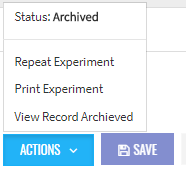
Set of Action for all of them is the same as for Completed status. Status “Submit\_Fail” has extended set of Actions:



“Reopen Experiment for Edit” make current Experiment with a status Open again. All previously entered data are saved.

“Resubmit for Signature”- allow to send the same version of the experiment to Signature service, Signature process is started from initial point in this case.

As soon as all members have completed signing, the experiment status changes to Archived.



* Repeat Experiment

When you click **Repeat Experiment**, the system creates a new experiment based on the current template with the corresponding serial number. In case the current template contains the following components:

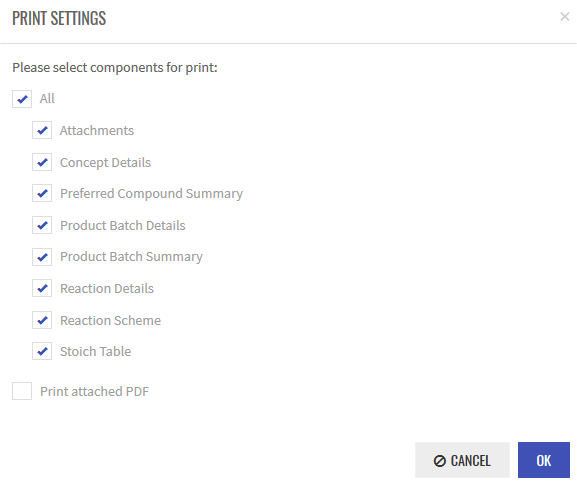
* Experiment Details
* Concept Details
* Reaction schema
* Stoichiometry Table
* Experiment Description

the new experiment will contain its’ content.

* Print Experiment

When you click “**Print Experiment”**, the “Print Settings” pop-up with a list of experiment components appears.

Select components to be printed.

1. The pop-up contains components available for current template.
2. There could be different attachments, but the application is able to print \*.pdf files only.

The PDF file downloads to the user’s computer .

* Version Experiment

When you click Version Experiment, the system copies all experiment content to the second version of the experiment. The first version gets additional v1 to the name. The second version gets additional v2 to the name etc. Status of the new experiment is Open. This option can be used to make a version of completed Experiment. Only one version for every Experiment is available. The next version can be created on the base of completed previous version.

1. The **Version Experiment** button is available in case experiment has not Open status (for example, Completed).

* View Record Submitted for Signature

When you click **View Record Submitted for Signature**, the PDF file downloads to the user’s computer.

## Components

Components are the sample forms for different aspects of experiments. These forms are combined in any order into experiment templates.

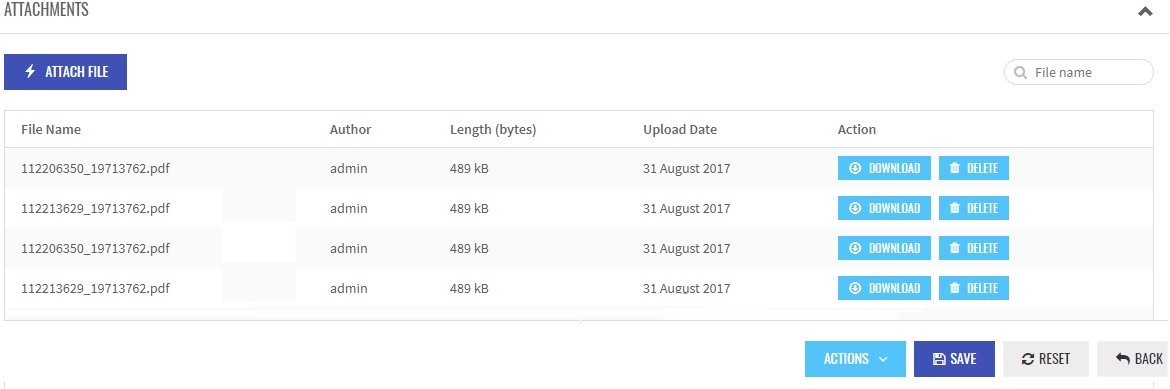
The following components are available in the system:

* Attachments
* Batch Structure
* Concept Details
* Experiment Description
* Preferred Compound Details
* Preferred Compound Summary
* Product Batch Details
* Product Batch Summary
* Reaction Details
* Reaction Scheme
* Stoichiometry Table

The following sections describe available components in the alphabetical order.

### Attachments

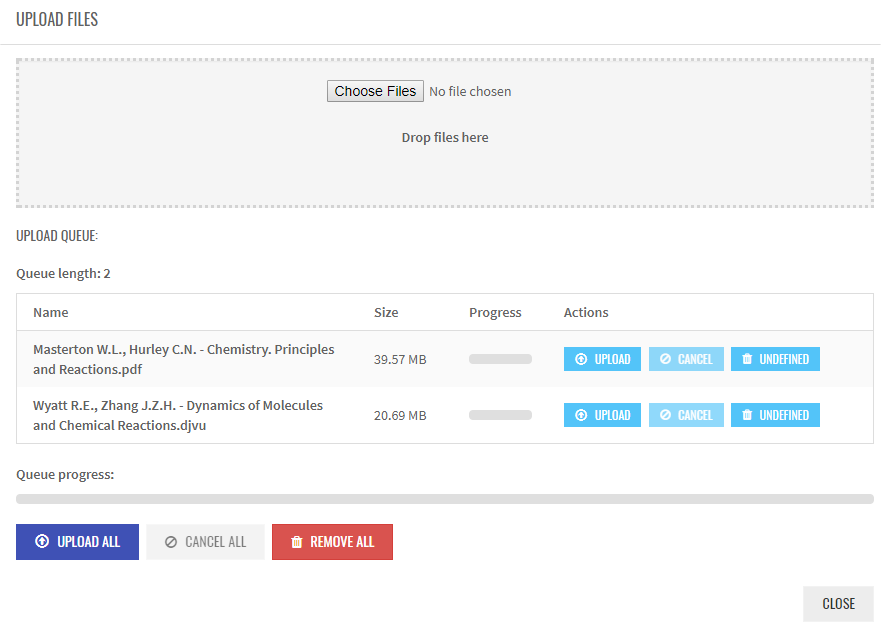
Allows to manage attachment of any kind of files related to this experiment.



To attach files to the experiment:

Click **Attach File**, which invokes the Upload Files popup.

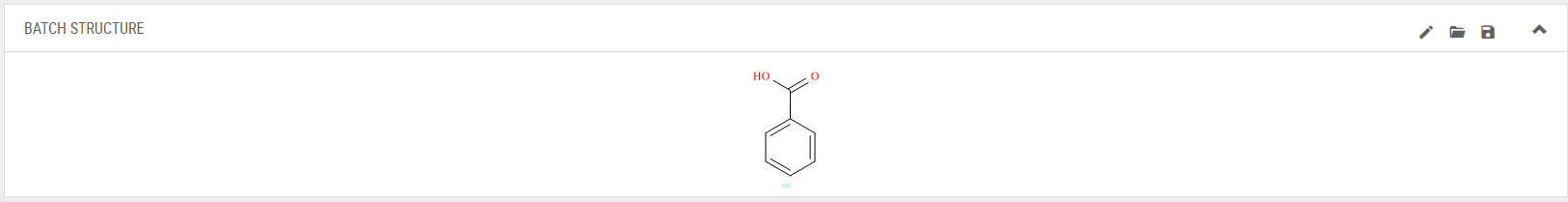
Click **Choose Files** to select required files from the computer.



Click **Upload All** or **Upload** to add files to the experiment, then click **Close**. The files will appear in the Attachments component.

### Batch Structure

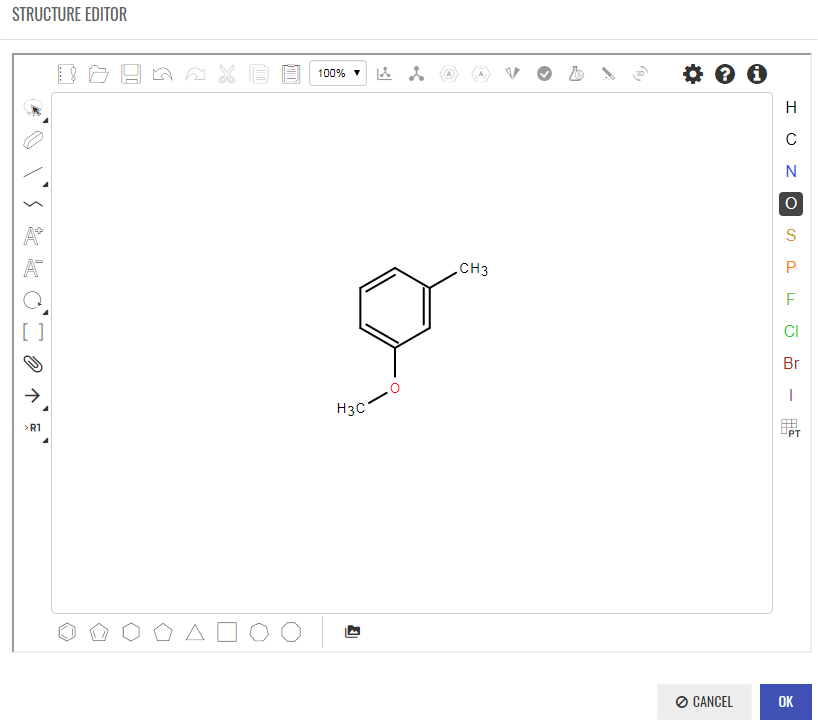
Allows user to draw, import, and export a batch structure.



To create the batch structure:

Click . The Structure Editor opens. See Ketcher user guide for the description of the Structure Editor.

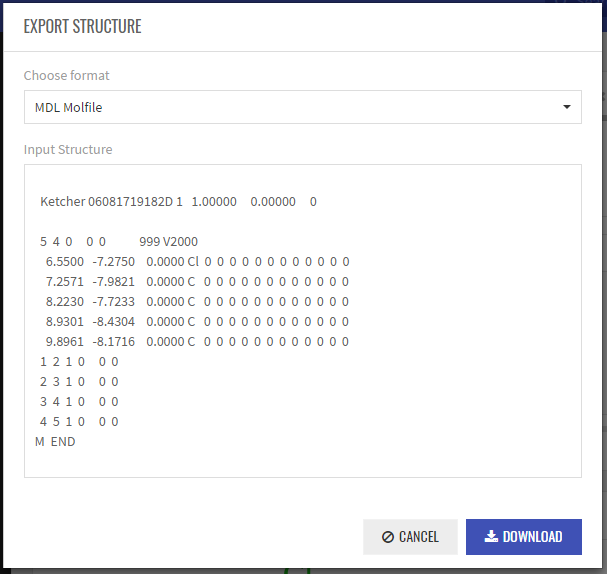
Create the structure and click **OK** to save the structure or **Cancel** to cancel the creation.



The structure appears in the Batch Structure component.

To export the batch structure:

Click . The Export Structure dialog opens.

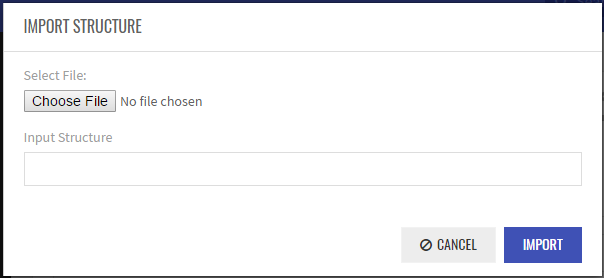


By default the file format is MDL Molfile.

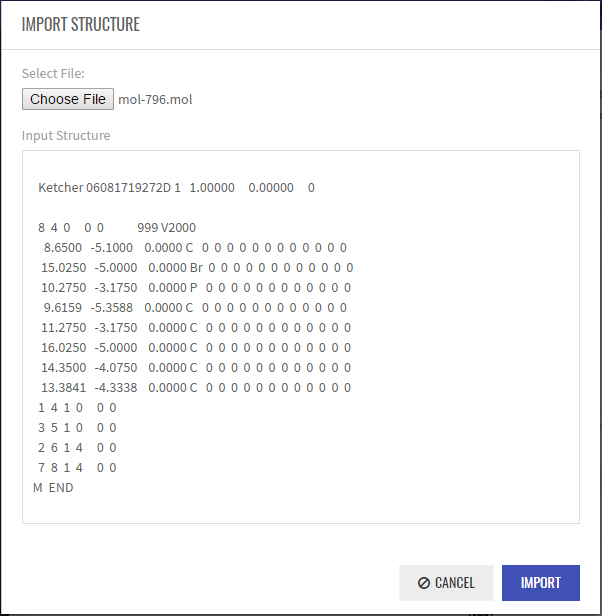
Click Download. File will be saved to default Downloads folder

To import a batch structure from the local drive:

Click . The Import Structure popup opens.



Choose the \*.mol file from the local driver. The structure preview appears in the Import Structure dialog below.

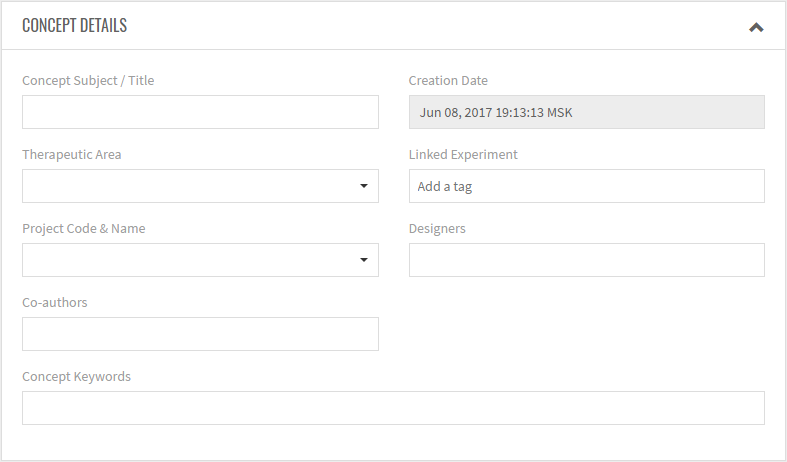


Click **Import**.

Structure appears in “Batch Structure” compound and its Mol Weight and Mo Formula are transferred to “Product Batch Details” and “Product Batch Summary” components if they are added to experiment template

### Concept Details

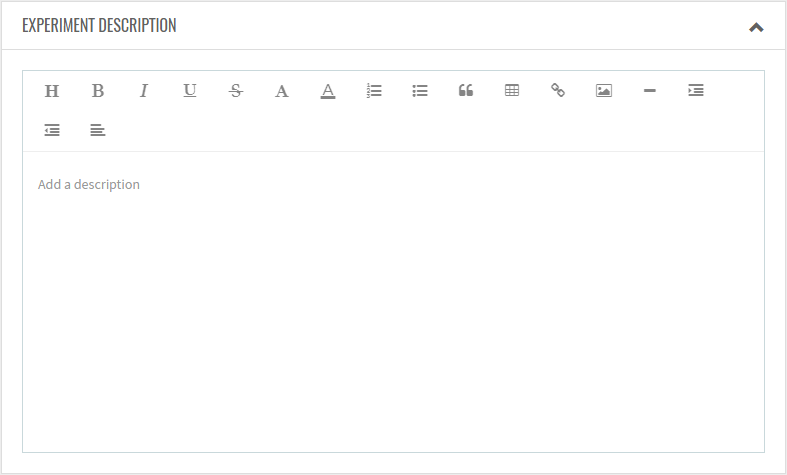
Allows a user to specify or select Concept Subject/Title, Therapeutic Area, Project Code & Name, Co-authors, Designers, Keywords, and Linked Experiments.



1. The Creation Date field is not editable.
2. The Therapeutic Area and Project Code & Name drop-down lists contain data from the corresponding dictionaries.

### Experiment Description

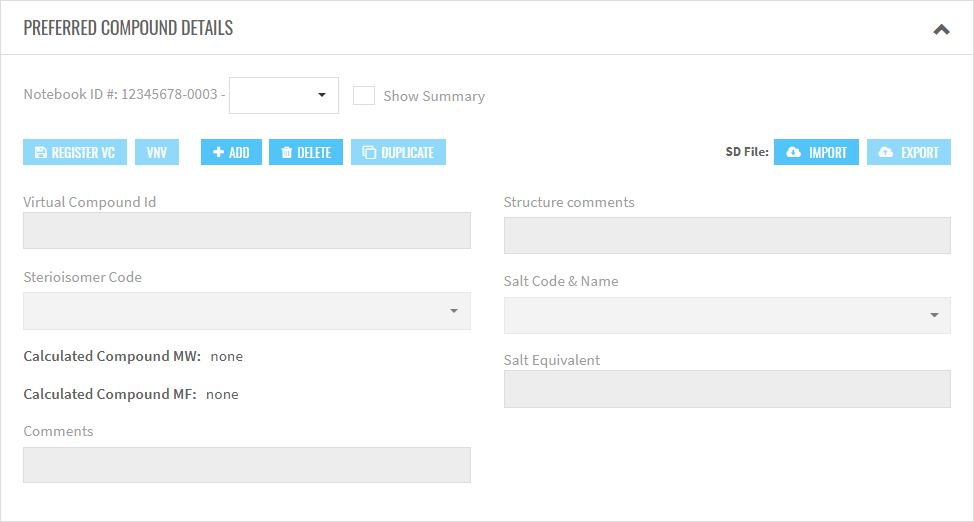
Contains a common text editor with the possibility of text formatting, inserting tables.

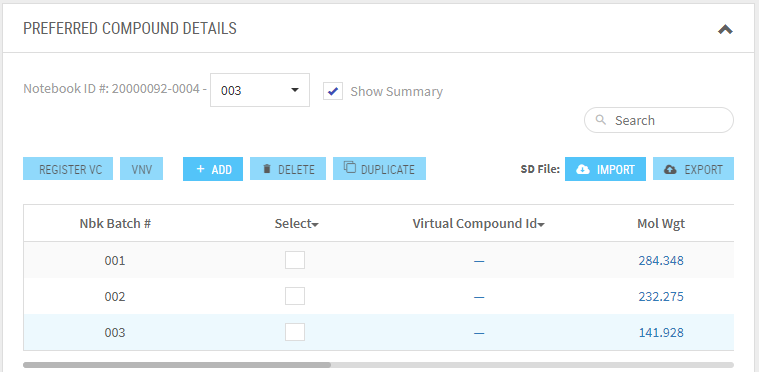


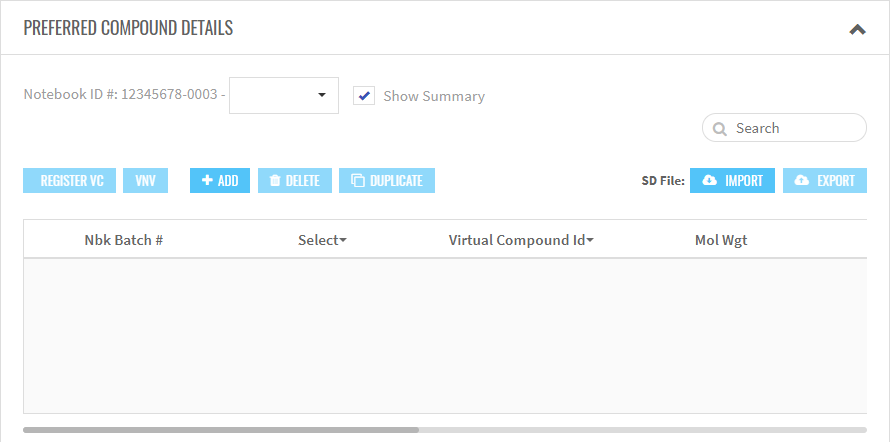
Click the text field to type like in other word processors: describe the procedure of the experiment, insert tables

### Preferred Compound Details

Provides details for an individual compound. Allows user to review, create, and edit batch details: Stereoisomer code, Comments, etc. Virtual Compound Registration (if allowed) is also executed here.



Select the **Show Summary** checkbox to show also the Preferred Compound Summary component below. You will be able to review compound in the table representation.

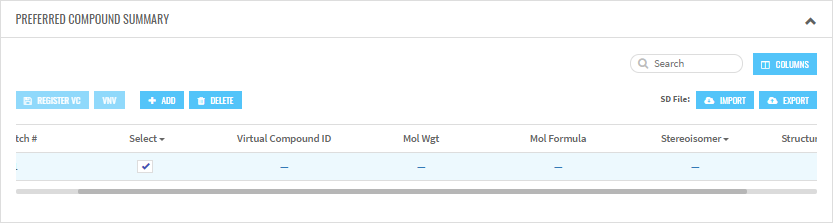


Fill in the Virtual Compound Id, Structure comments, and Comments text fields.

Select the Stereoisomer Code from the drop-down list.

### Preferred Compound Summary

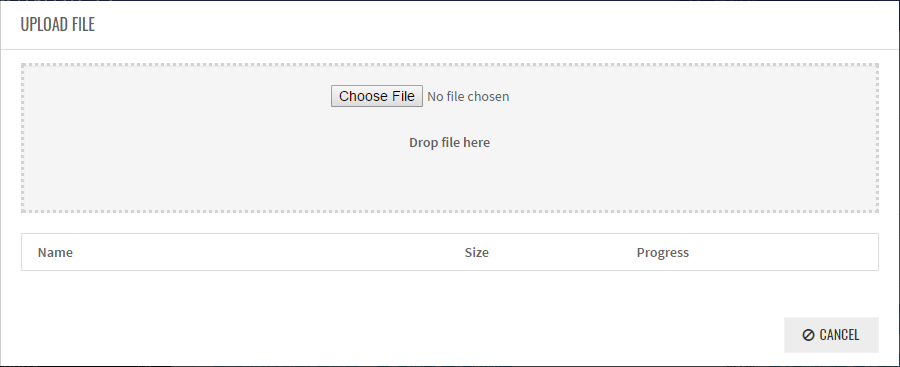
Allows user to review, create and edit compounds details in table: Stereoisomer code, Comments, etc. Virtual Compound Registration (if allowed) is also here.



* Click **Add**. The new row appears in the table.

To import an SD file:

Click **Import**. The Upload File window opens.



Choose an \*.sdf file from the computer or drop it to the area. The new files appear in the table.

Click **OK**. System adds new batches to the table; batches contain structures from the SD file and any properties assigned to these structures in the SD file.

To delete a compound:

Select the row. The **Delete** button becomes available.

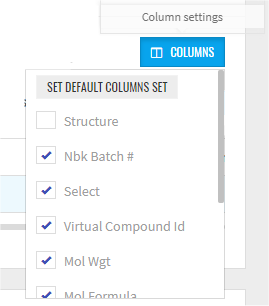
Click **Delete**. The row disappears from the table.

To create an SD file:

Select the row. The **Export** button becomes available.

Click **Create SD File**. The \*.sdf file downloads to your local computer.

Click **Columns** to manage columns settings.



Click **VNV** to verify the designated stereoisomer code and the same existing batches in the system.

1. By default the **VNV** button is available for those customers who have a special service, so that Indigo ELN application can integrate with it.

### Product Batch Details

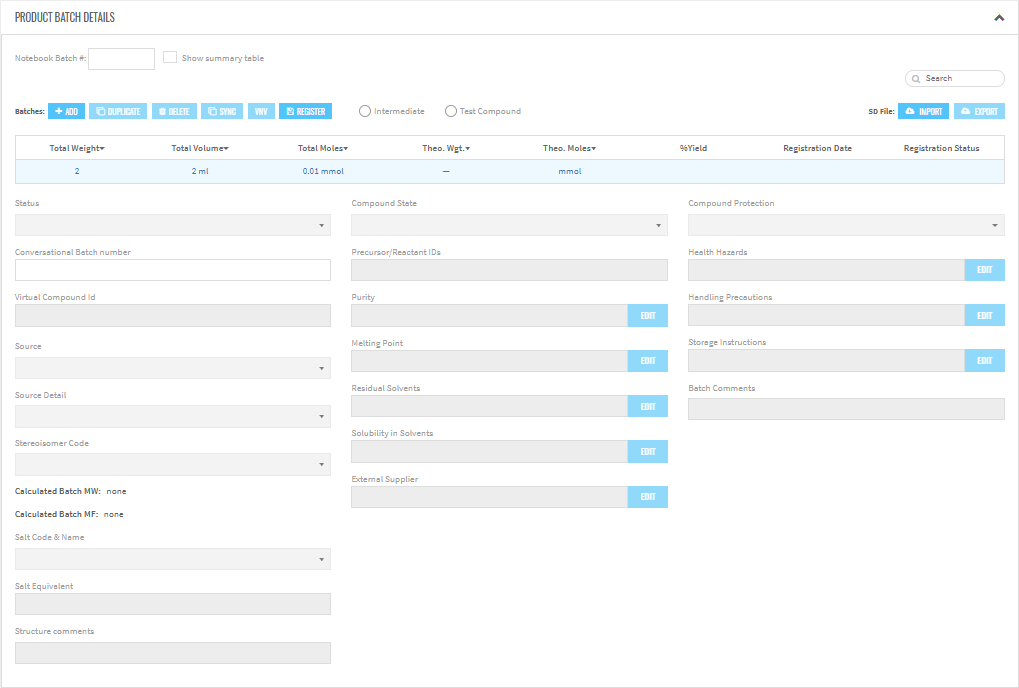
Provides details for the individual batch. Allows user to review, create, and edit batch details: Total amount weight, Yield%, Stereoisomer code, Purity, Solubility, Hazards, etc. Batch Registration (if it is allowed) is also executed here. Batches can be added by “Add” button, duplicated by “Duplicate” button, added by synchronization with Intended Reaction Products section of Stoichiometry Table using “Sync” button and imported from local .sdf file by “Import” button

Batch can be deleted by checking “Select” in Summary Table (“Show summary table” need to be checked) and pressing “Delete” button.

**Note**: registered batches cannot be deleted

For more information see 4.4.8

1. You can see Product Batch Summary Table in case you select the **Show summary table** checkbox.



Select the compound status: Intermediate or Test Compound.

Edit the fields and click **Save**.

1. The Product Batch Details table contains the Theo. Weight and Theo. Moles from the Stoichiometry Table. The user should enter manually the real amounts of the batches. System calculates **%Yield** according to the provided amount and theoretical value.

Fill in the following fields:

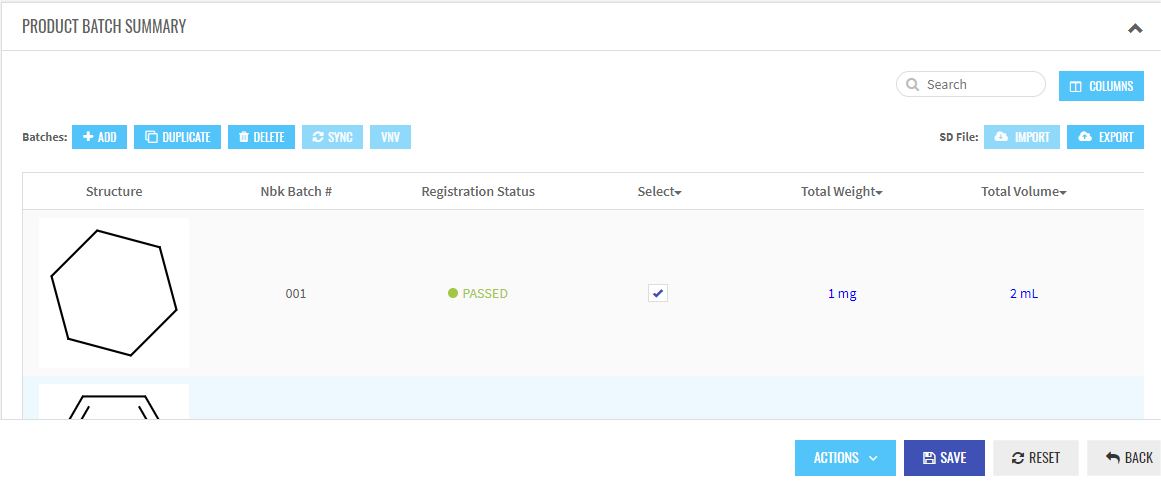
* Source, Source Detail, Stereoisomer Code, Salt Code & Name, Salt Equivalent, Structure comments, Compound State, Compound Protection, Batch Comments. See Section 2.3.6 for information about this fields.

1. Status, Virtual Compound Id fields are not for manual enter, can be populated by customer related information.

### Product Batch Summary

Represents all batches in a table format. Allows user to review, create, and edit batch details.

* Click **Columns** to select properties to be displayed, e.g. Total weight, %Yield, Stereoisomer code, Purity, Solubility, Hazards, etc. Batch Registration (if it is allowed) is also executed here.



To add a new batch:

* Click **Add**. The new batch appears in the table.
* Click **Sync**to create a batch for each intended product on the right of the reaction arrow.

1. The new row contains the populated structure field, Mol Weight and Formula. The Salt Code and EQ fields will contain information in case you have assigned these fields to the Indented Reaction Product.

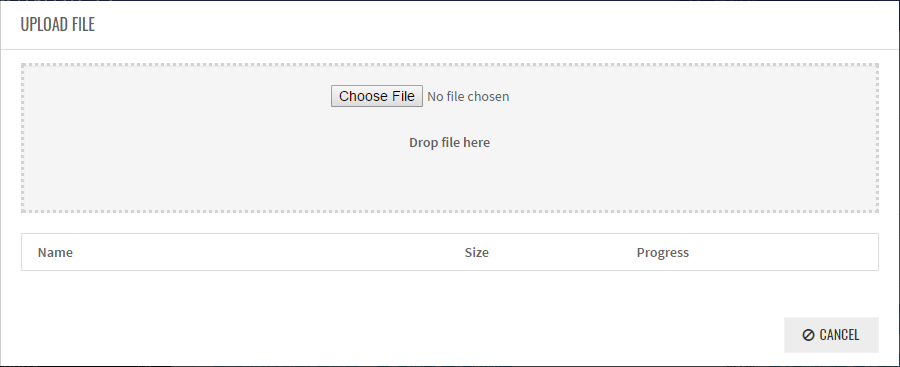
To duplicate or delete a batch:

* Click the check box in the Select column. The **Duplicate** and **Delete** buttons in the component become available.

1. You cannot delete registered Batches.

To import an SD file:

Click **Import**. The **Upload File** dialog opens.



Choose a \*.sdf file from the computer or drop it to the area. The new files appear in the table.

Click **OK**.

The new row appears in the Batch Summary Table. The new row has the Structure and other fields filled in, in case they exist in the selected file. The new structure of the new batch appears in the Batch Structure component.

To Register Batch(es):

Select a batch;

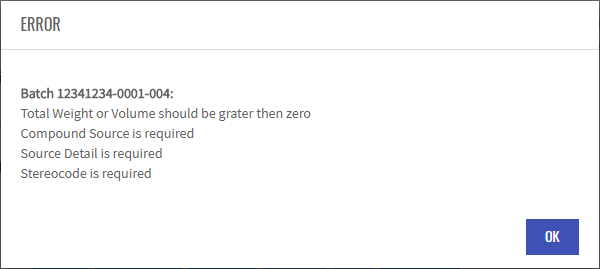
Fill in all necessary fields:

* Total Weight
* Source
* Source Details
* Stereoisomer code
* Structure comment for some Stereocodes
* Salt Code and Salt EQ (if needed)

Click **Register**.

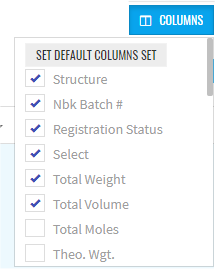
The system saves the experiment automatically. The batch gets the In Progress status. In case of successful registration the registration gets the Pass status. The registration date field contains the todays date and assigned Conversational Batch number.

1. The system shows the error message in case the registration failed.
2. In case there are empty mandatory fields, the error message appears.



1. The user can send several batches to registration.
2. The **Register**button is available in case the system has integration with the external Registration service.

Click **Columns** to select columns for display.



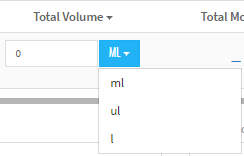
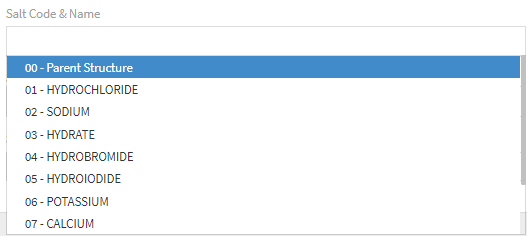
Fill in the batch fields:

1. The following fields have the drop-down list of the possible values:

Total Weight, Total Volume, Total Moles, Theo. Wgt., Theo. Moles, Compound State, Salt Code, Stereoisomer Code, Source, Source Detail, Compound Protection, Intermediate/Test Compound.

1. The following fields have the pop-up windows:

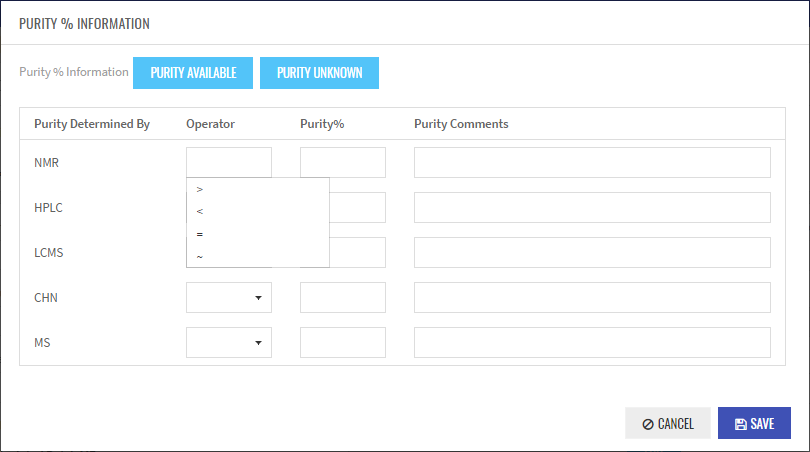
Purity, Melting Point, External Supplier, Health Hazards, Residual Solvents, Solubility in Solvents, Storage Instructions, Handling Precautions.

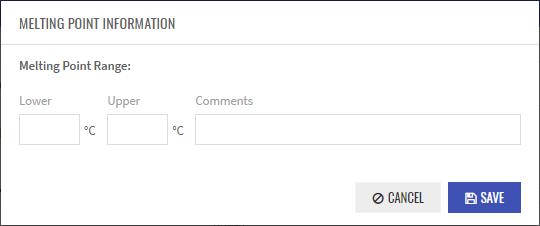
Some fields have the drop-down list of the possible units and text field. The data in the text field changes depending on the selected unit.

The following fields have the pop-up window:

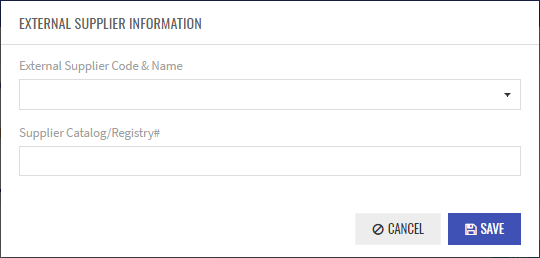
* Purity. To change the set of the possible analyze methods see Section 5.4 Dictionaries.



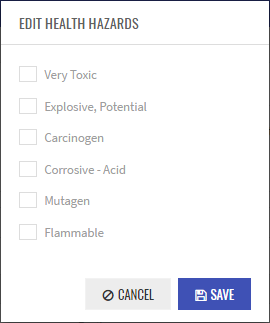
* Melting Point



* Ext Supplier. To change the set of the possible supplier codes or analyze names see Section 5.4 (Dictionaries).



* Hazards. To change the set of the possible hazards see Section 5.4 Dictionaries.

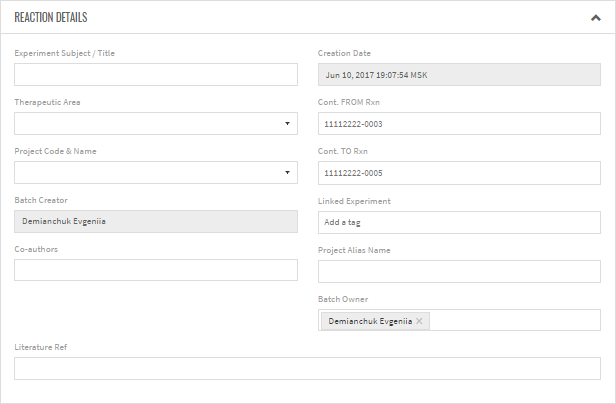


Click **VnV** to verify the designated stereoisomer code and the same existing batches in the system.

1. By default the **VNV** button is available for those customers who have a service for Stereocode validation, so that Indigo ELN application can integrate with it.

### Reaction Details

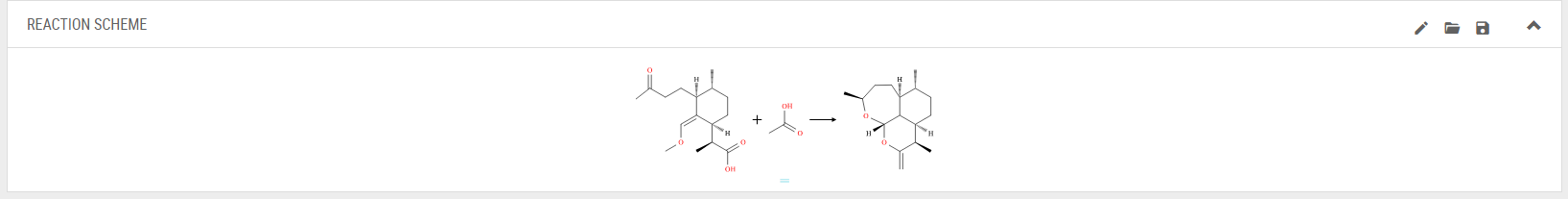
Allows user to specify Title, Therapeutic Area, Project Code, Co-authors, Literature References, Keywords, Link to Previous “Cont. FROM Rxn” and Future “Cont. to Rxn” Experiments, and Link to any Experiment.



1. The Creation Date field is not editable.

### Reaction Scheme

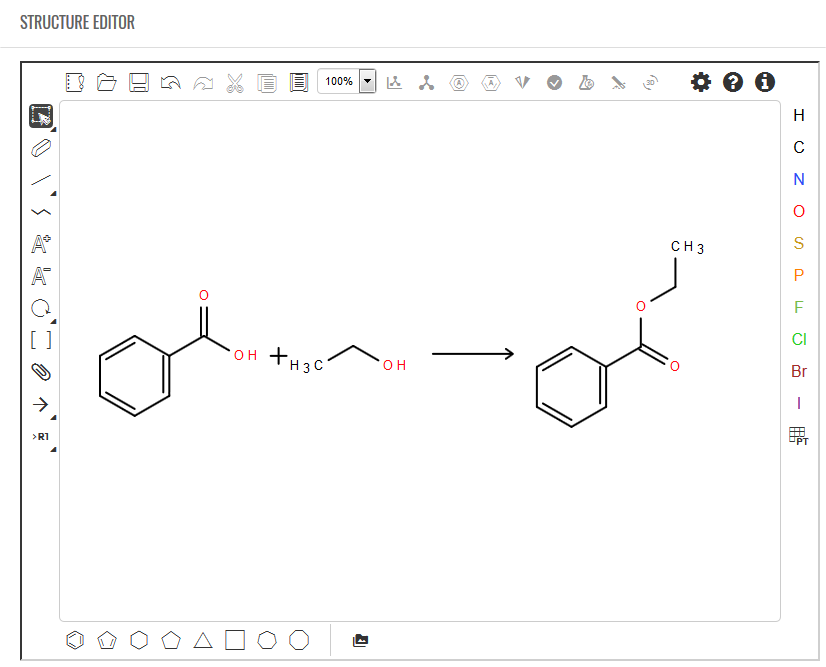
Allows user to draw, import, and export a reaction scheme.



To create the reaction scheme:

Click . The Structure Editor opens.

Draw the structure using the editor’s toolbars and click to clear the canvas.



To export the reaction scheme:

Click . The Export Structure window opens.

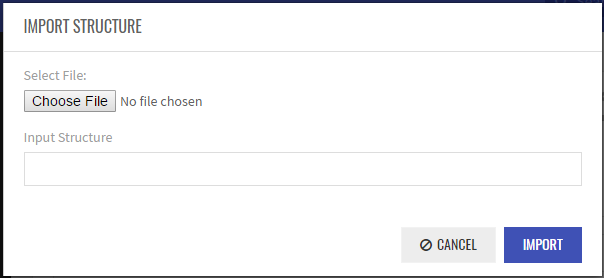


By default the file format is \*.rxn. The Export Structure pane contains the \*.rxn file. This \*.rxn file may be copied or downloaded to the local hard drive.

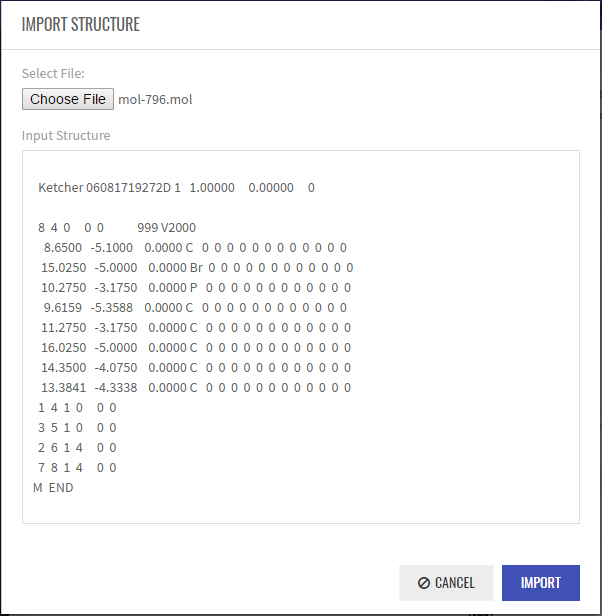
Click Download.

To import reaction scheme from the local driver:

Click . The Import Structure window opens.



Choose the \*.rxn, \*.mol or \*.sdf file from the local driver. The Structure preview appears in the field below.

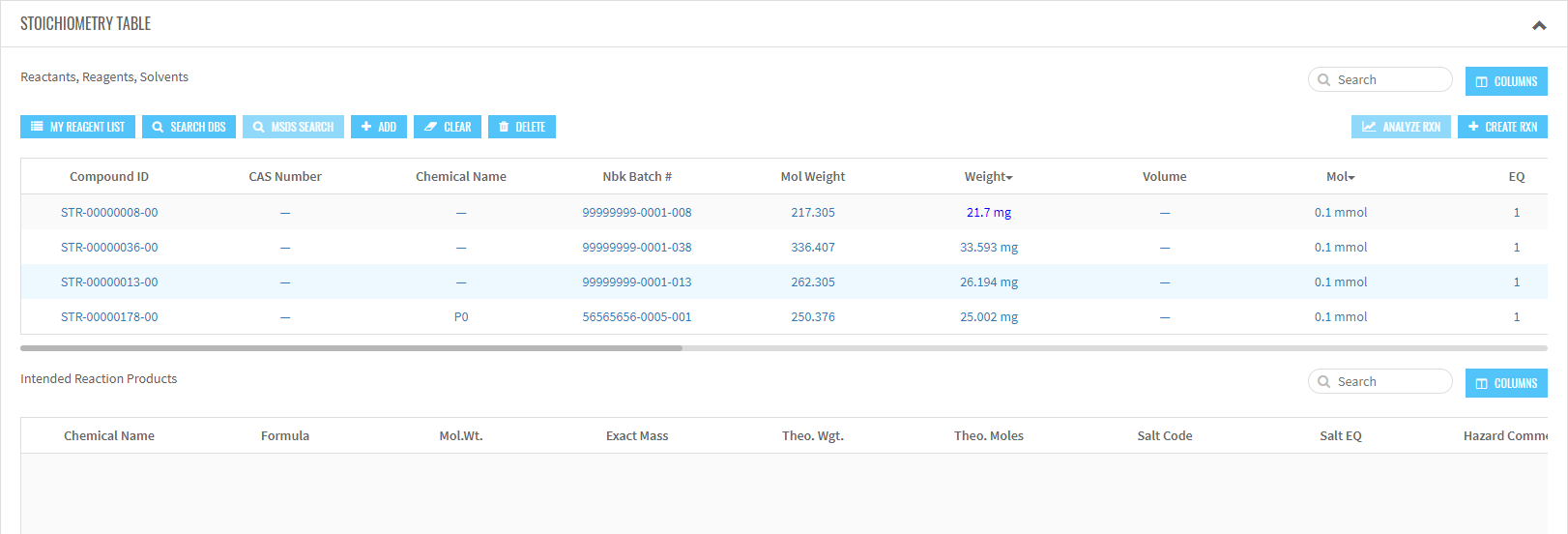


Edit the file if needed.

Click **Import**.

### Stoichiometry Table

Allows user to specify Reactants, Reagents, and Solvent using automatic reaction scheme analysis or manual search in database(s). Stoichiometry calculations of the starting compound amounts and Theoretical amounts of the Intended Reaction Products are executed here.



#### Stoichiometry Table

The Stoichiometry Table contains list of Reactants, Reagent and Solvents used in reaction. You can find a Predicted reaction product displayed on Reaction schema also in Intended reaction products. Intended Products are added automatically from the Reaction Scheme (it is the only way to add Intended Reaction Products

The user can manage the stoichiometry table in the following ways:

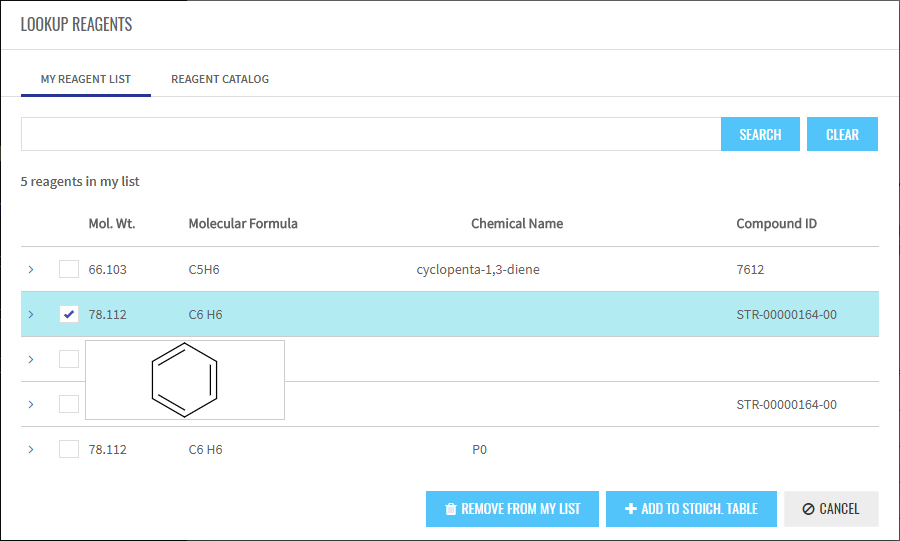
* Use Analyze RXN button (see further)
* Populate Compound information in the table through My Reagent List, Search DBs, retrieve by Compound ID and Nbk Batch# in empty rows
* Add new empty rows
* Delete rows.
* Clear rows
* Drag rows
* Drag columns
* Use “ Columns” button in upper right corner to show/hide desired columns or reset to default view

To fill the Stoichiometry Table through the reagent list:

Click **My Reagent List**. The Lookup Reagents window opens.

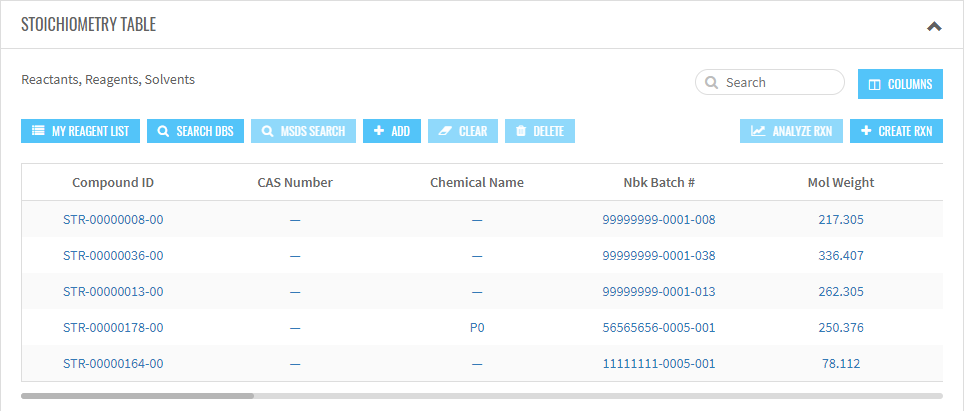
1. Reagent List contains reagents which the user has chosen before.

Select reagents from the list.



Click **Add to Stoich.Table**. New reagents appear in the Stoichiometry Table.

Click **Cancel** to close the Lookup Reagents window.



To fill the Stoichiometry Table through reagent catalog:

Click **Search DBs**. The Lookup Reagents window opens.

Choose catalog/catalogs to search in.

Reagent catalog contains possibility to select Data Base to search in. By default we can search only in application database. Any integrated external Reagent Catalog will be also listed here (example of such integrated DB is “PubChem”).

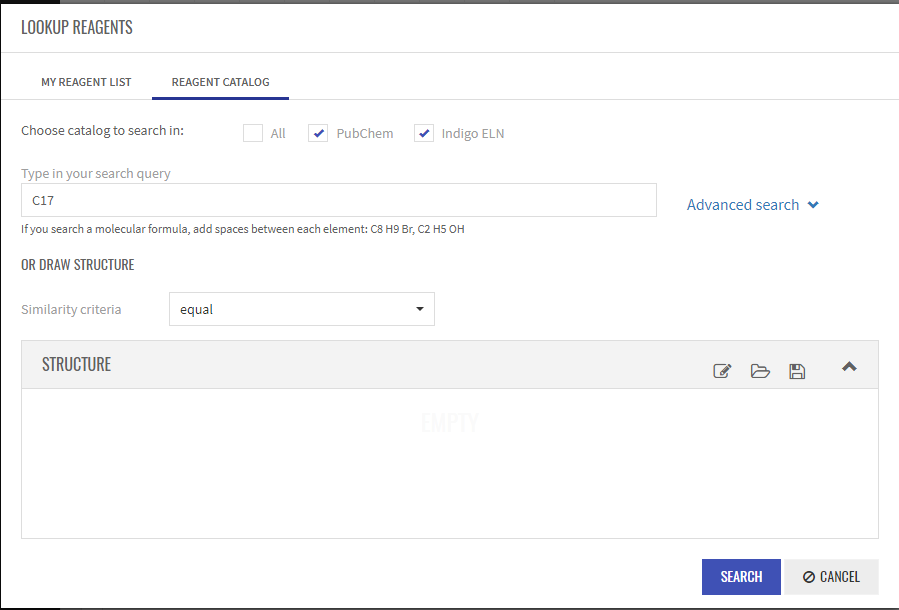
**Note:** “My Reagent List” and “Search DBS” opens the same dialog window, but different Tabs

1. By default the search is available only in the application database. You can select any integrated external Reagent Catalog from the list (example of such integrated DB is “PubChem”).
2. My Reagent List and Search DBS buttons open the same dialog window, but different tabs.

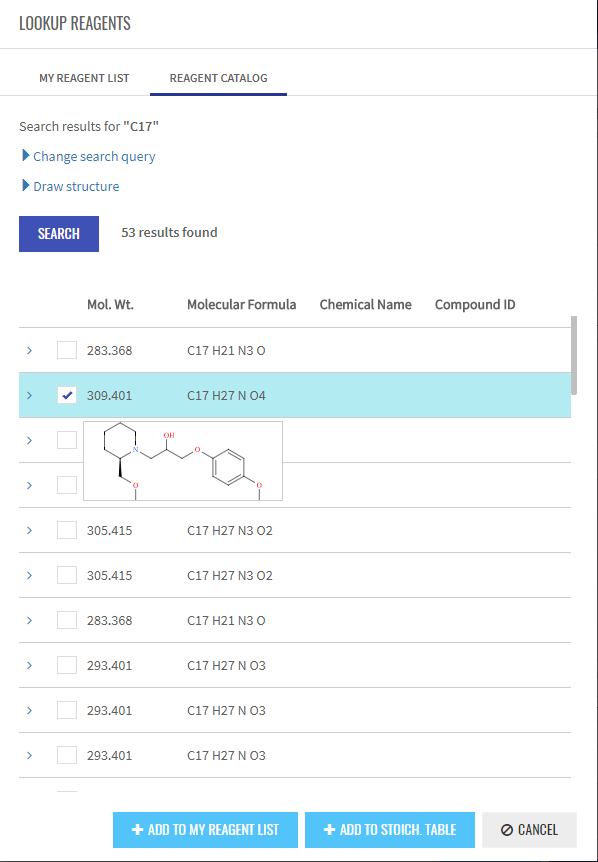
Type in your search query or draw structure.

1. To specify the search query click **Advanced Search**.

Click **Search**.



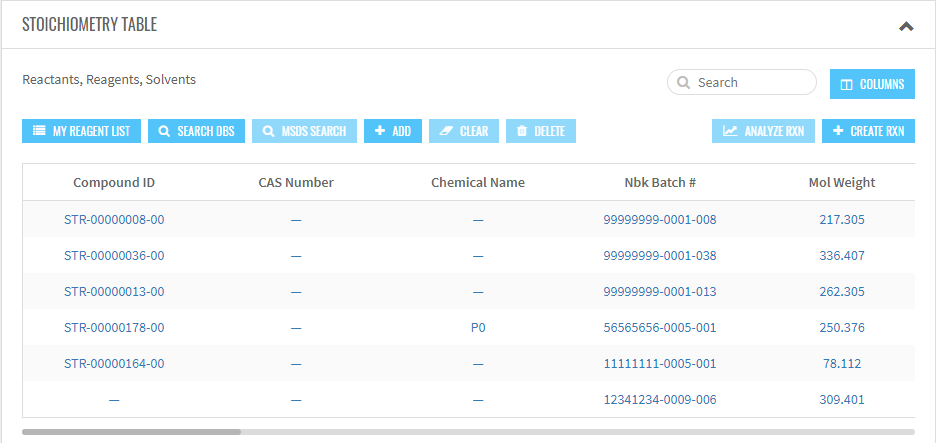
Select reagents from the list.



Click **Add to Stoich.Table**. New reagents appear in the Stoichiometry Table.

Click Add to my Reagent List if needed.

Click **Cancel** to close the Lookup Reagents window.



To add reagent form DB select one of the following options:

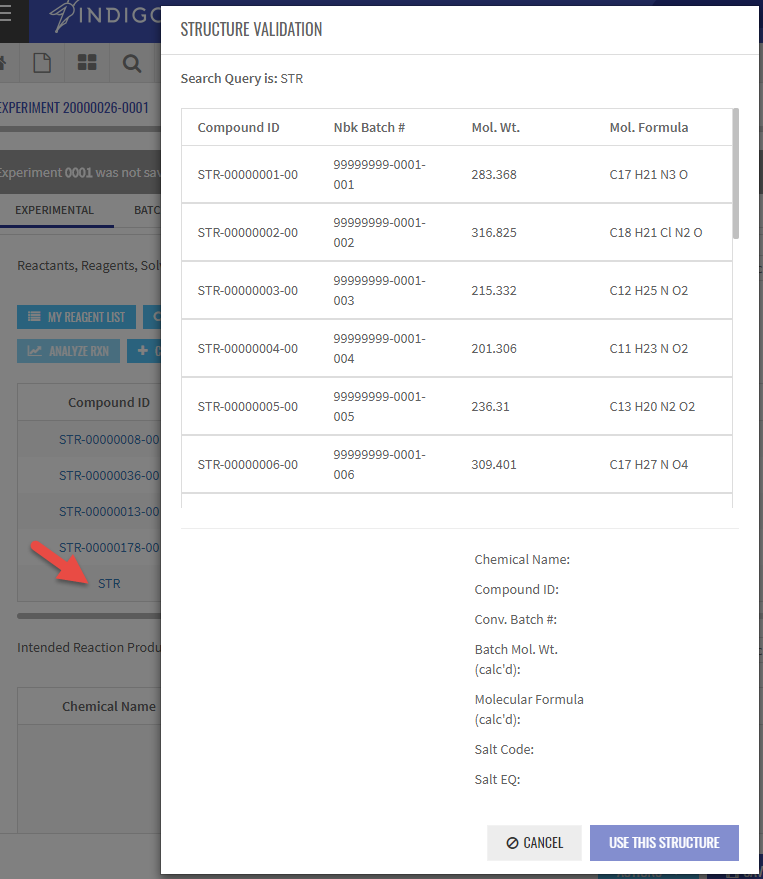
Fill in NBK Batch# in format *notebook #-experiment#-batch #*. System prompts user to select desired batch from drop down list when the user starts to type NBK Batch#.

The information about this batch appears in other columns. By this method the system retrieves the following information for the batch: Mol Weight, structure (in tool tip), Mol Formula, Salt Code/EQ (if they were assigned to the batch).

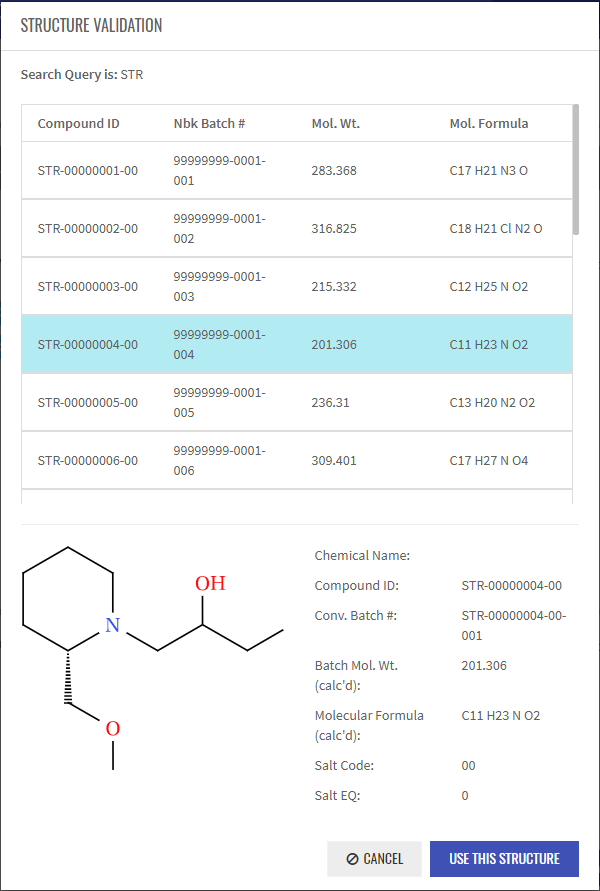
1. Salt Code, Salt EQ and Hazards comments appear in the table if they were assigned to the batch. Compound ID appears in case compound was registered in registration service through Indigo ELN.

Fill in Compound ID

In case several batches have the same compound ID the validation window opens.



Select the needed compound and click **Use this Structure**.



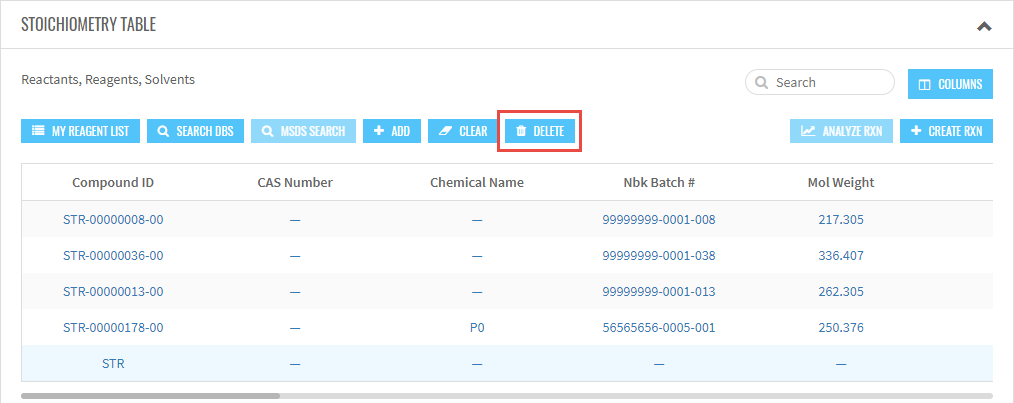
The information about this batch appears in other columns. The system retrieves the following information: Mol Weight, structure (in tool tip), Mol Formula.

1. Salt Code, Salt EQ and Hazards comments appear in the table if they were assigned to the batch. NBK# appears in case compound was registered in registration service through Indigo ELN.

To delete rows form the table:

Click the row.

Click **Delete**.

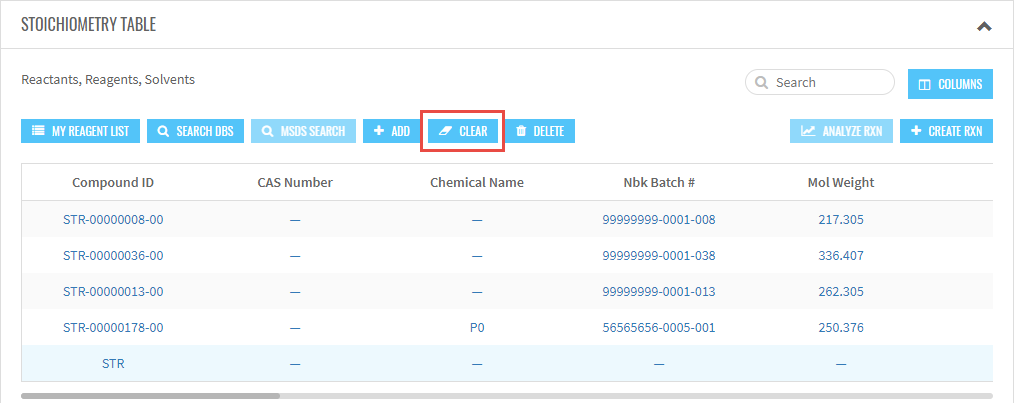


The row disappears.

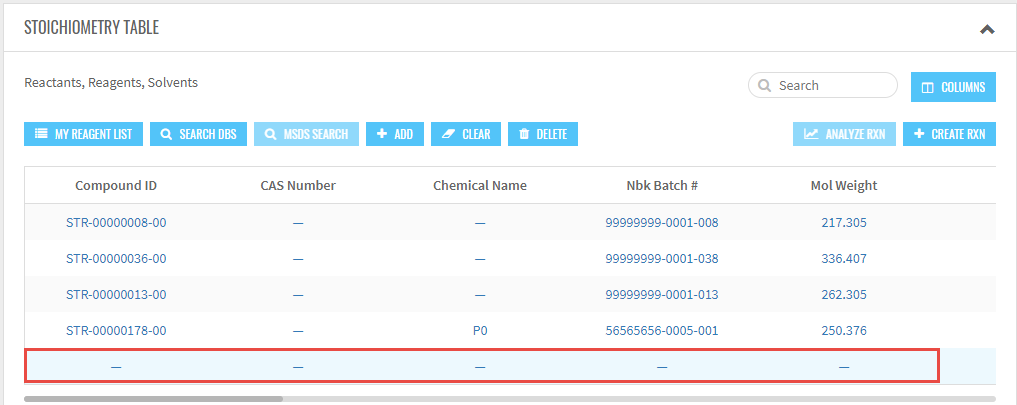
To clear the row:

Click the row.

Click **Clear**.



The row becomes empty.



To add new empty row:

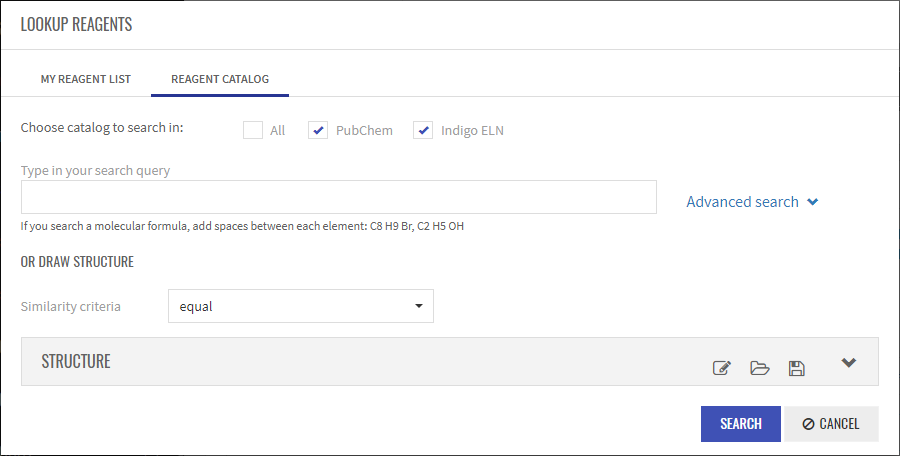
Click **Add**. New row appears in the table.

Fill in all necessary fields.

#### Search DBs

Allows to search compound in internal and integrated databases by criterion or set of criteria, or by structure. To find new reagent:

Click **Search DBs**. The Lookup Reagents window opens.



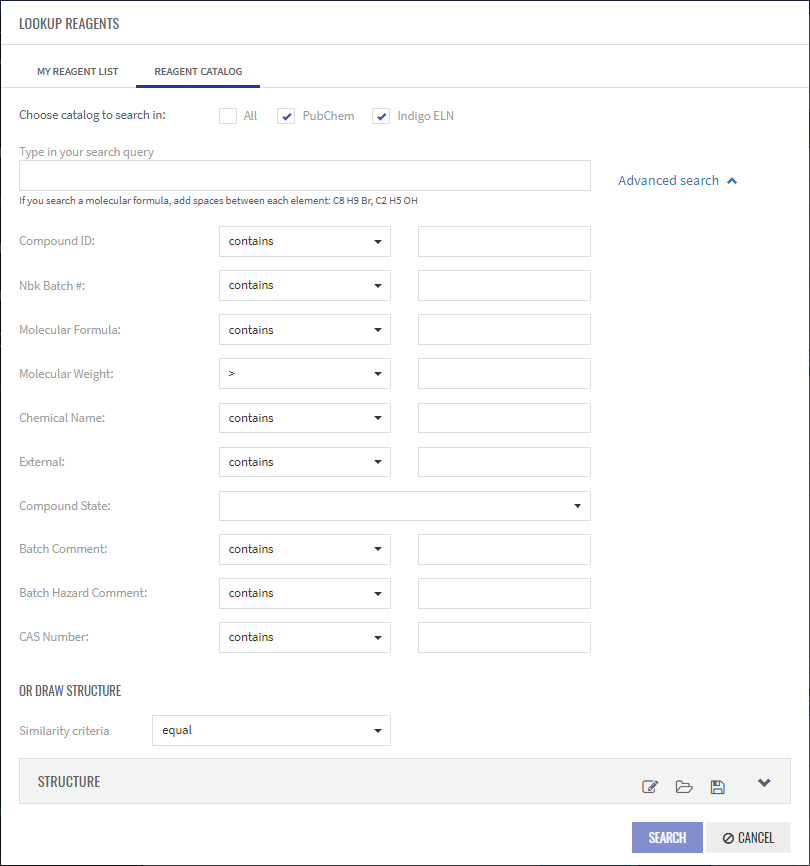
Click the checkbox to choose catalog to search in.

1. The checkboxes correspond to the reagent databases the application is integrated with.

To find the reagent type the reagent Compound ID, mol. Formula, chemical name or any other useful information in the text field.

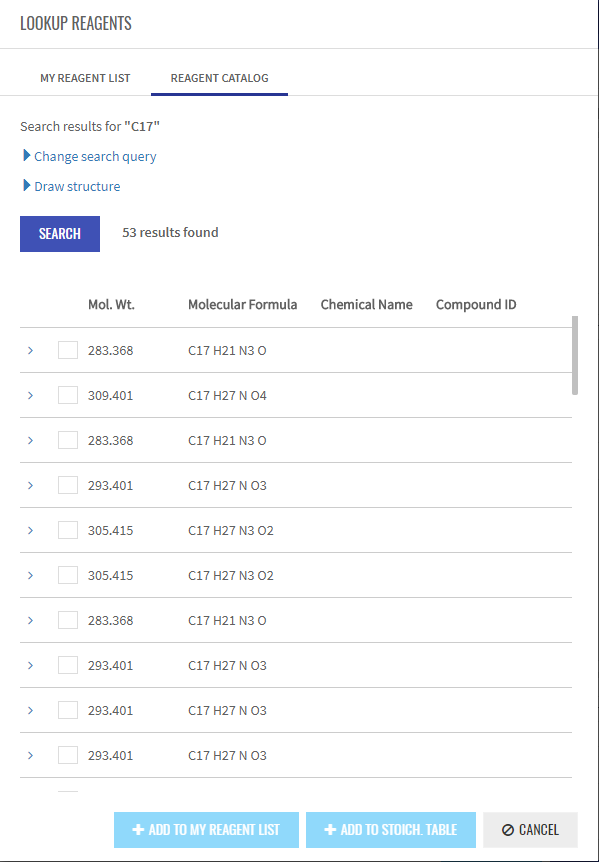
1. To create the search query type spaces between each element.

Click **Advanced search** to open additional filters.



You can also search by structure. Click **Structure** to open the molecular editor.

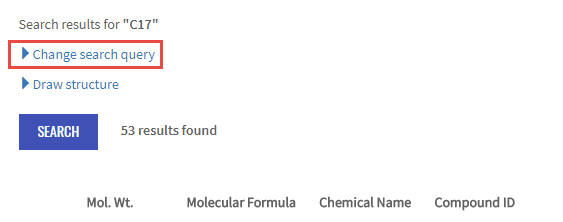
Click **Search**. The search results appear below.



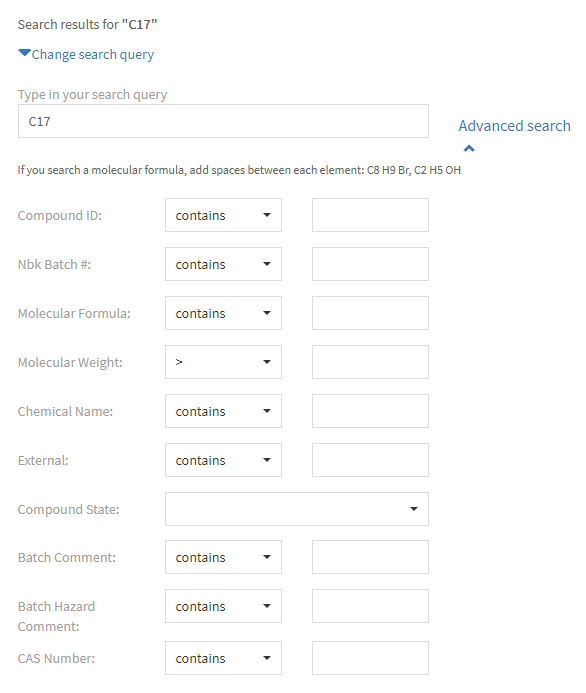
You can change search criteria on the Reagent Catalog tab.

To change the search query:

Click Change search query.



The new area opens.



Edit the reagent name in the text field and any advanced characteristics if needed.

To search the reagent by structure click **Draw Structure**.

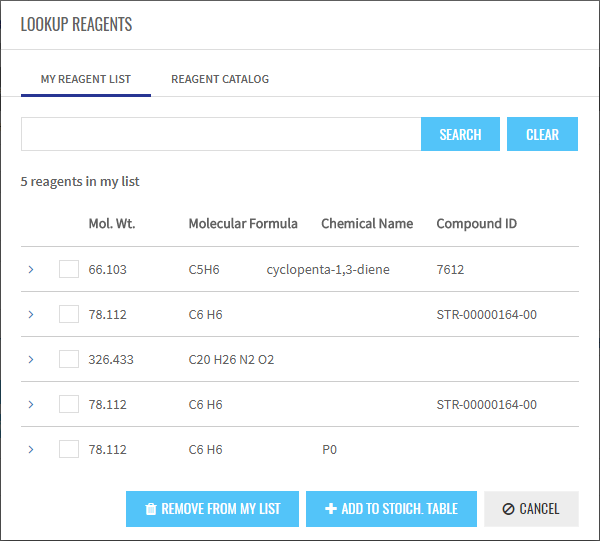
Ketcher editor opens. User can execute search with selected similarity criteria. See description of the structure editor in Section 4.4.3.

#### Reagent List

The Reagent List contains some reagents previously selected by user in search DB results and added to this list for future quick access to them. In case user changes the reagent information in this list, the new information appears in all further experiments that contain this component and does not change in already existing entities.

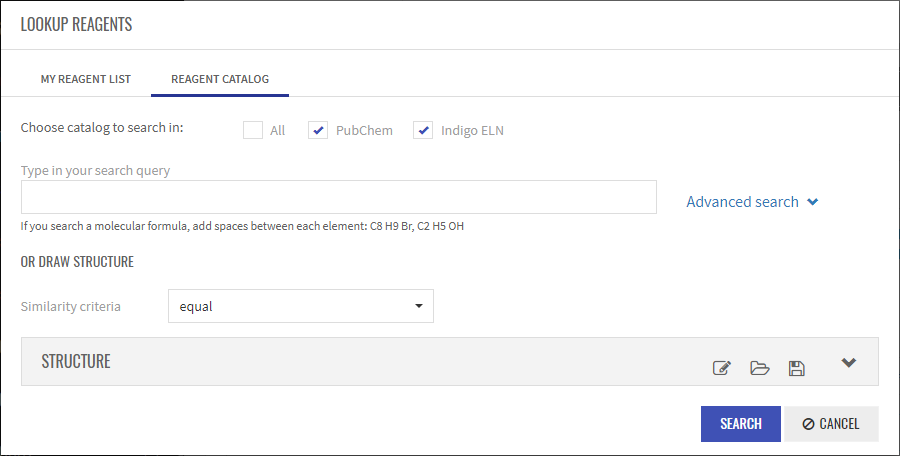
To manage the reagent list:

Click **My Reagent List**. The Lookup Reagents window opens.

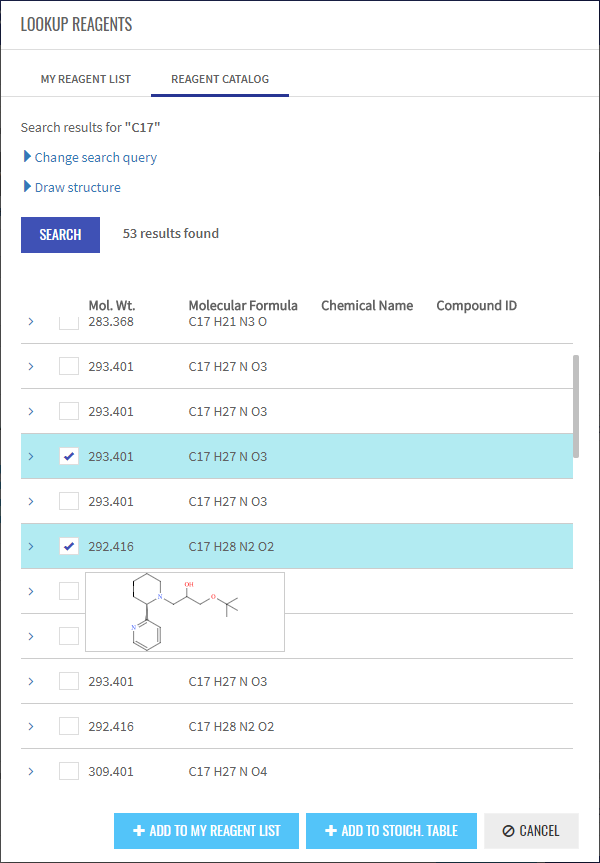


To add reagent in the list:

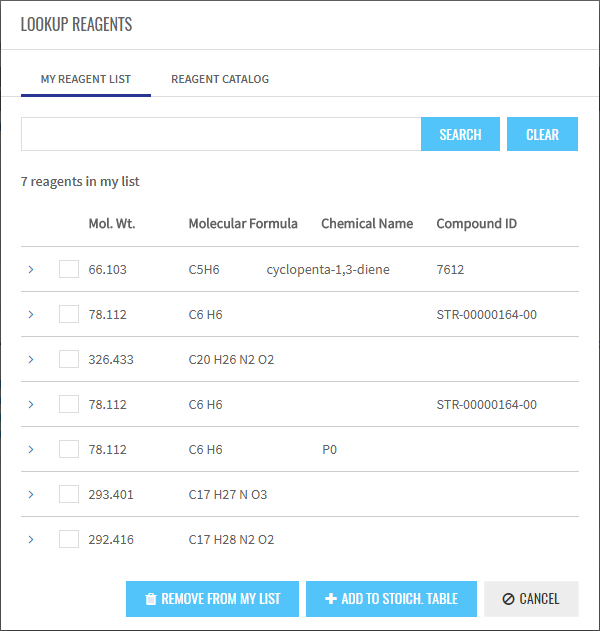
1. Find reagents in DBs. See section 4.4.11.2 for instructions.



1. Select reagents.

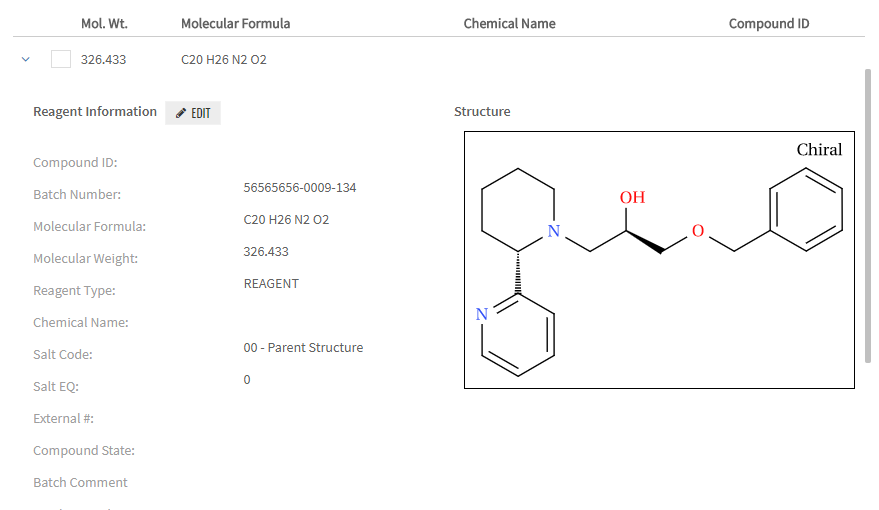


1. Click **Add to My Reagent List**. New reagent appears in the list on My Reagent List tab.

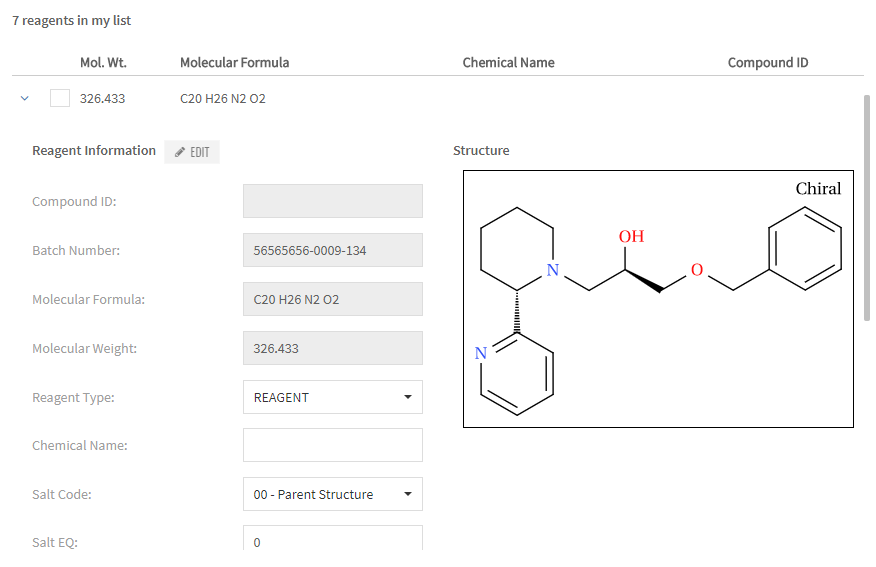


To see full information about the reagent:

1. Click the arrow in the reagent line.



Click **Edit** to edit information about reagent.

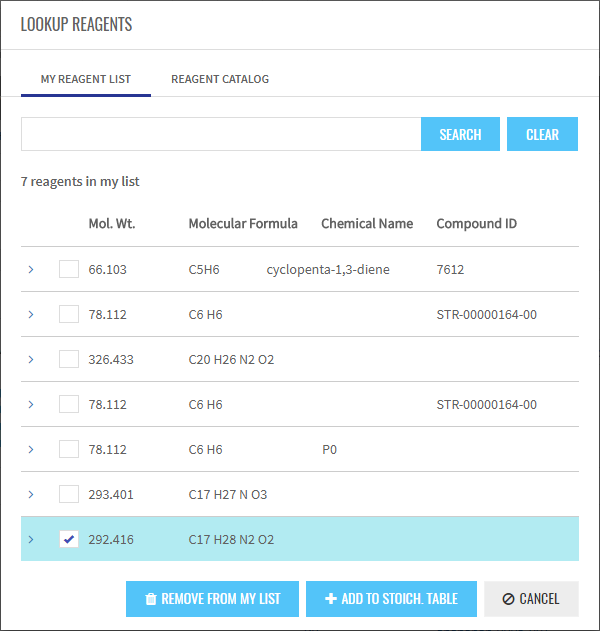


1. The reagent information changes in all further experiments that contain this component and does not change in already existing entities.

To remove reagent from the list:

Open My Reagent List tab.

Select the reagent in the list.



Click **Remove from My List**. The reagent disappears.

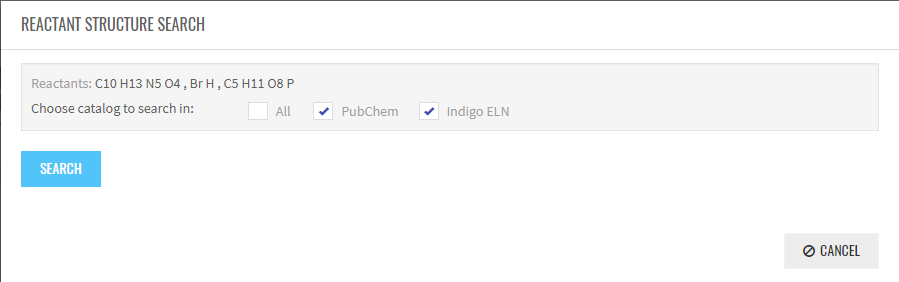
#### Analyze Rxn and Create Rxn

Reaction Scheme and Stoichiometry Table components are related to each other and provide information to each other if they are in one experiment template. In case they are in one template, the user use them to populate each other. There rea two methods to fill this components:

* **Method A**: Transfer information from Reaction Scheme to Stoichiometry Table.

Draw or import reaction schema in Reaction Scheme component. The **Analyze Rxn** button in Stoichiometry Table becomes available.

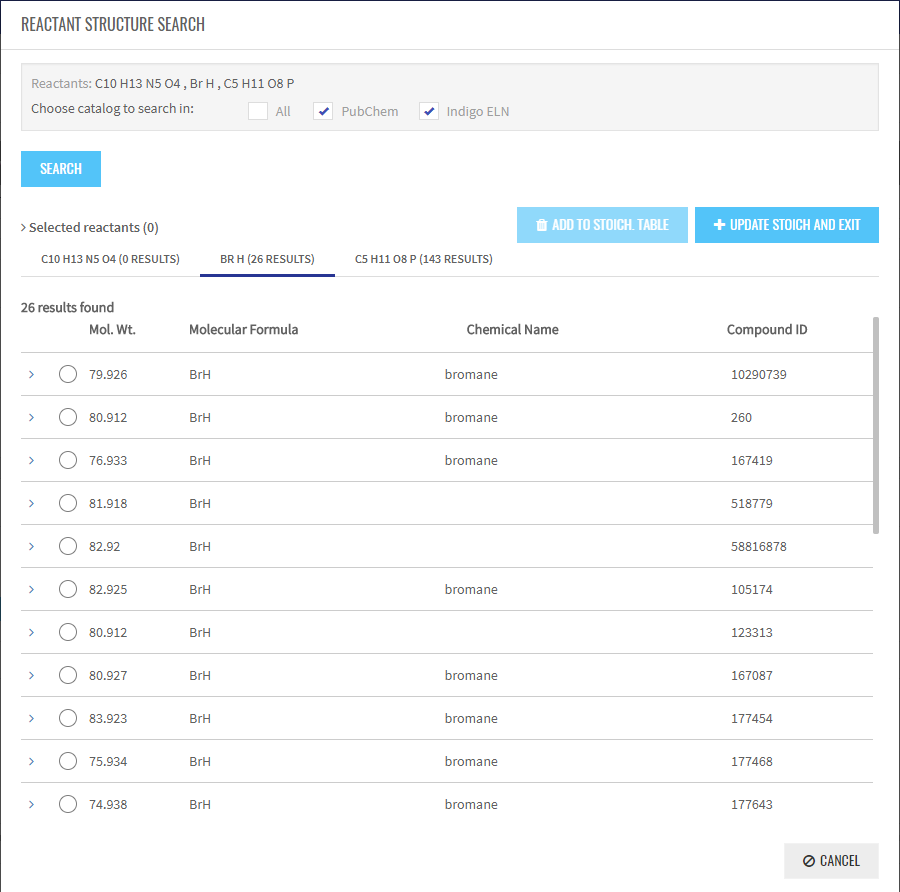
Click **Analyze Rxn**. The Reactant Structure Search window opens.



Select databases to search in.

Click **Search**. The system executes substructure search to find appropriate reactants in selected internal and integrated databases. Search results appear in the list below.

1. Analyze Rxn search supposes structure search with Substructure similarity criteria only. User cannot affect this setting.



For each reactant on reaction schema system provides search results on separate tabs. Select the reactants from database corresponding to reaction schema on each tab.

Click **Add to Stoich. Table** to add found selected reactant to Stoichiometry table

The new row with data for selected reactant appears in Stoichiometry table.

1. User can select only one reactant on each tab.

Click **Update Stoich. And Exit** to populate Stoichiometry table by Mol Weight and Mol Formula of the reactant corresponding to structures drawn in reaction schema. This works in case the reactant was not found in databases. If some of reactants are found and some are not, the **Update Stoich. And Exit** button adds selected search results for defined reactants and Mol Weight and Mol Formula for nonfound.

Add other solvents and reagents to the Stoichiometry Table by any way described in previous section.

* **Method B**: Transfer data from Stoichiometry Table to Reaction Schema.

Populate Stoichiometry table by any way described in previous section. Set RXN Roles for added compounds.

Click **Create Rxn**. The Reaction scheme component shows reactants and the arrow.

1. Create RXN option is available only for reagents containing Molecular Structure
2. Only rows with RXN Role values “Reactant” appear in Reaction Schema, Reagents and Solvents do not appear in reaction schema. If any of the row with RXN Role “Reactant” has no Structure in tool tip, it is also omitted in Reaction schema.

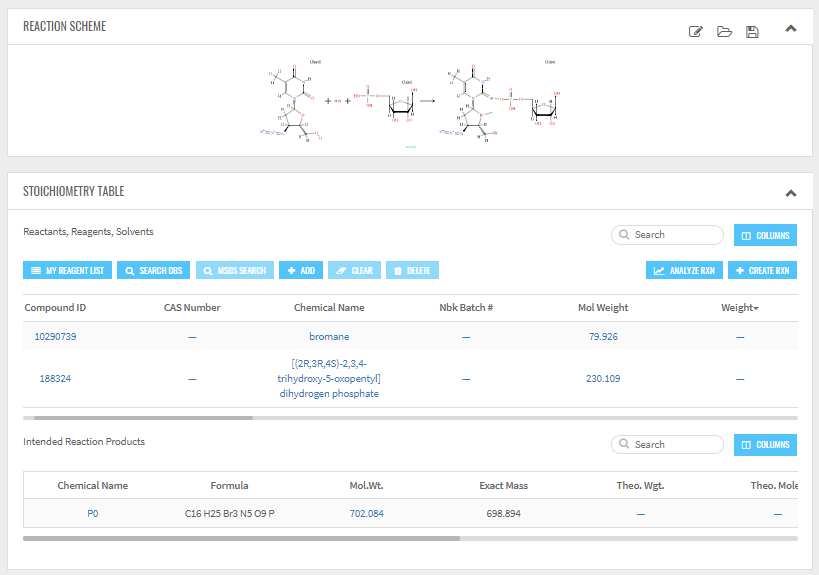
Open reaction schema in editor and draw reaction products to populate Intended reaction products table.

#### Intended Reaction Products

The Intended Reaction Products area contains the information automatically added from Reaction Scheme. Table shows Theoretical amounts of the Intended product calculated on the basis of amount of limiting Reactant.

Intended Reaction product Table contains row for each drawn product. Products are described with MolWeight, Mol Formula and structure in the tool tip when we hover under Chemical name column.

To get some information about the intended products in the table make steps from the Section 4.5.1.4.



# Administration menu

The administration menu contains four tabs:

* Users
* Roles
* Templates
* Dictionaries

## Users

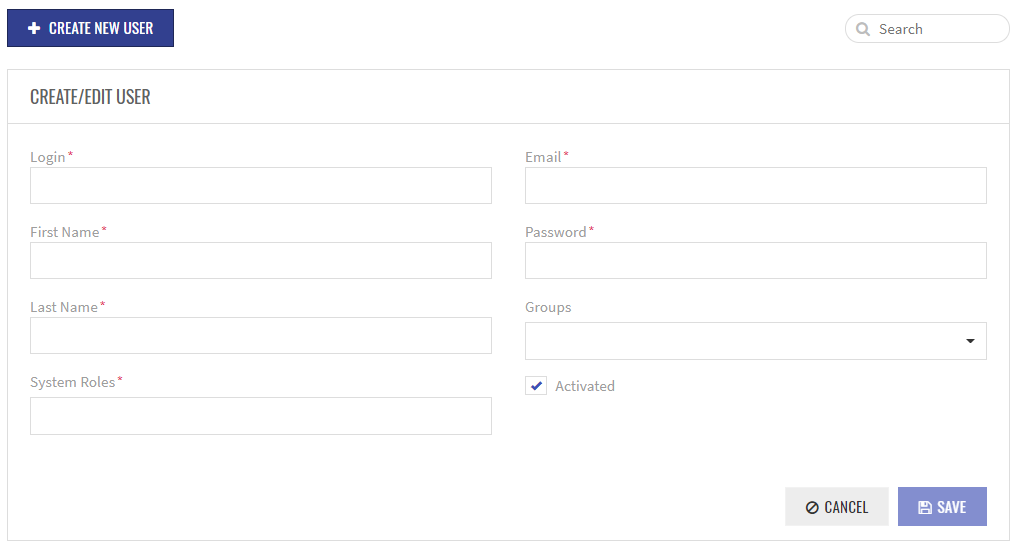
The Users tab contains the table with the information about users.

To create a new user:

Click Create New User.

To edit a user:

Click **Edit** on the right of a particular user in the list. The Create/Edit User box opens.



In the lower part of this box there is the list of existing users, same as in the initial view of the Users tab.

Fill in the following fields (mandatory fields are marked red):

* Login (unique within the system)
* First Name
* Last Name
* System Roles
* Email
* Password

1. The password should contain minimum 6 symbols with at least one capital letter and at least one digit.

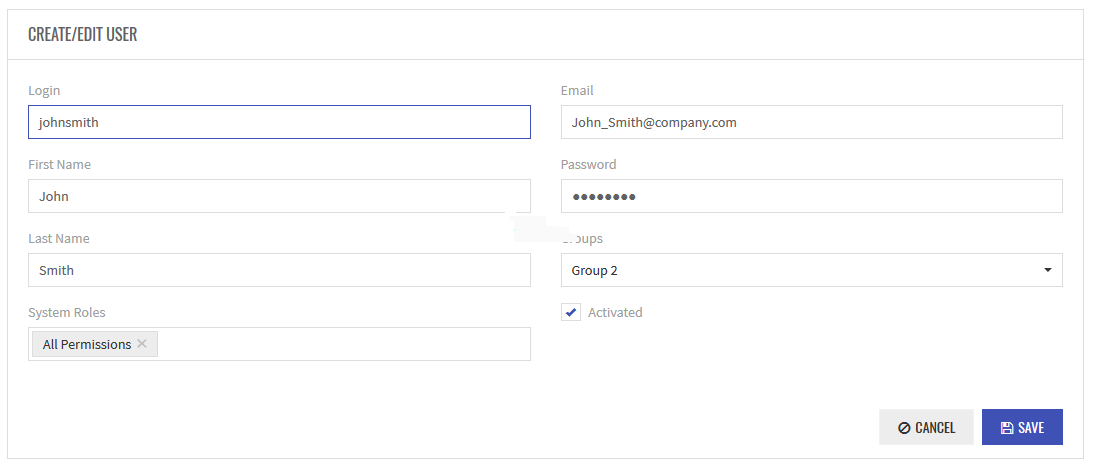
* Groups

Click **Save**.

To edit the user’s profile:

Click **Edit** to the right of a particular user’s name on the Users tab. The Create/Edit User page opens.

Edit the necessary fields.

Click **Save**.

The user could be deactivated if there is no necessity for his/her activity in the application.

To deactivate the user:

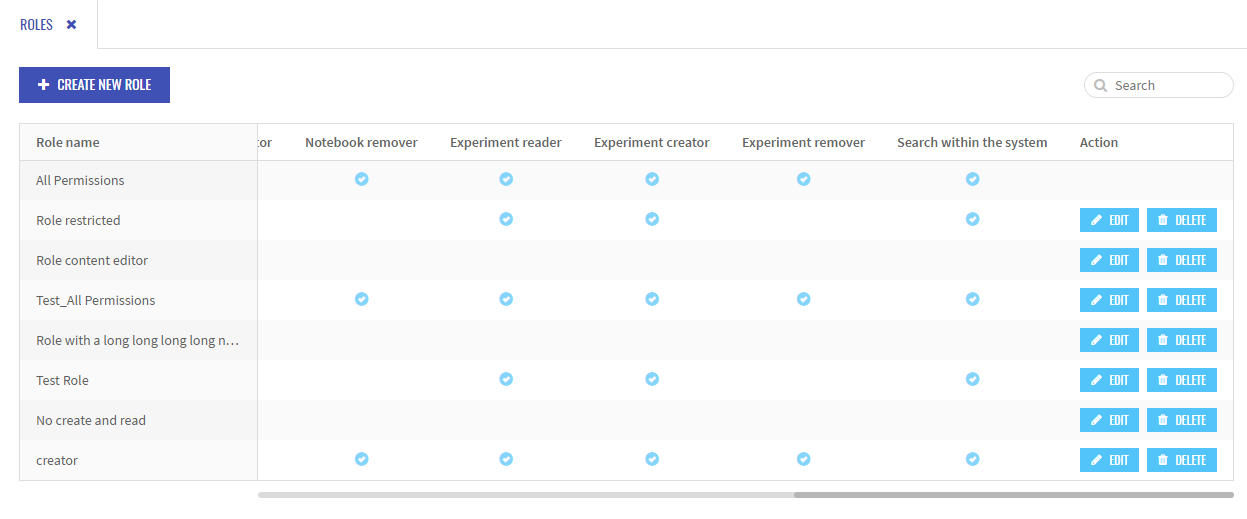
Click **Activated** in the list of users.

Or click **Edit** and deselect the checkbox **Activated**.

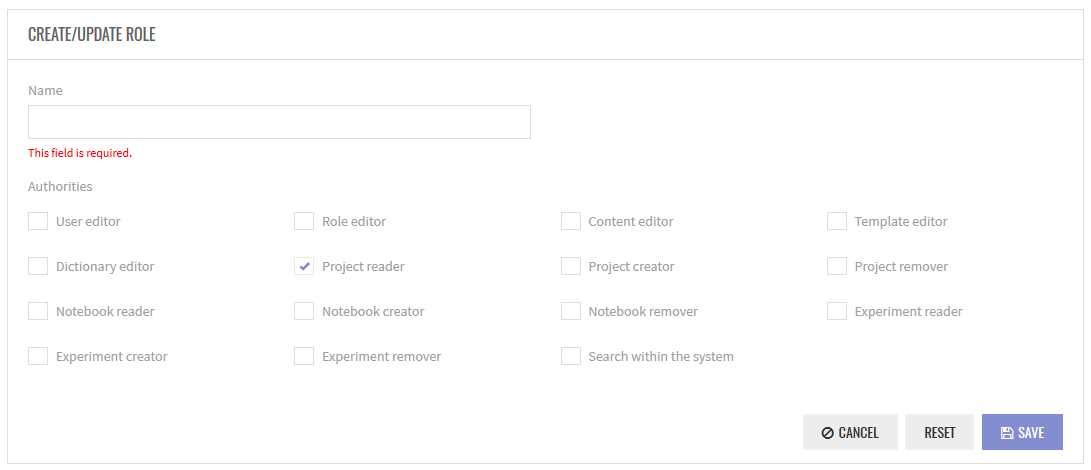
The status changes to Deactivated. The user is not able to enter the application. All his entities are available in the All Projects section. The content editor user can share these entities with other users.

## Roles

The Roles screen contains a table with all roles in the application.



To create a new role:

Click **Create New Role**. The Create/Update Role screen opens.

Type the name of the role in the Name text field (mandatory).

Mark the checkboxes to assign the authorities.

1. The Entity creator role includes the Entity reader permissions.

Click **Reset** to undo all changes, if needed.

Click **Save** to save a new role.

To edit an existing role:

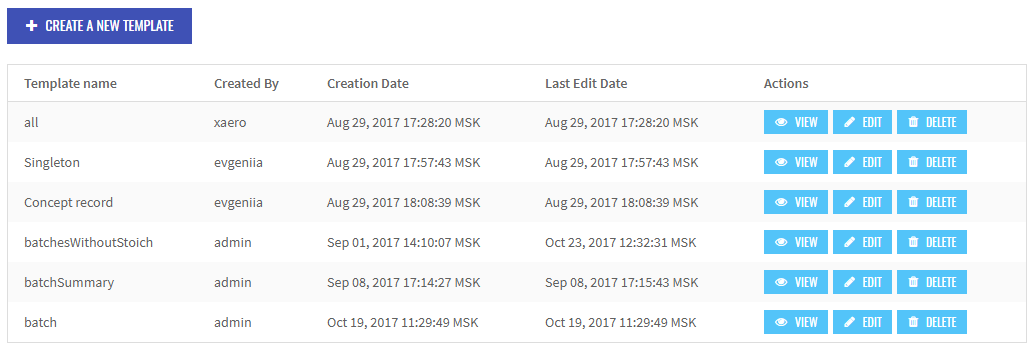
Click **Edit** on the Roles tab to the right of a required role. The Create/Update Role screen (see above) opens.

Edit the required authorities or change a role name.

Click **Save**.

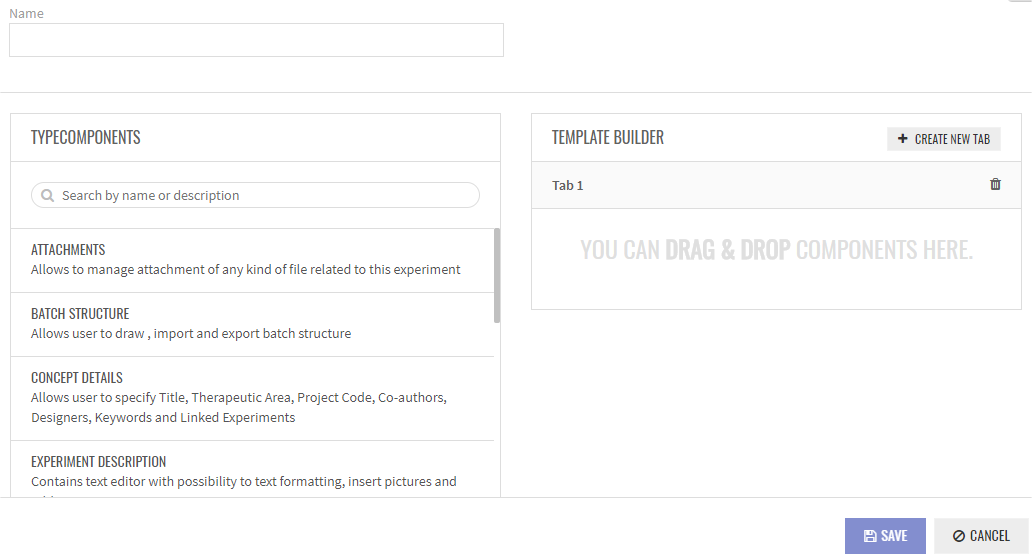
To delete a selected role, click **Delete**.

## Templates

The Templates tab contains the information about templates for the experiments (see Introduction and Section 4.3 Manage Experiments).

Use buttons in the Actions column to View, Edit, or Delete a template.

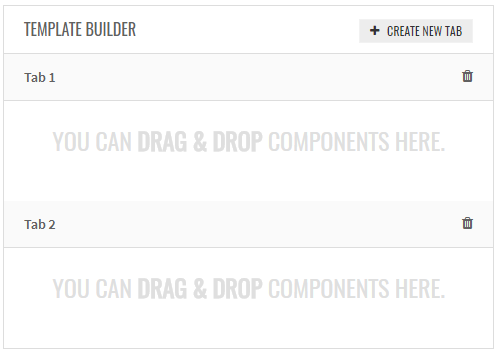
To create a new template:

1. Click **Create a New Template**. The New Template tab opens.

Type the Name in the corresponding text field.

Select components in the Type Components area and drop them into the Template Builder area to change their order.

Click **Create New Tab** in the Template Builder upper right corner to add a new tab.



Click the tab name (by default you have name of the tab - Tab 1) to edit it.



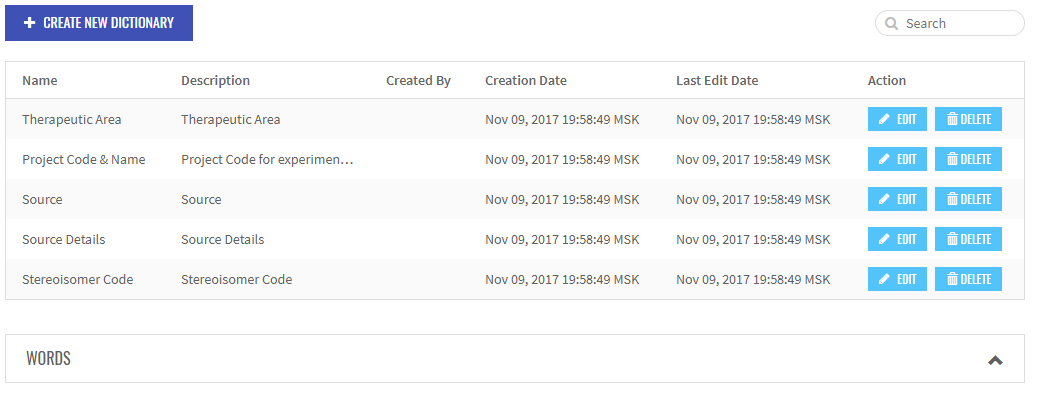
Drag and drop tabs to change their order.

Drag components from Template list on the left to the Template builder for each tab.

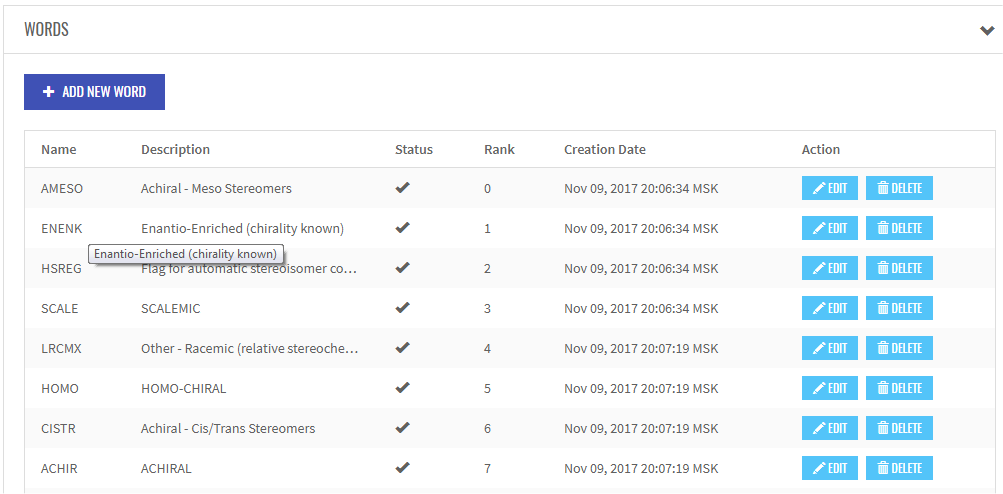
Use the **Show Preview** button to review added components and its position in template.

Click **Save**.

## Dictionaries

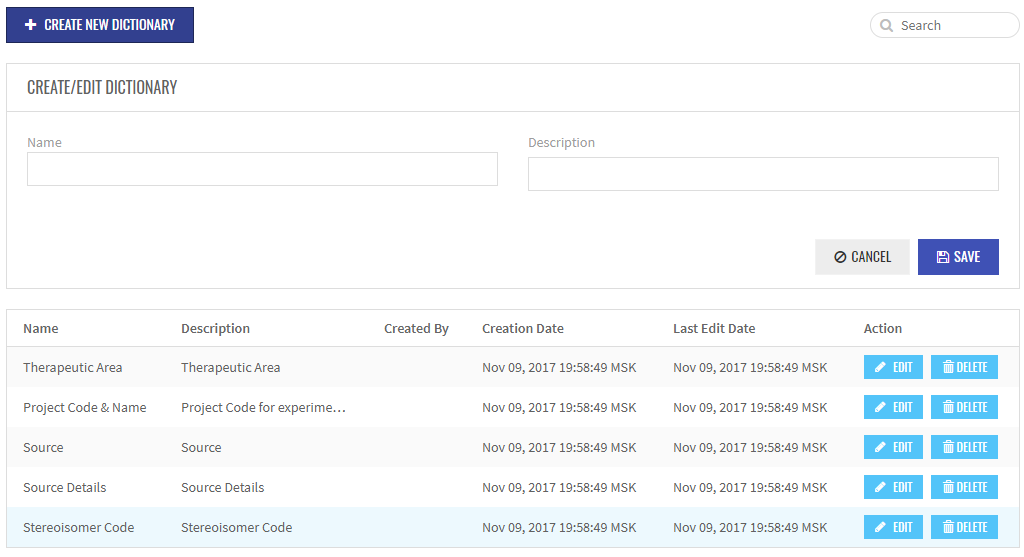
Dictionaries collect items that appear in the drop-down lists of the application. Users can create and edit dictionaries in the Dictionaries tab. You can see the list of available dictionaries using the corresponding command on the Administration menu.

The tab has two panes, the list of Dictionary drop-downs (see above) and a list of items in these drop-downs (Words):



To create a new drop-down:

1. Click **Create New DIictionary**. The Create/Edit Dictionary pane opens above the list of existing dictionaries.

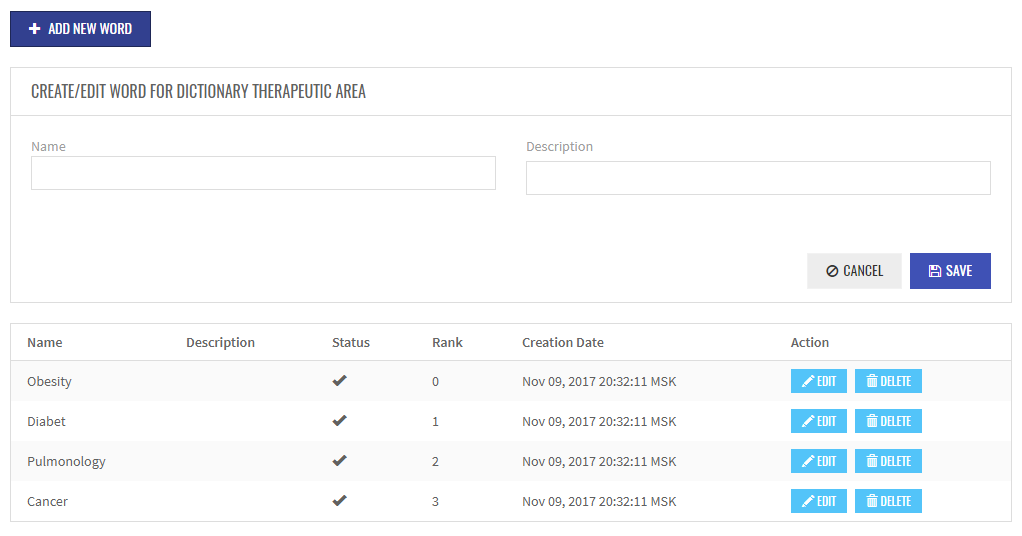


1. Type the Name and Description for the drop-down in the text fields.
2. Click **Save**.

Next, you have to add words to the dictionary. You can also use this algorithm to add words to any dictionary in the list.

1. Select any dictionary from the list above.
2. Click **Add New Word** at the Words pane of the tab.

The Create/Edit Word for Dictionary <NAME> area opens.



1. Type the Name and Description of the word.
2. Click **Save**. A new word will appear in the table.
3. Repeat these actions to add other words to the dictionary.



To edit a word in the list, click **Edit**.

To delete a word, click **Delete**.