Mbook 4.0 Manual

Last Revision: 26th-Feb-2025

Mbook 4.0

by MESTRELAB RESEARCH

This is the manual of Mbook 4.0

Mbook Manual

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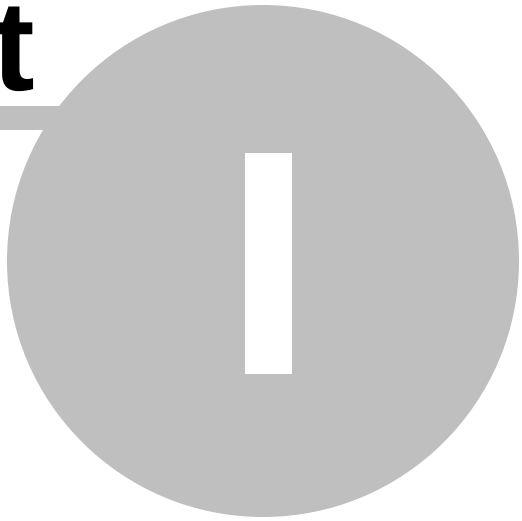
Part



1 Introduction

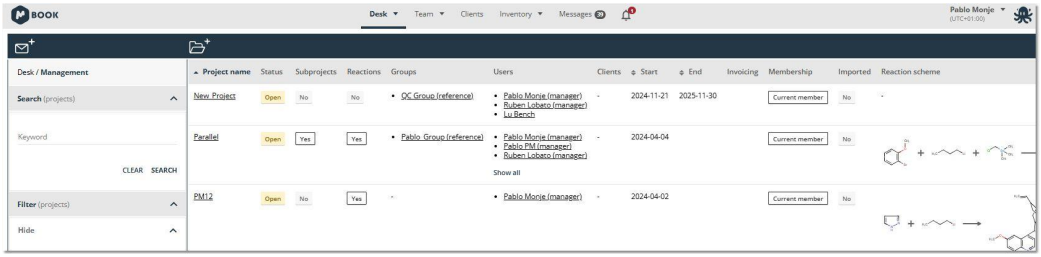
ABOUT MBOOK MANUAL

This manual describes the features included in Mbook. Mbook is an Electronic Notebook (ELN) that will help you to enter, archive, search and report your chemical experiments and reactions, including analytical, spectroscopic and other types of data.

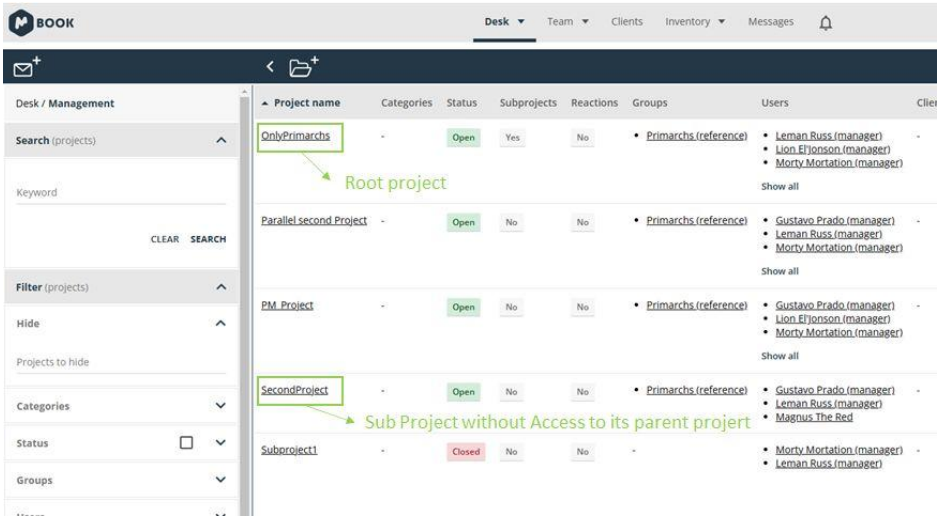
- Different levels of users: Project Manager, Group Manager, Bench Chemist and more
- Input any type of information related to your chemistry: graphical representation of a reaction, stoichiometric calculations, experimental write-up, purification procedures, spectroscopic characterization, analytical data, physical, chemical, biological, and pharmacological properties, health and safety information, literature/bibliographical documents and more
- Chemical structures, numerical data, text, images, spectroscopic data, binary files, etc.
- Its own large editable database of typical chemical reagents, with relevant physical and chemical properties to facilitate the setup of your reactions or experiments
- Its own, optimized chemical structure drawing package
- Communications within your organization (user to user, user to groups, etc.)
- Powerful and fast structure and text-based searches
- Interfacing with external databases to search for relevant information and properties
- User-tailored reporting
- Cloning of experiments and easy modification of pre-existing structures/information

1.1 Definitions

- **Groups:** Set of users who will carry out a project.
- **Projects:** Tasks created by privileged roles that contain a set of reactions.
- **Reactions:** Set of experiments within a project.
- **Experiments:** Each of the tests, typically run by the Chemist, within a reaction containing a reaction scheme, a stoichiometry table and a reaction write-up section.
- **Desk:** Work area containing the list of projects and a view of the experiments of interest.



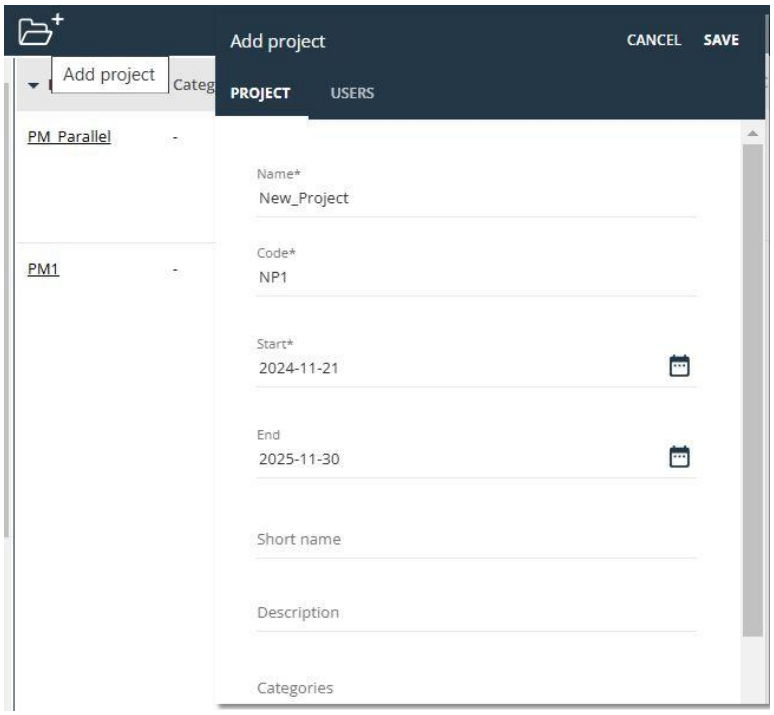
The displayed projects are root projects or subprojects (if the user does not have access to the parent project):



The table has an horizontal scroll, being the 'Project Name' column sticky. The project list can be sorted by 'Project Name', 'Start date' and 'End date'.

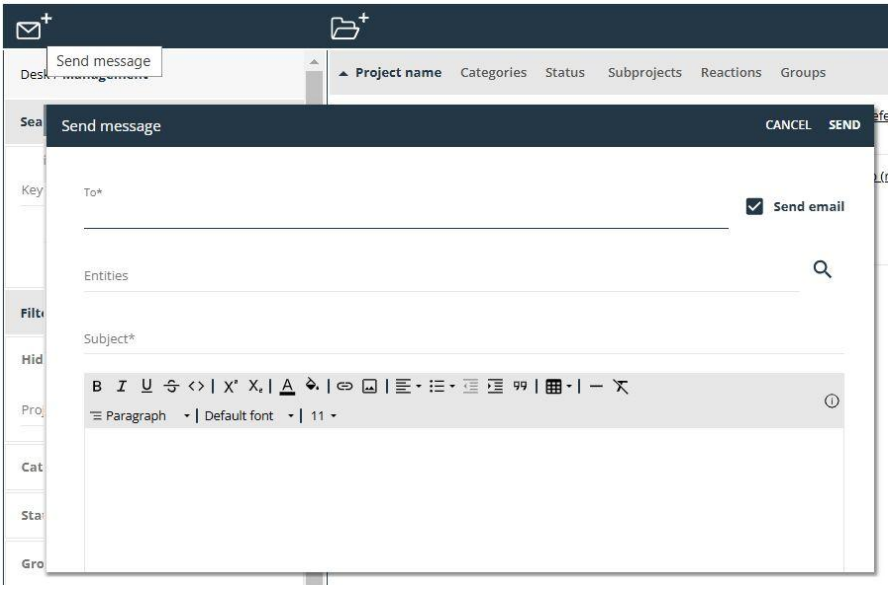
You can search by keywords and use the desired filters (hide, categories, status, groups, users, clients, date, invoicing or membership), which will be kept in the registry.

From this panel, you can also add a new root project by clicking on the 'Add project' button.

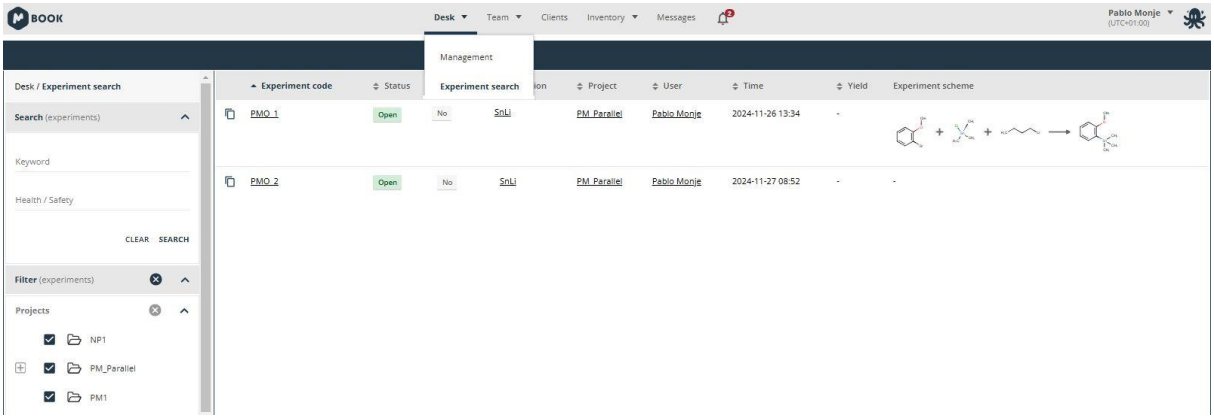


Clicking on the project or group name will allow you to navigate through the project and group dialogues respectively. Besides, you can display user and client details by clicking on the user or clients name.

Clicking on the 'Send message' icon will allow you to send messages:



From the Desk scroll down menu you can also search and filter by experiments by using the 'Experiment Search' option:



- Inventory: Set of compounds, stockrooms and suppliers.

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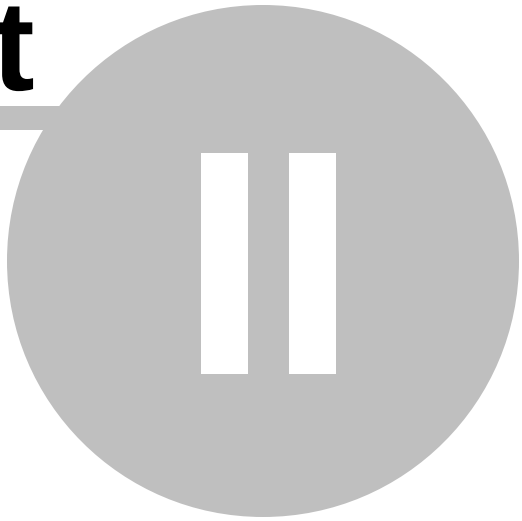
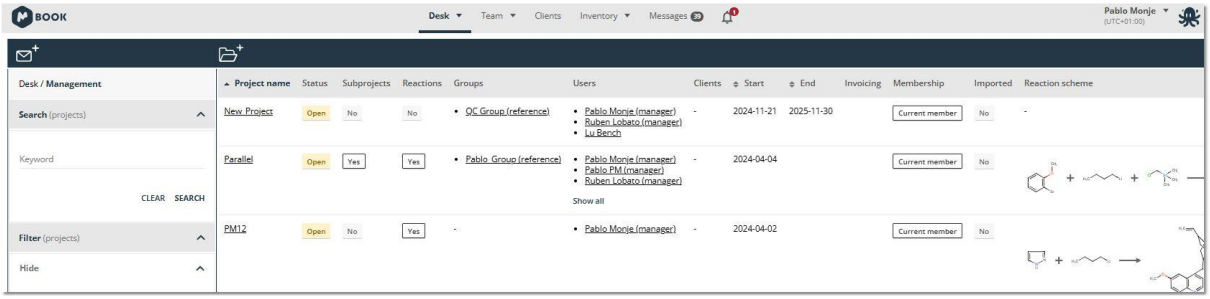


2 Starting with Mbook

You can use your Internet browser to connect to your server just by typing something like the address below into the search field:
http://SERVER_IP_ADDRESS:PORT/ELN/

After having entered the applicable username and password, you will be presented with the GUI:



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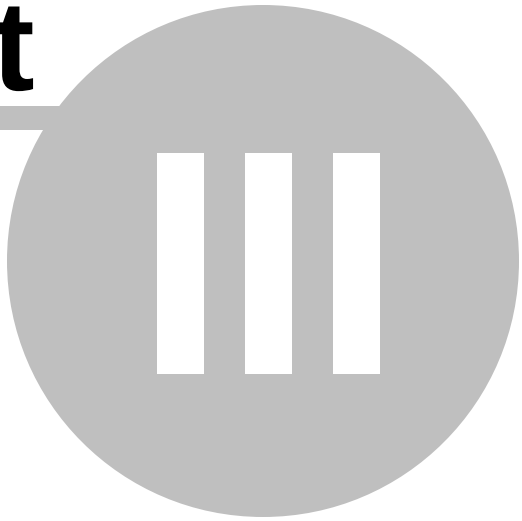


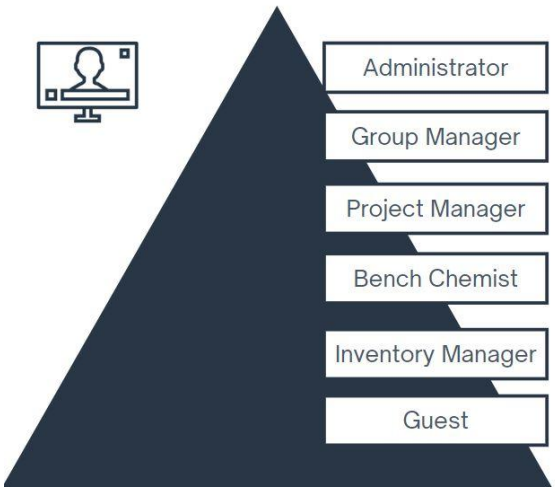
3 Users and Groups Configuration

Before you start creating users and groups, we strongly recommend you read the descriptions of the six user role types within Mbook ELN below.

Please note that understanding the differences between an Admin and a Group Manager is very important to this preliminary configuration step.

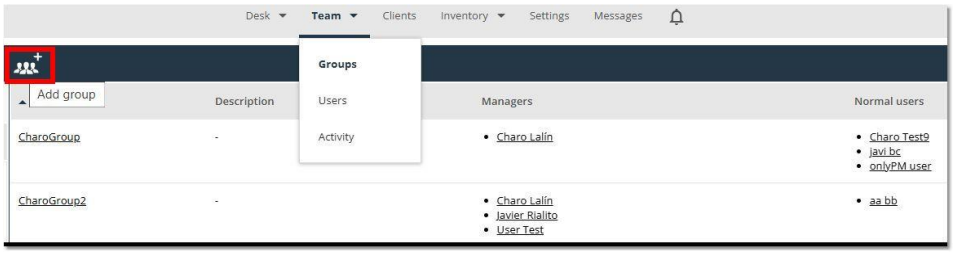
3.1 User Roles

Mbook offers a range of roles that can be assigned individually or combined to tailor each user's privileges according to the organization's needs (Administrator, Group Manager, Project Manager, Bench Chemist, Inventory Manager, or Guest).

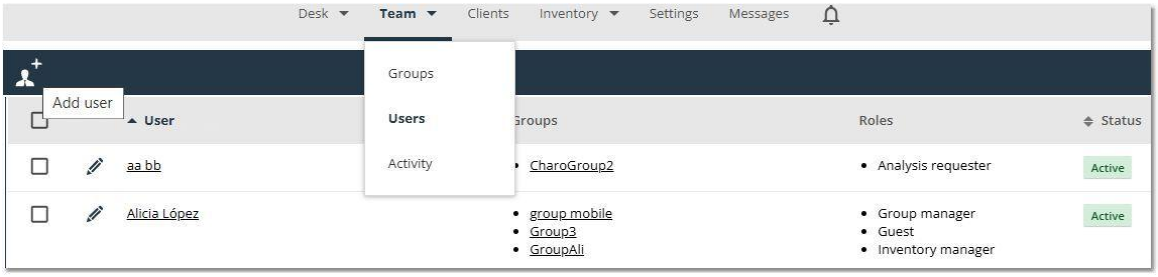


- **Administrator:**

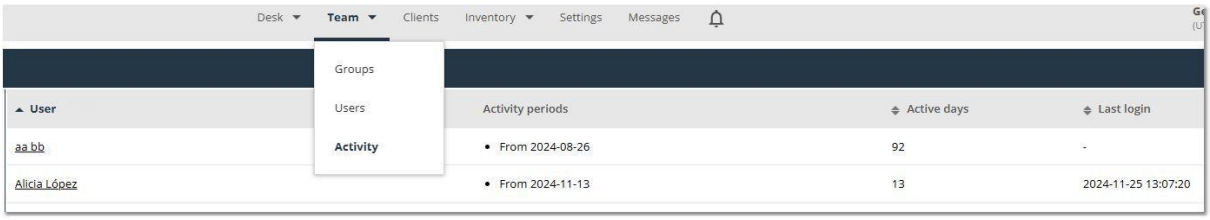
This role is for authorized users in management roles and is key for the initial configuration of Mbook. A user with administrator rights is automatically created for new organizations when they start using Mbook (but we do not charge a license for it). The administrator cannot create or work with projects, reactions or experiments. An administrator, however, can create groups that are completely independent from each other, which a Group Manager cannot do.



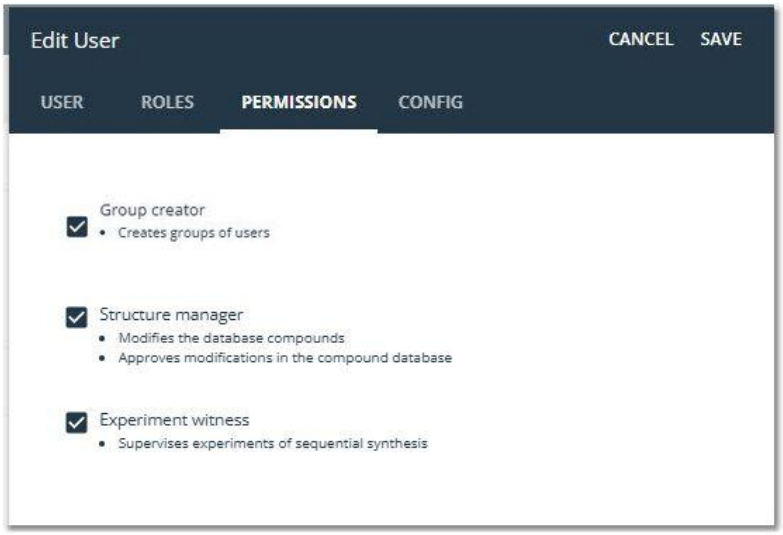
From the admin account you can also activate/disable users:



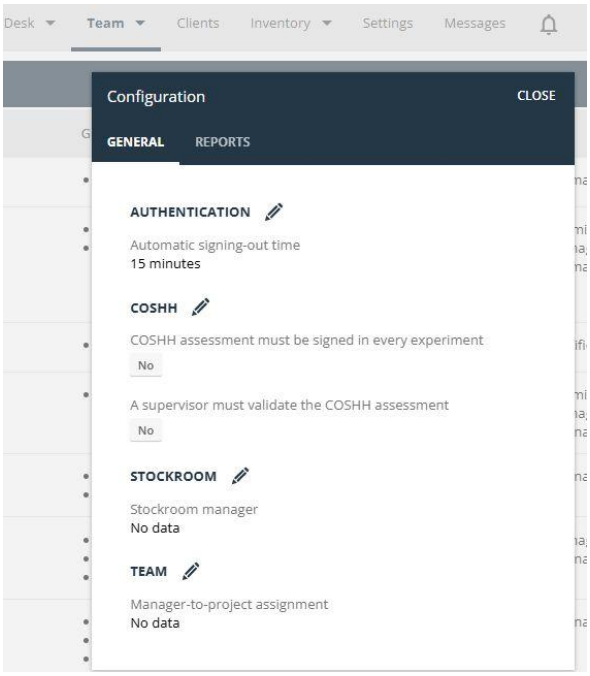
and to check user's activity (with the option to apply some filters as usual):



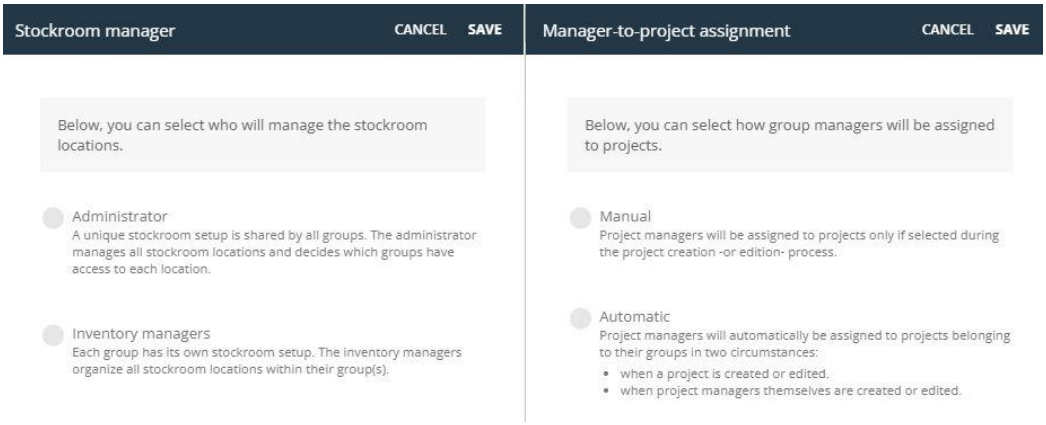
Admins can also change user's details, roles, permissions and COSHH configuration to other users :



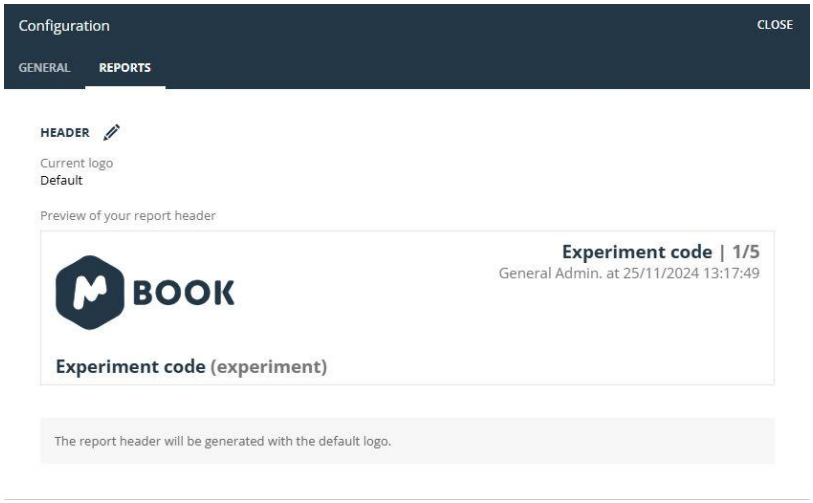
From the settings tab, the admin can control the automatic logout time (Minimun value: 15 minutes; maximum: 12 hours) and select some COSHH settings:



From here the admin and also choose the desired configuration for the Stockroom manager and also how the Group Manager will be assigned to the new created projects:



Clicking on the Reports tab will allow the admin to select the desired report header:



If your group is small, then this role is rarely needed. It is useful for organizations that have several sites or very distinct working groups within a lab, for example, separate groups for analytical and synthetic chemistry.

In the future, we expect the administrator role to become more important in Mbook as we add functionalities that will require an authorized user to supervise them.

- **Group Manager:**

The Group Manager role is intended for team leaders with management and lab responsibilities. The Group Manager can create users, groups (if the Admin allows), and clients (but not reactions or experiments). In addition, Group Managers can assign additional permissions to other users so they can be made responsible for inventory, safety, or structures.

A Group Manager can be removed from a group or project only by himself, other Group Manager or by an Admin user (and can remove others Project Managers or Bench Chemists users from a project or group).

Witness and approval of experiments are also parts of the permissions granted to Group Managers by default, as well as being able to designate other users who can also witness and approve.

> ***NOTE:*** *When a compound has associated experiments, the user can modify the existing one which implies an approval request (by message) to all the structure managers (only one approval will be needed). If the modification is approved, a message will be sent to the users responsible of the experiments and to the associated project managers. In case of closed experiments (or equivalent), they will be opened again. There is no automatic modification of the experiment. These modifications (if any) are the responsibility of the owner of the experiment.*

- **Project Manager:**

This is a suitable role for staff members that own projects but are not in charge of teams and do not have management responsibilities. As such, Project Managers can create and manage projects, but not users, groups, reactions or experiments; they can, however, assign an existing user to their projects. Project Managers can also witness and approve experiments.

A Project Manager can be removed from a project by himself, other Project Manager or by a Group Manager. However, a Project Manager can't remove a Group Manager from a project but can remove others Bench users from a project.

- **Bench Chemist:**

This role is designed to for chemists that have neither management responsibilities, nor ownership of projects. A Bench Chemist can create reactions and experiments, but not groups or users. They can also witness experiments and manage the supply of compounds (bottles). By default, Bench Chemists will only see their own experiments in the Desk Panel navigation tree, but this can be modified if required.

- **Inventory Manager:**

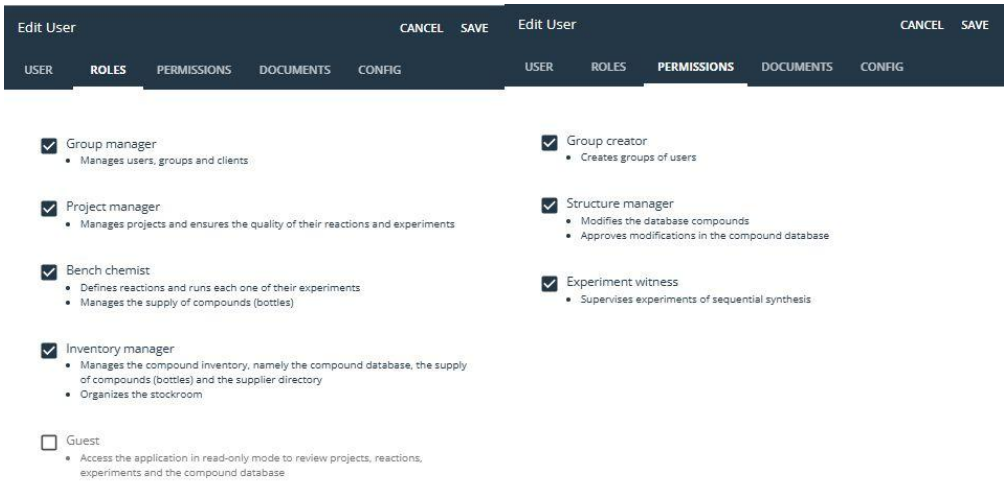
This role is designed to manage the compound inventory, equipping users with tools to organize the stockroom, including maintaining the compound database, tracking the supply of compounds (bottles), and managing the supplier directory.

For further information about the Inventory Manager, please follow this link.

- **Guest:**

This role was added to Mbook in version 2.1 following requests for such from various Contract Research Organizations (CROs). CROs wanted to be able to prove their expertise in certain processes to potential clients, or to show existing customers the progress on their projects via the CRO. With this in mind, Guests only have permission to see projects or groups that they have been granted access to.

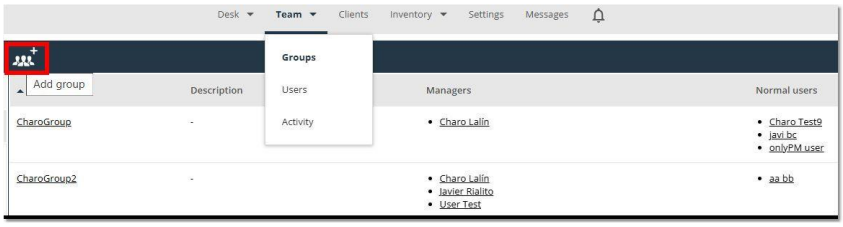
In addition to these roles, Mbook offers the possibility of further customization of permissions by allowing Group Managers to designate Inventory or Structure Managers and to allow the same user to have a mix multiple roles.



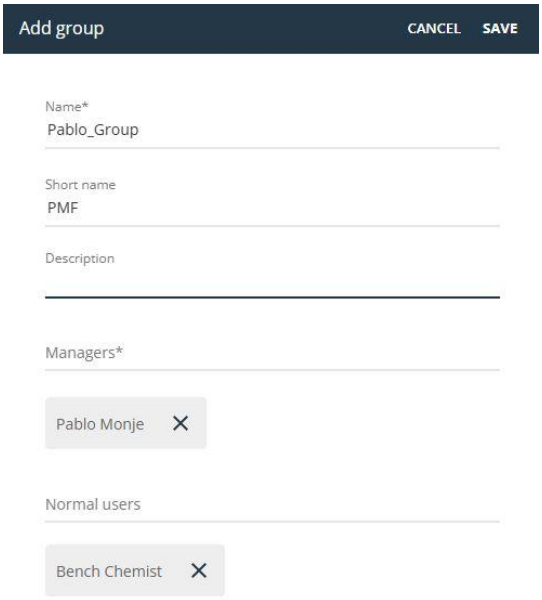
3.2 Create Users and Groups

ADMINISTRATOR - How to create a group and a user?

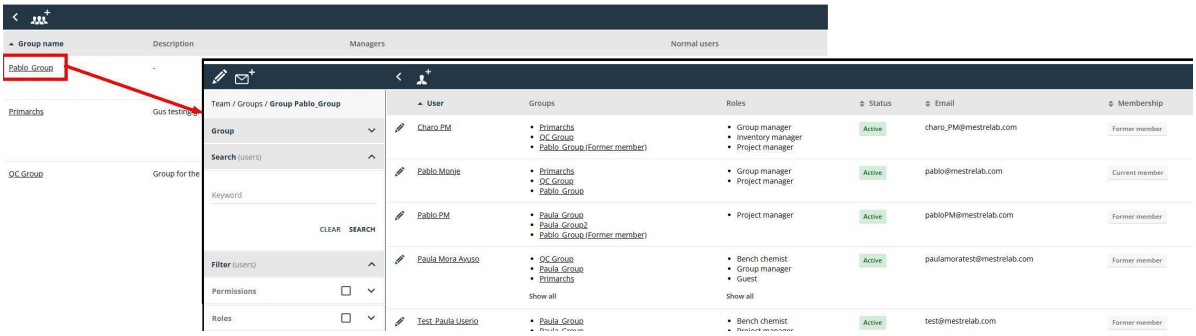
Click on the Add group button under the 'Team/Groups' section to create groups and and organize users as an initial stage.



The Group can then be defined by filling in the form so invoked and can then add any existing managers and users as desired:

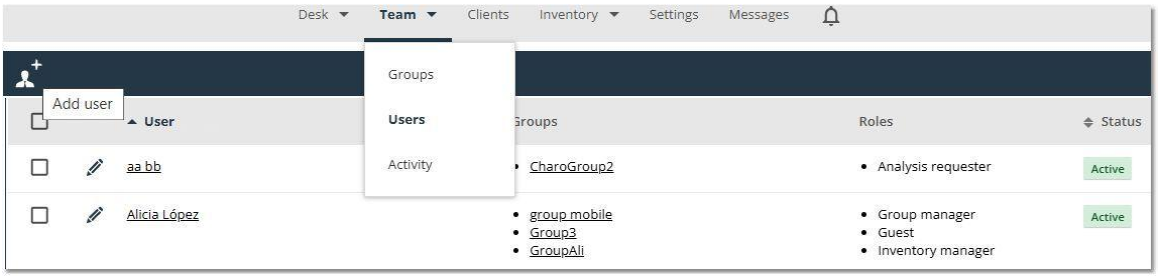


Once some groups have been created, you will find them listed on the Groups panel. You can click on any of them to list the users associated with a particular group:

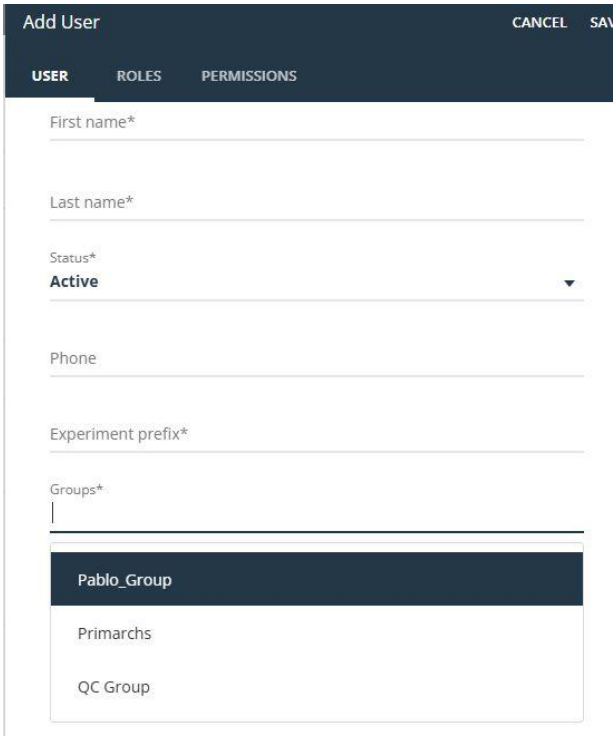


New users can be added to any existing group, just by clicking on the group (or on any existing user in the group) and then selecting the 'Add User' tool:

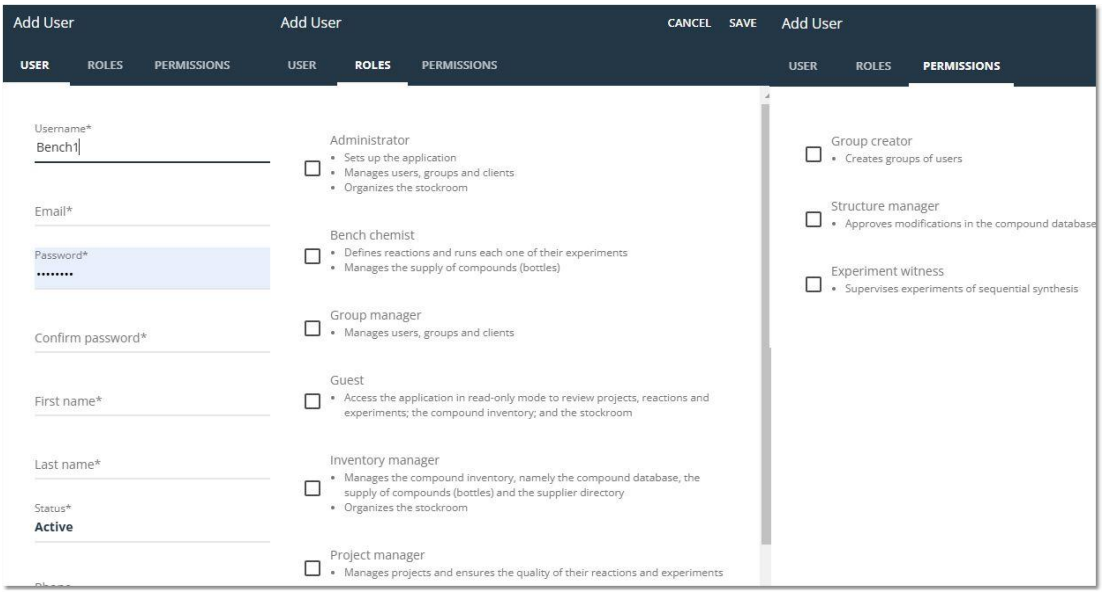
You can also create a user, by clicking on the 'Add User' button (under the 'Team/Users' scroll down menu):



From here, the Administrator needs to enter a username (with a valid email address), password, role, etc... Admins can also assign new users to any existing group:

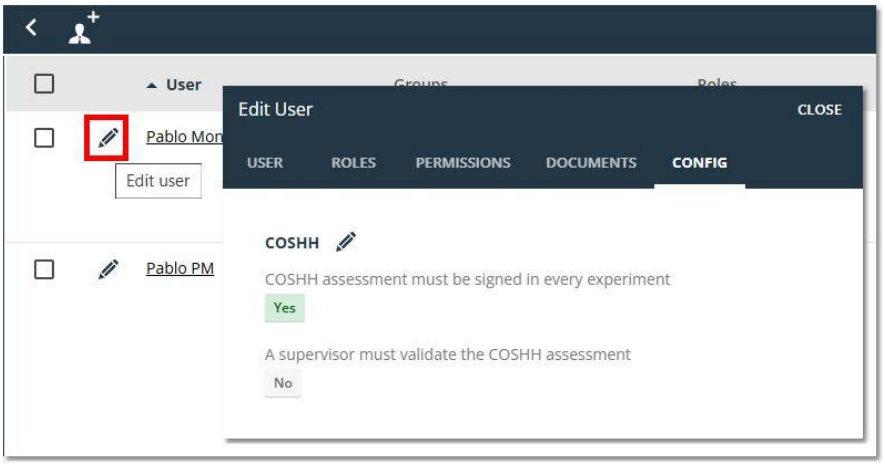


From here the Administrator can also select the desired roles and permissions:

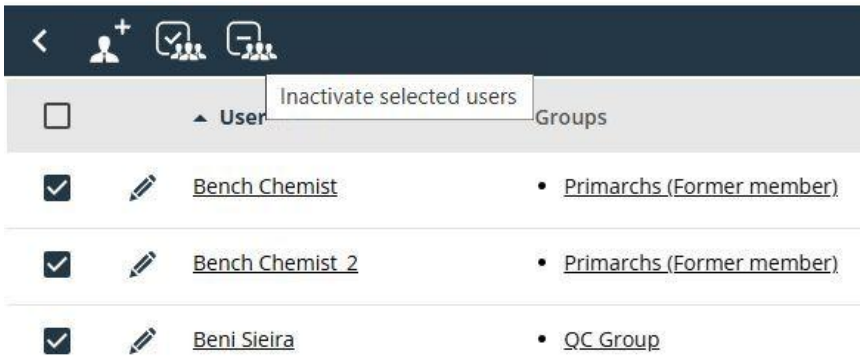


The Prefix field can be used to automatically generate experiment codes for experiments created by the user.

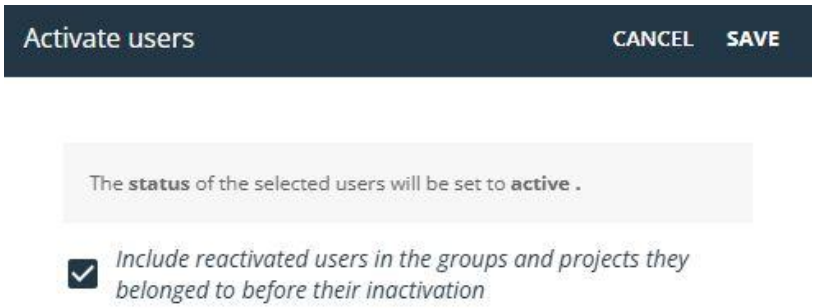
Clicking on the Edit User button will allow you to change user details, roles, permissions, add documents and modify COOSH configuration:



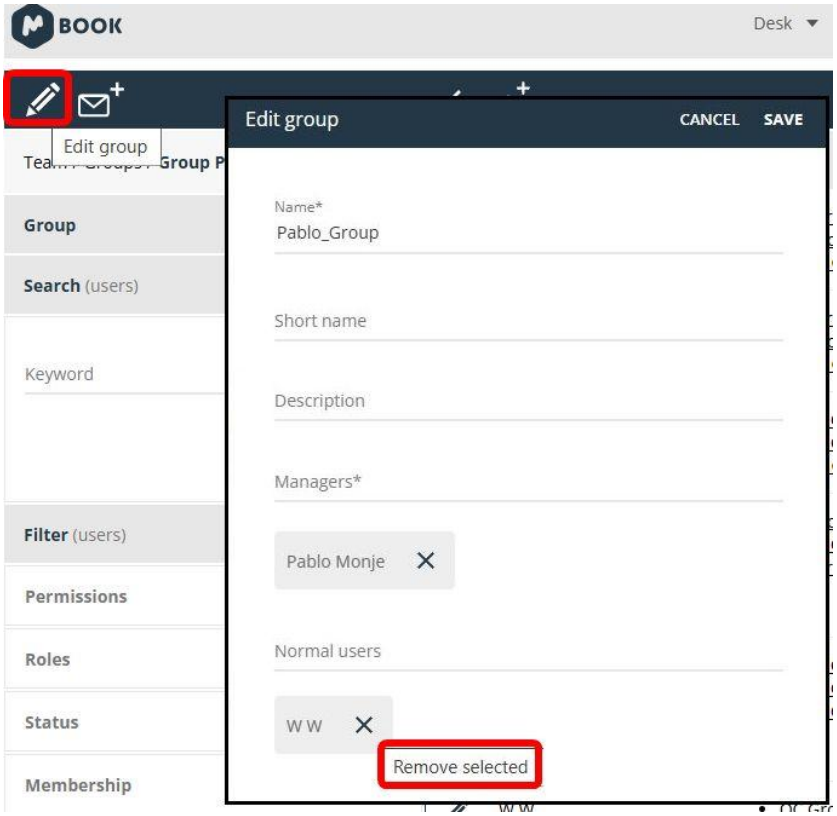
You can activate/inactivate several users at the same time by using the "Activate/Inactivate users" buttons:



Note that when a user is inactivated in this way, he/she will be removed from all groups/projects at once. When the user is activated again, you will have the capability to include him/her back in the groups/projects he/she belonged to before their inactivation.

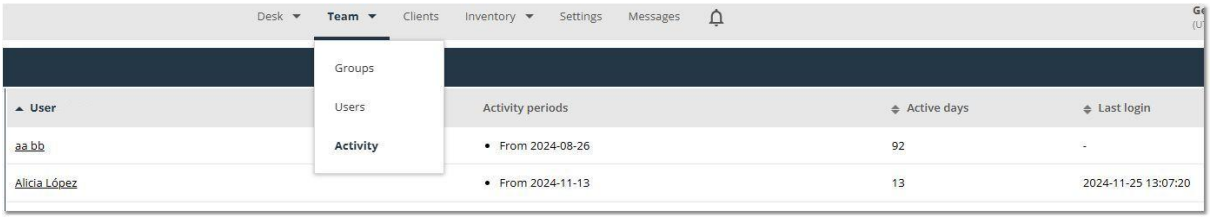


Users can be linked to or disabled from groups (and projects):



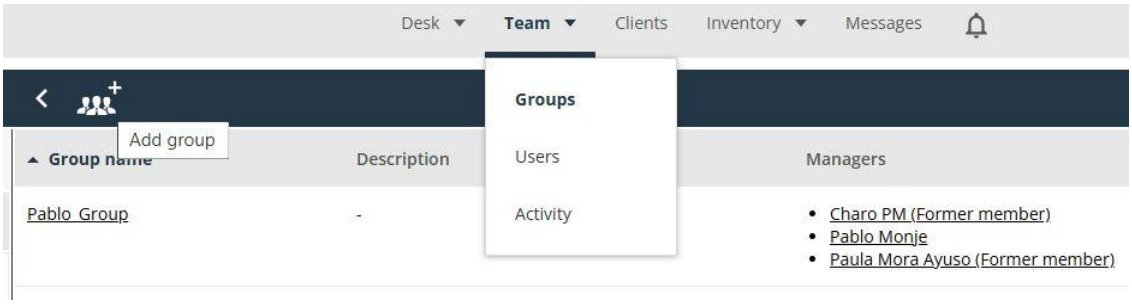
If a user is disabled from an existing group (or project), the remaining users and groups will still be able to see the data created by that user (whose name will appear in italics under the navigation tree).

Click on the 'Team/Activity' button to check some relevant information about the users:

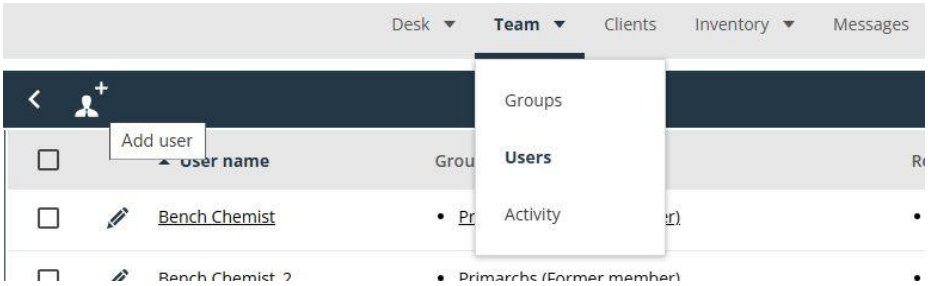


GROUP MANAGER - How to create a group and a user?

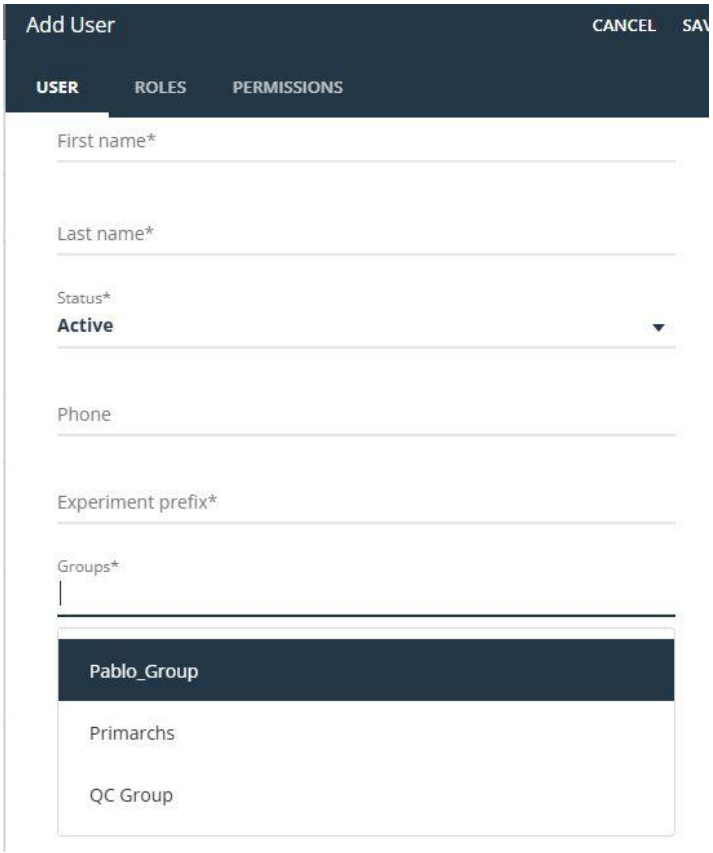
A Group Manager can also create users and groups (if the admin allows), among their other possible duties. As can be seen in the screenshot below, the Group Manager has different active tabs than an Administrator.



Then you can create users (as we described above for the admin role):



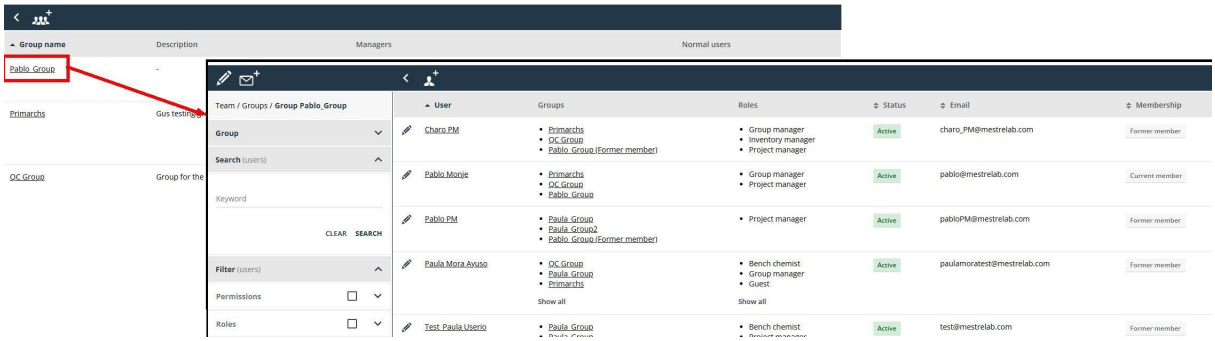
When the group manager is creating a new user, it is also possible to assign him/her to any existing group:



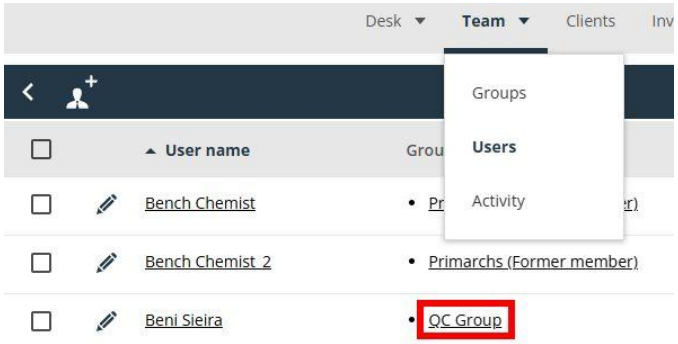
Please note that a Group Manager can also assign individual privileges to any user, for instance, as an Experiment Witness, an Inventory Manager, or a Structure Manager.

3.3 Managing Groups and Users

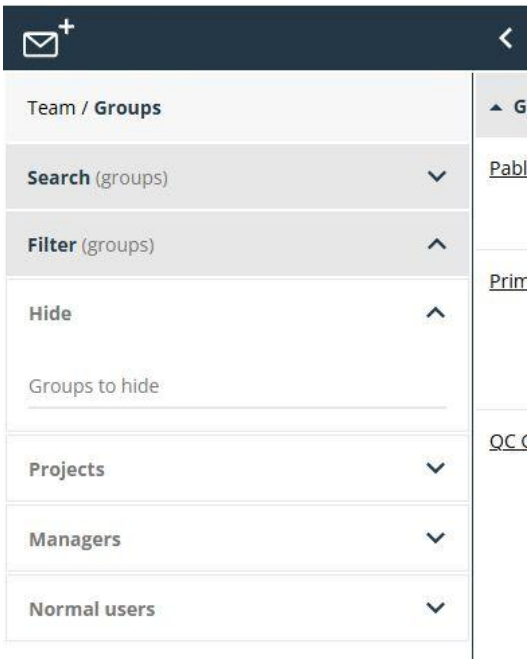
Left clicking on the group name will display the group's users and will allow you to send messages to all users or edit the current group. From here, you can also check the group documents:



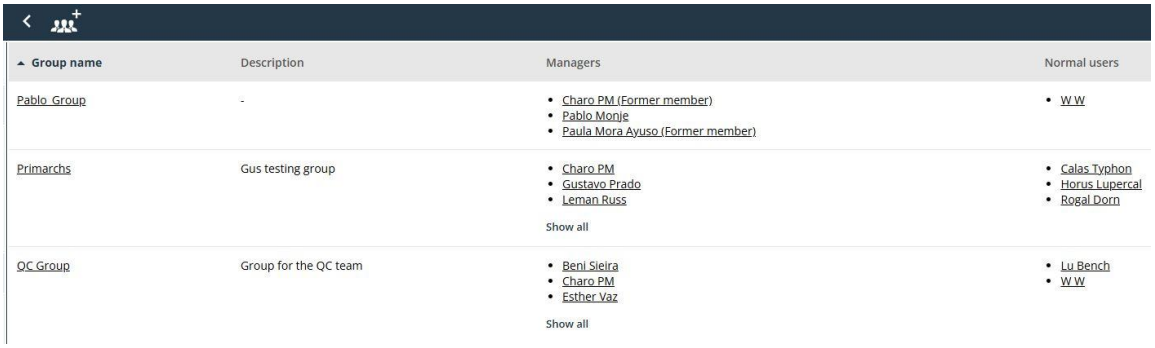
You can also manage the groups by clicking on the Group name from any table or component that allows it (for example from the Users list):



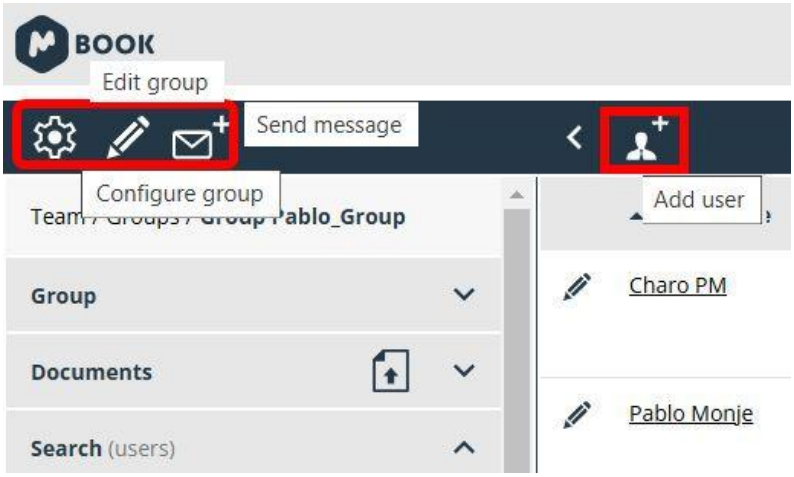
The groups page is divided in two sections, on the left side you will find a collapsible dialog which will allow you to search and filter groups by projects, managers and normal users:



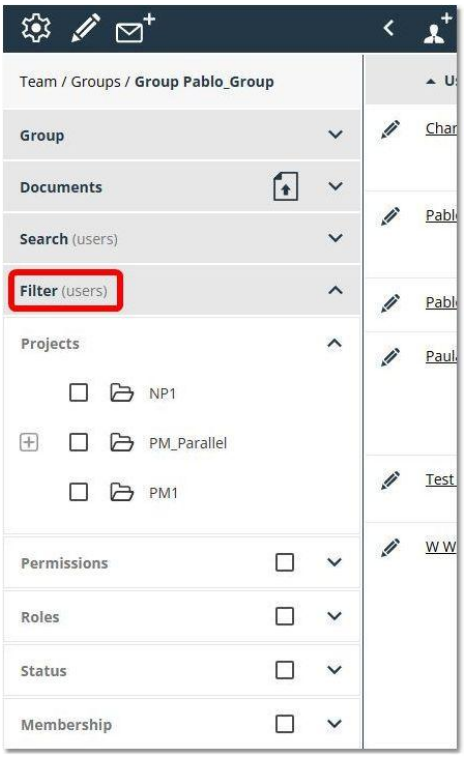
On the right side, you will find the groups list with information about the name, description, managers and normal users:



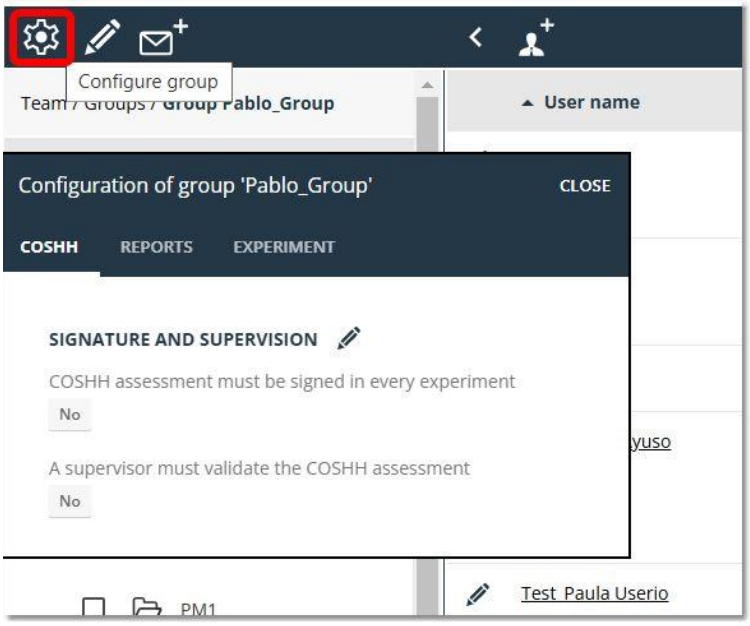
Once you have selected any group, you will find a button to configure the group, to edit its details, to send a message to another user and to add users:



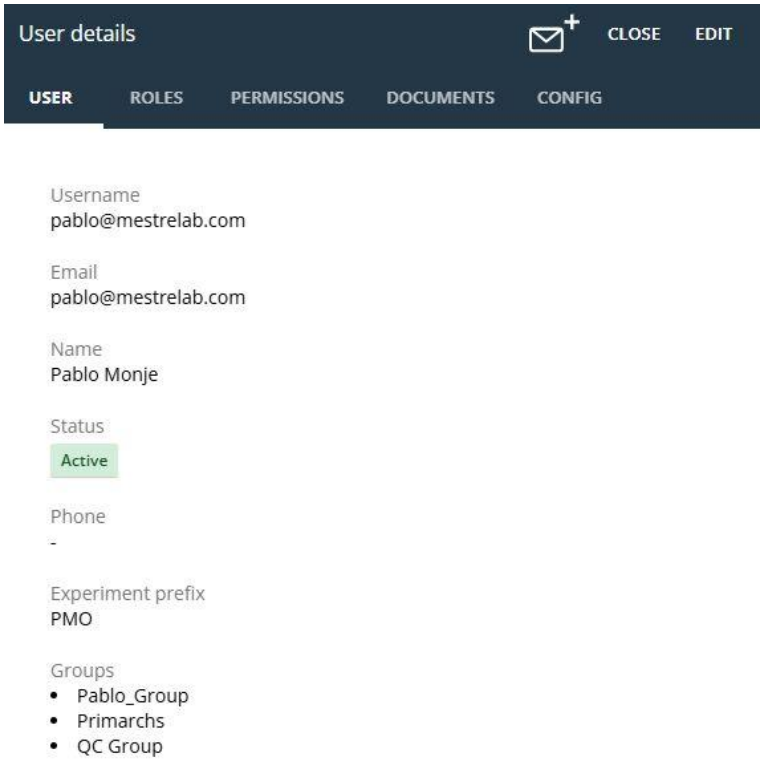
From the left panel you will also be able to find and upload documents (general, health/safety, bibliography, etc) and to search and filter users by project, permissions, roles, status and membership:



Click on the 'Configure Group' button: to select 'COSHH assessment' settings, a signature footer and custom settings for the stoichiometric table:

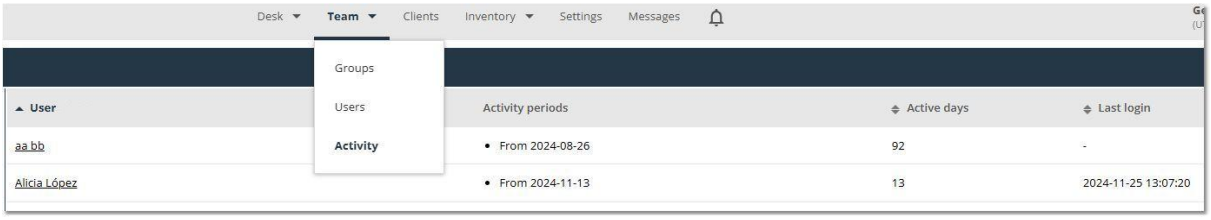


Left clicking on any existing user will display all user details (roles, permissions, documents and COSHH configuration):

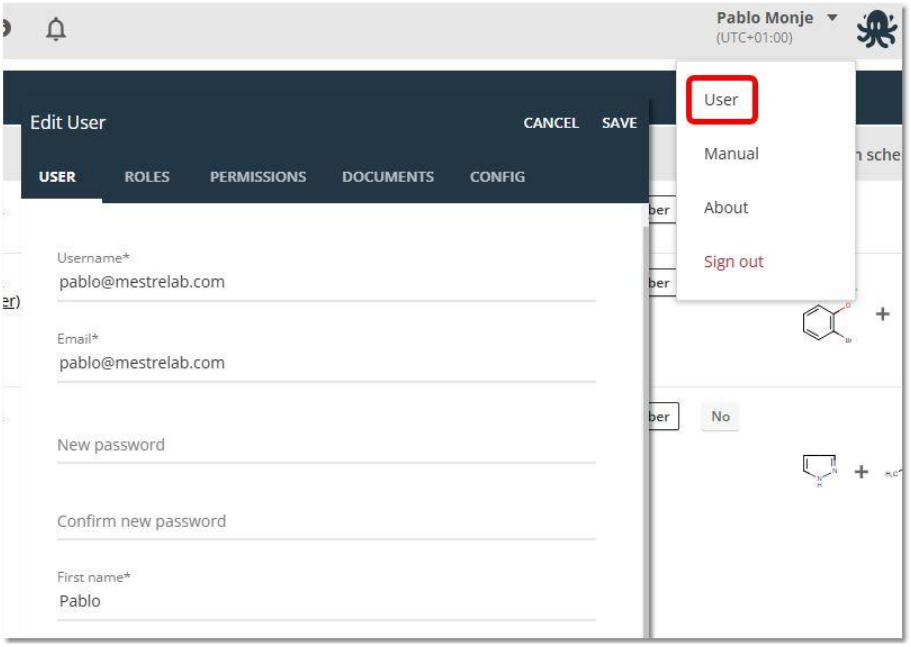


Clicking on the 'Edit User' icon will allow you to edit a given user's details (password, status, role, etc.):

Click on the 'Team/Activity' button to check some relevant information about the users:



Every user can edit his/her own information by selecting 'User' from the top right scroll down menu and clicking on 'Edit¡:



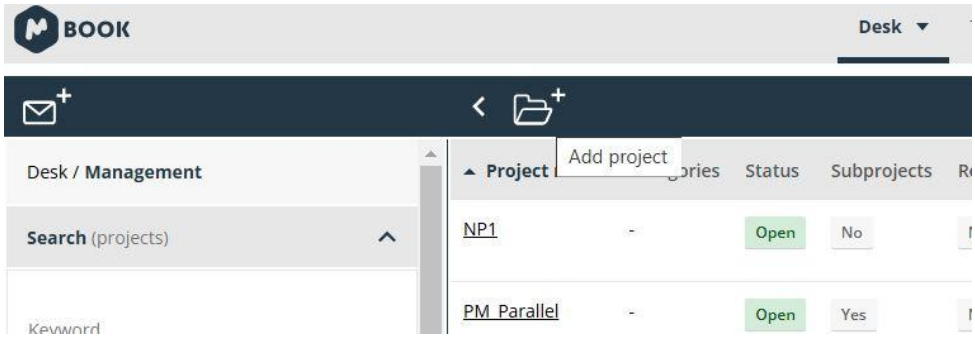
From the same scroll down menu, you will be able to get the manual and to check the Mbook version.

Part

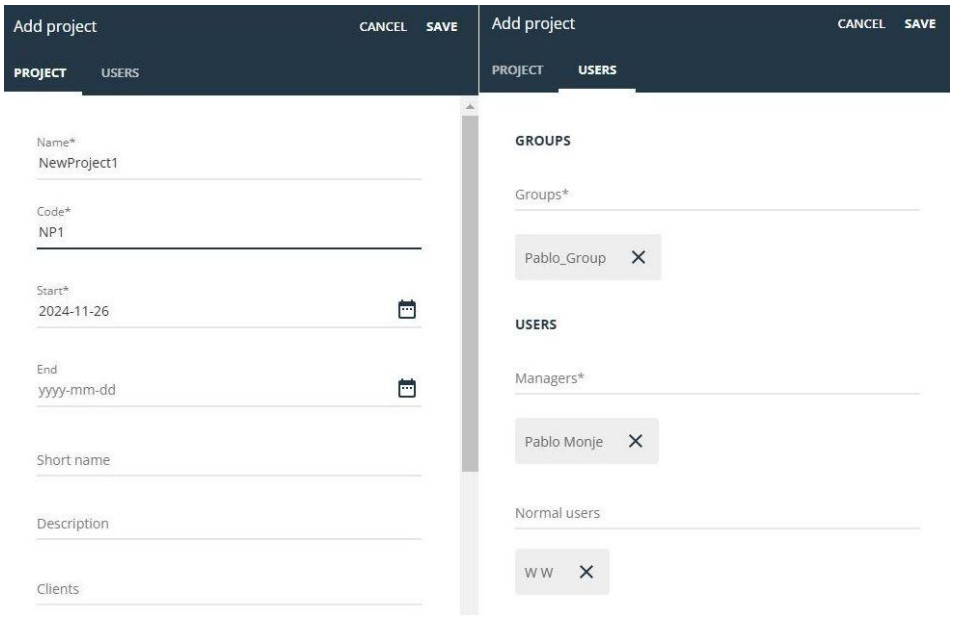
4 Creating Projects

How to create a Project?

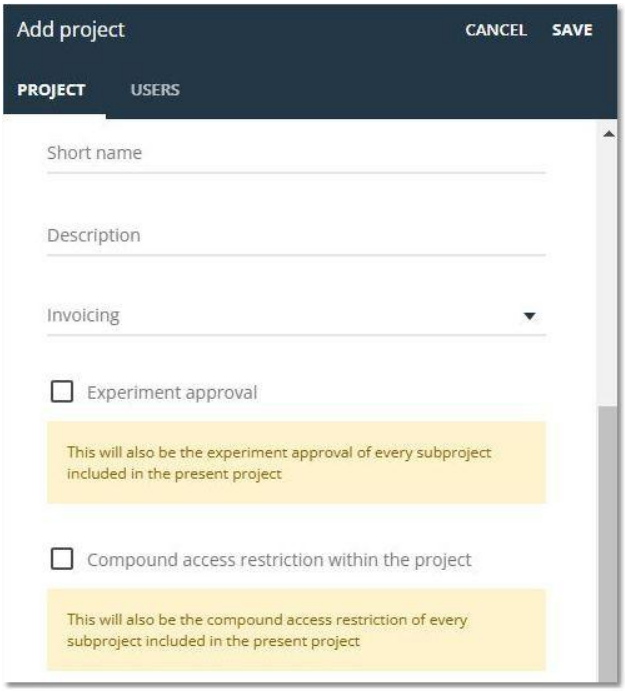
Once a group has been created, a 'Group or a Project Manager' will be entitled to create a project, just by clicking on the 'Add Project' button from the 'Desk/Management':



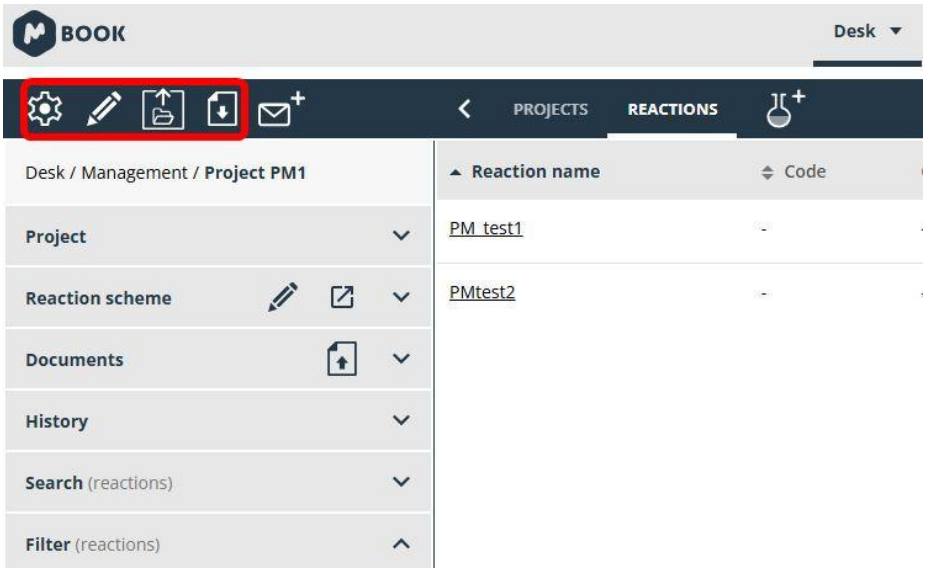
To add a new Project, the group manager will need to type a 'Project Name' and 'Project Code', 'Start Date' and the groups and users involved in the new project:



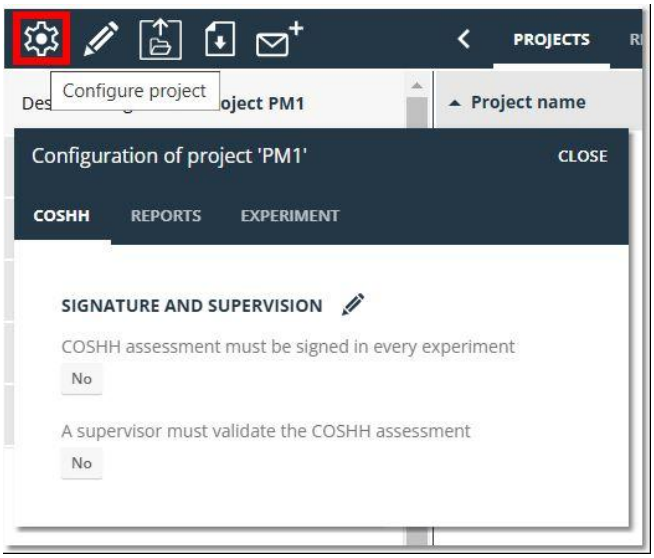
Check the 'Experiment Approval' box if you want that the Group Manager must approve the project experiments. If the 'Compound access restriction within the project' option is selected, the new structures added to the project experiments will be only visible to their project members. If this option is not selected, all the members of the group to which the project belongs will have access to the structures, regardless of whether they belong to this project or not.



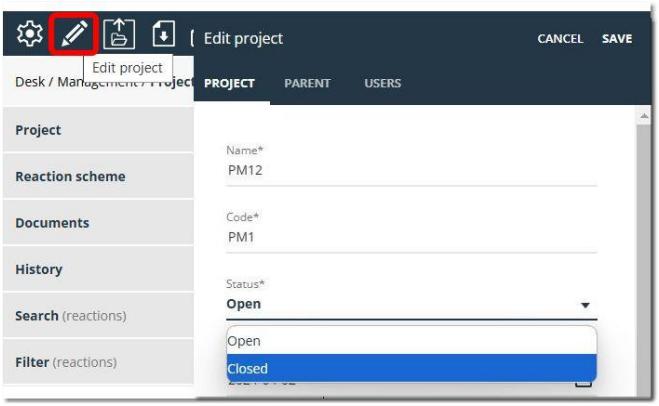
Once you have created the desired projects, these will become listed in the right panel. A user only has access to view and search the projects in which he/she is involved.
Clicking on the Project Name will allow you to configure, edit, export, or download its report:



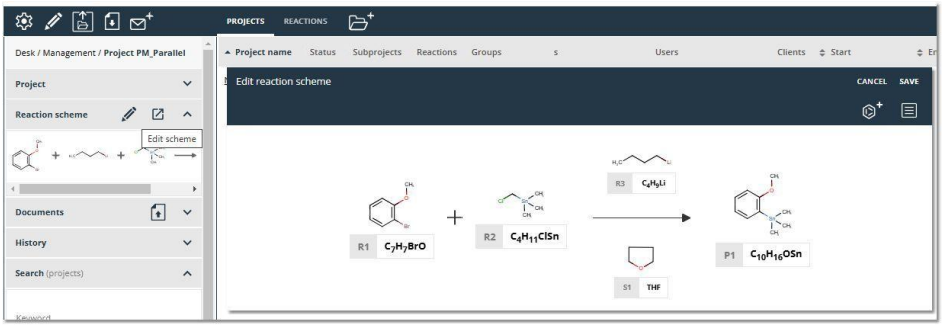
Clicking on the 'Configure Project' button will allow you to set up the COSHH assessment, the signature footer reports and the stoichiometric table:



For reasons of integrity, it is not possible to delete projects. However, you can 'Edit the project' and change the status (from **open** to **closed**):

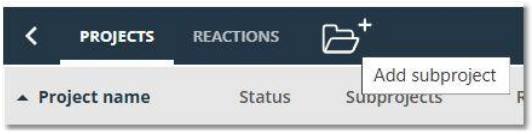


You can define a reaction scheme for your project:

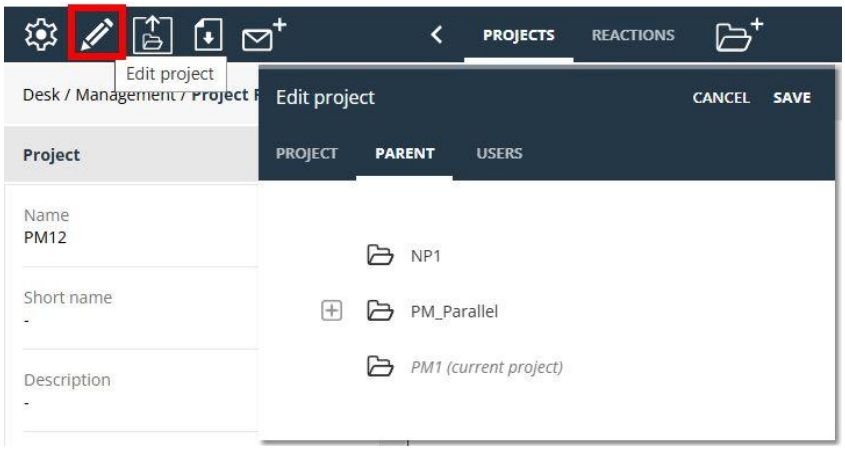


You will also find certain collapsible tabs that allow to check information about the project, reaction scheme, documents, history, search, filter.

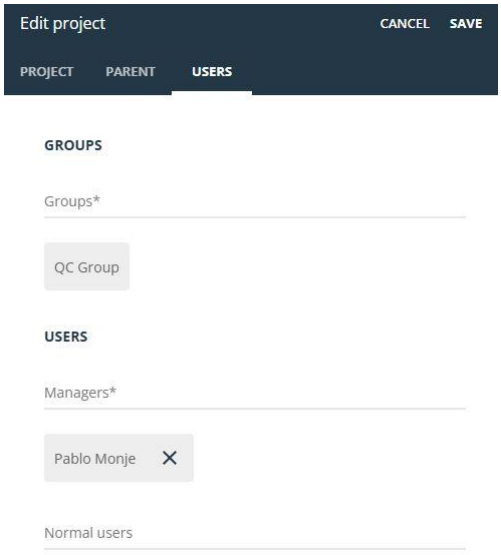
Subprojects can be created just by clicking on the 'Add Subproject' button (from the parent project panel):



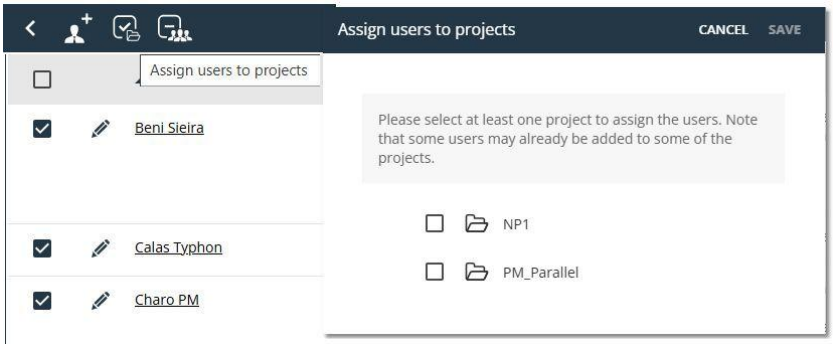
You can change the parent project by clicking on the 'Edit Project' button and using the 'Parent tab':



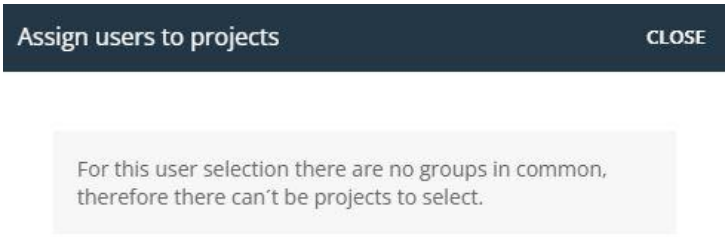
Selecting the 'Users' tab will allow you to edit the Groups and users associated to the project:



From the Team/Users tab, if you check the boxes of several users belonging to the same group, you will be able to assign them to the desired projects at the same time.

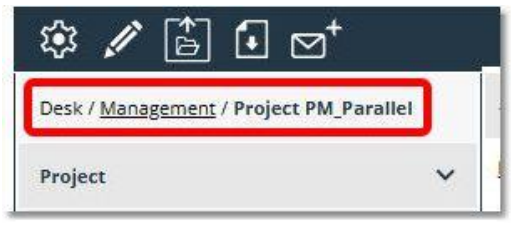


If the selected users do not belong to the same group, you will get this error message:

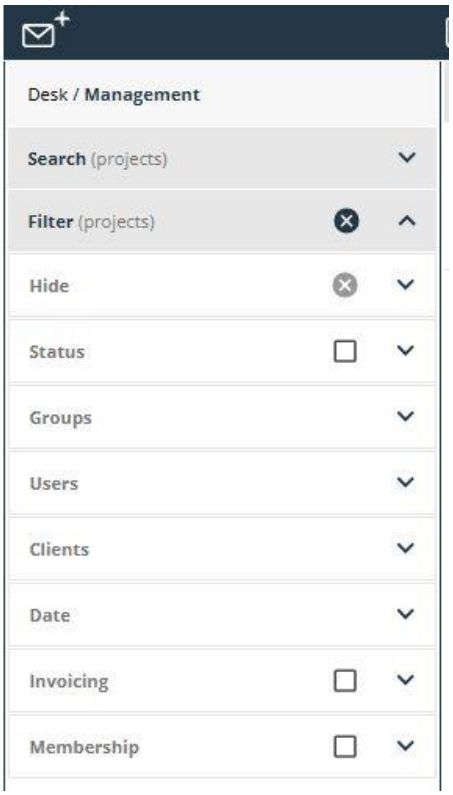


If there are no projects associated to the users, you will get this message:

The breadcrumb displays the hierarchy of all the parent projects (if any). Clicking on a project name redirects the user to the corresponding project page:

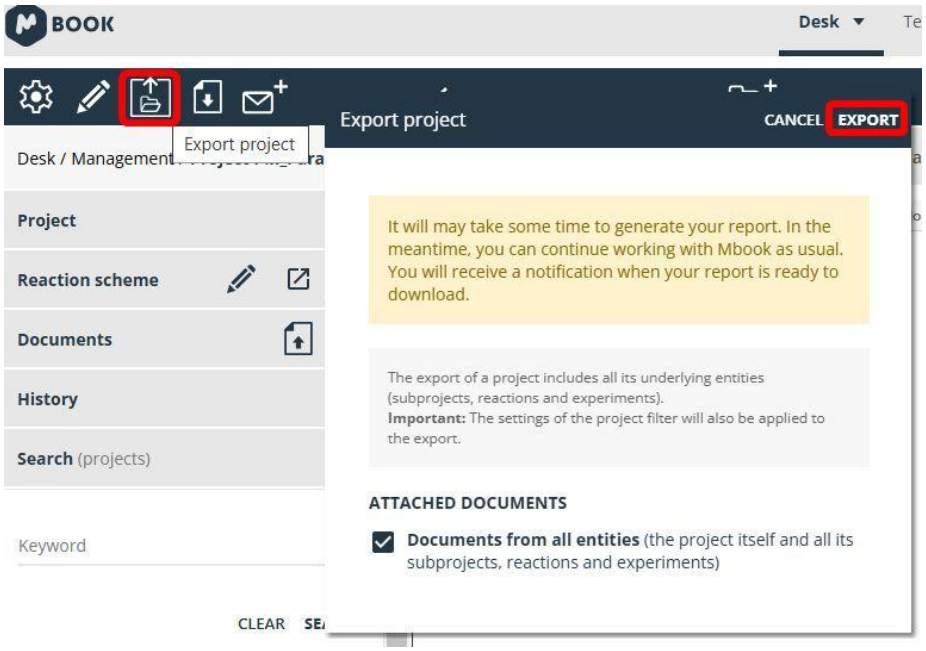


You can search by projects by using keywords and filter them by name, status, groups, users, clients, date, invoicing and membership:

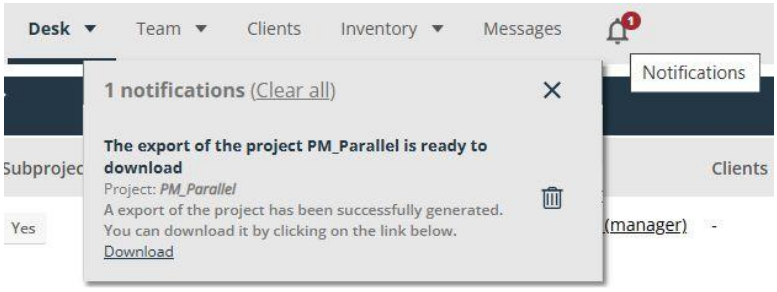


4.1 Export Projects

You can export an entire Mbook project with its subprojects, reactions, experiments and documents, just by clicking on the "Export Project" button (only available for Group or Project Managers).



Once the export is complete, you will get a notification displayed on your screen that allows you to download it as a zip archive.



You will also receive an email with the notification.

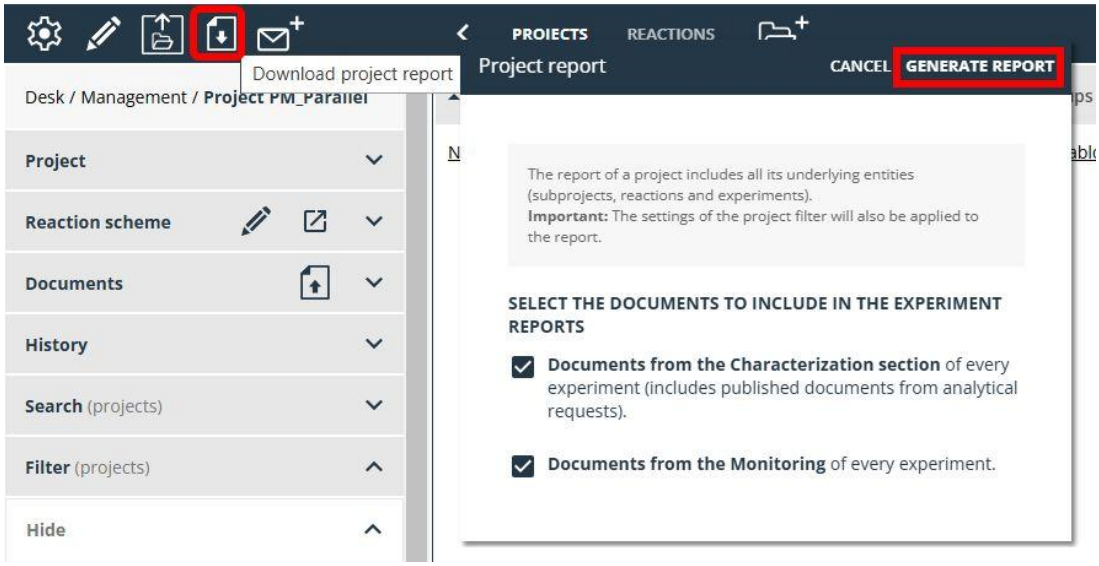
The generated ZIP file will contain:
-an XML file for the project
-a folder for each reaction
-an XML file for the reaction
-a folder named 'experiments' containing a ZIP file for each of the experiments in this reaction
-this ZIP file (experiment) contains two files: an XML file with the experiment, and a SDF file for the experiment
- a recursive list of the folder/subfolder structure mapping the same structure for the project (subprojects/reactions/experiments)

Each of the XML files contains a property, 'buildNumber', that includes the version and release information for the Mbook Instance generating them.

You can import single experiments by following the instructions described in this chapter.

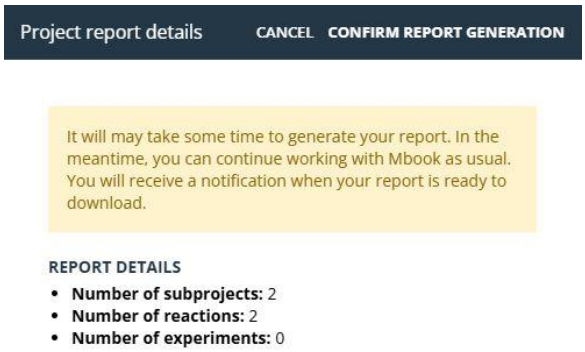
4.2 Report Projects

Group and Project Managers can generate PDF reports for an entire project (including subprojects, reactions, and experiments) just by clicking on the 'Download Project Report' button. After that, a new pop-up dialog will be displayed to allow you to select which documents included in the experiments within the project will be included in the PDF report.



As usual, clicking on the filter button will allow you to filter 'Projects' by, 'Categories', 'Status', 'Groups', 'Users', 'Clients', 'Dates, etc. The selection chosen will be used to generate the project report (in an otherwise identical manner to the reaction project and its filter).

Clicking on the "Generate report" will display a summary window that includes the number of subprojects, reactions, and experiments:



You will receive a notification once the report is complete and can continue working as usual with Mbook in the meantime.

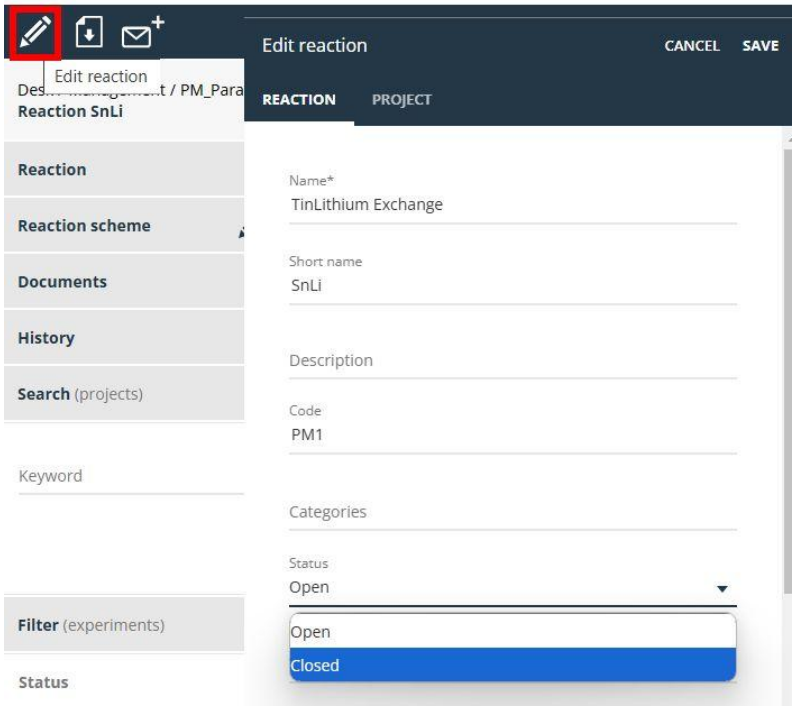
The project report is saved in the form of a zip archive (with the name of the project) containing a PDF file with a summary of the project and several folders (one per reaction).
Inside each reaction folder, you will find a reaction PDF report and the experiments folder, containing the individual PDF reports.

Part V

5 Creating Reactions and Experiments

Selecting any of the available projects in the left panel and clicking on the appropriate button will allow you to add reactions:

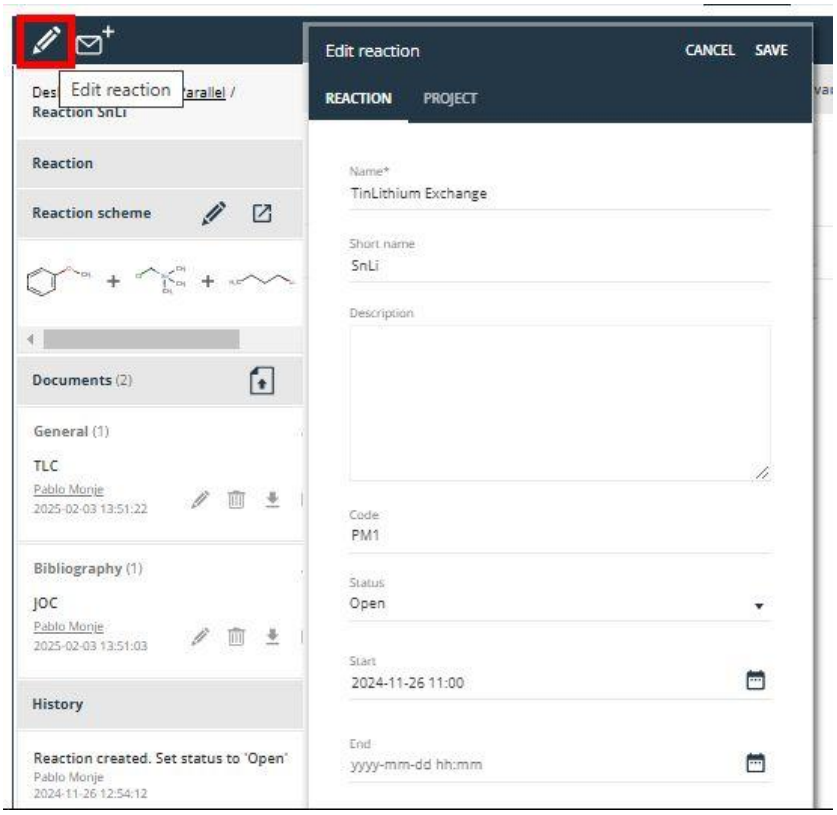
For reasons of integrity, it is not possible to delete reactions. However, clicking on the reaction name will allow you to 'Edit the reaction' and change the status (from **open** to **closed**).



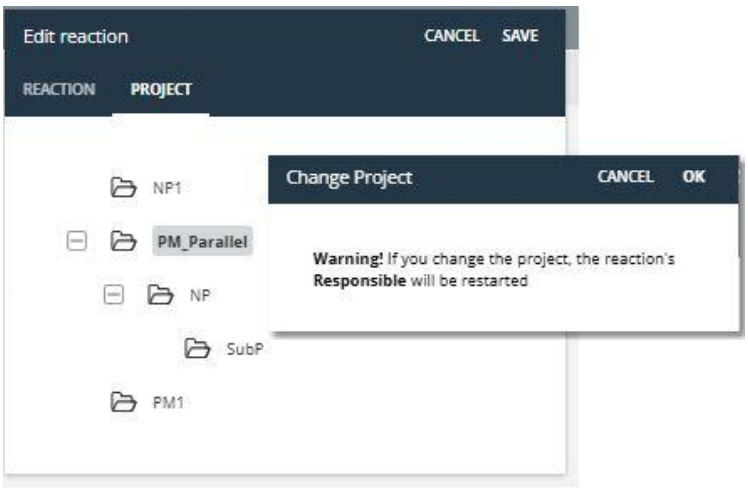
You can find the list of reactions under the 'Reactions' tab:

Clicking on the Edit reaction button will display the reaction dialog in the edition mode. This dialog contains two tabs, Reaction and Project. From the reaction tab, there is a form to be filled by the user

with the current values of the reaction: Name (mandatory), Short name, Description, Code, Categories, Status, Type, Optimization Type, Start, End, Invoicing and Responsible.



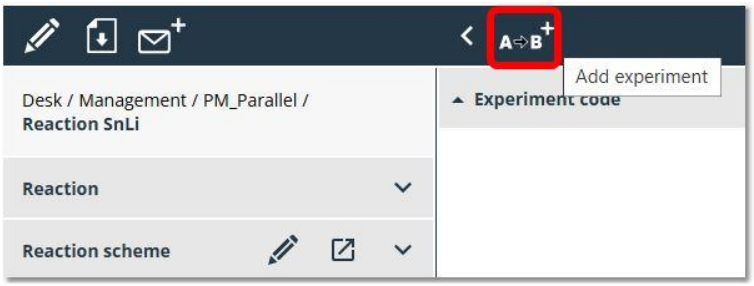
From the project tab, you can move the reaction to a different project. The current project will be highlighted in the tree. Selecting a different project in the tree displays a warning message to advise that the responsible user will be deleted. After clicking on OK, the reaction will be moved to the indicated project.



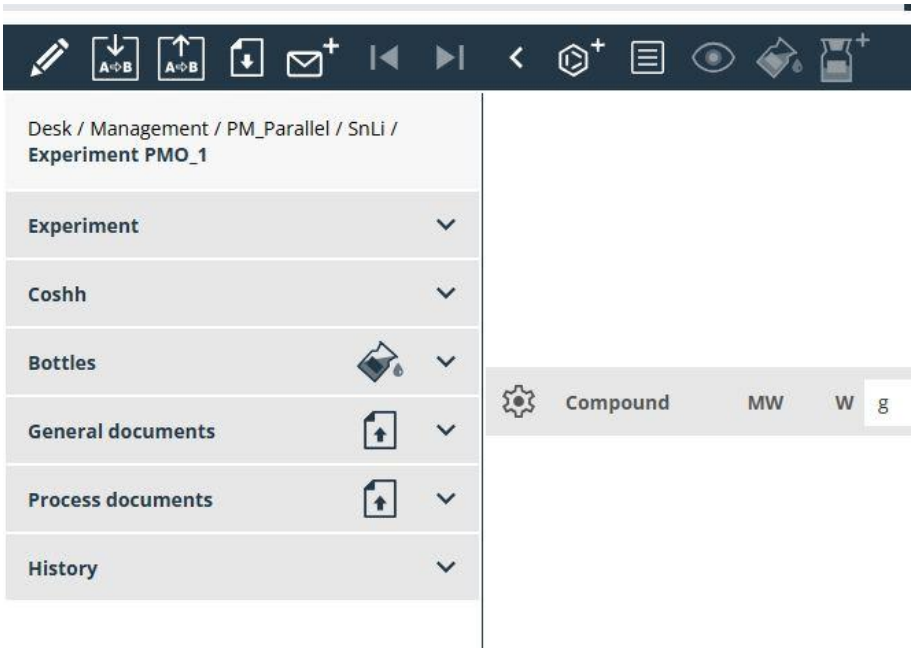
You can add a reaction scheme and upload some documents (general of bibliography) from the left tabbed menu:

In the History section, you can find a list of events through the lifecycle of the reaction. Each entry displays an informing message, the user who performed the action and the date:

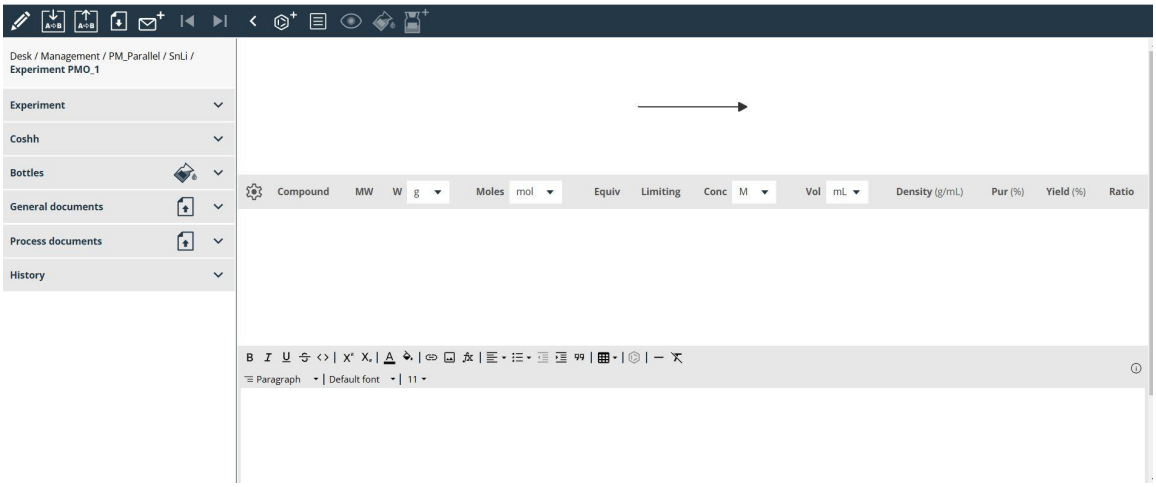
Once you have created the reaction, you will be able to add experiments just by clicking on the reaction name and selecting the 'Add Experiment' option:



In the example below, we have created an experiment called ‘PMO_1’ in the ‘SnLi’ reaction of the ‘PM_Paralell’ project:

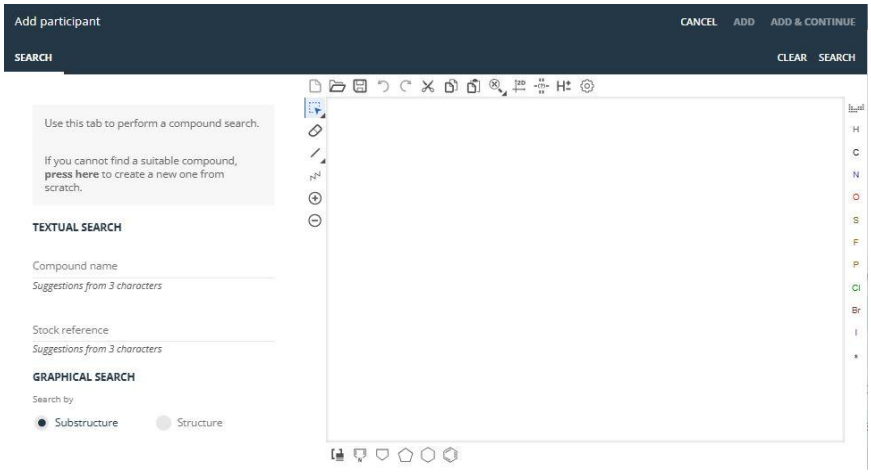


The next step is to add information about the experiment (reagents, products, amounts of reactants, solvents and products, reaction description, etc.):

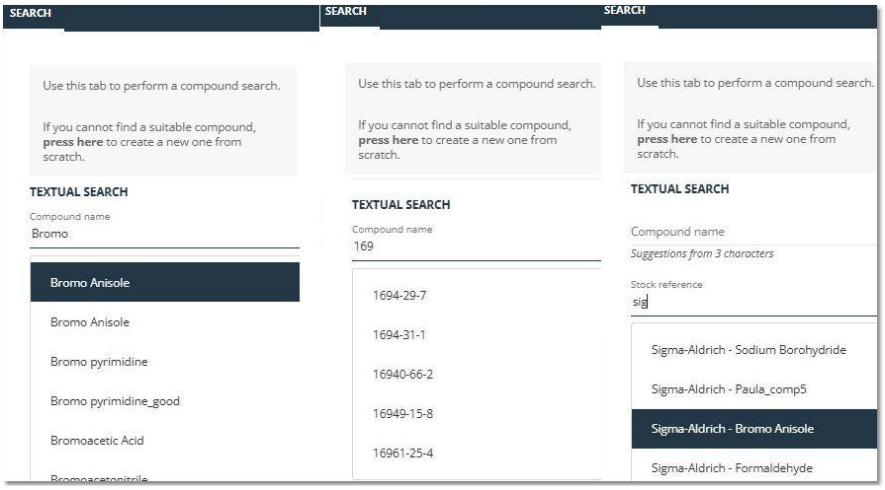


You will find a toolbar  to add participants, select experimental conditions (temperature, time, pressure, pH, etc.) , show/hide (reactants, solvents, and/or products), assign sources or create bottles.

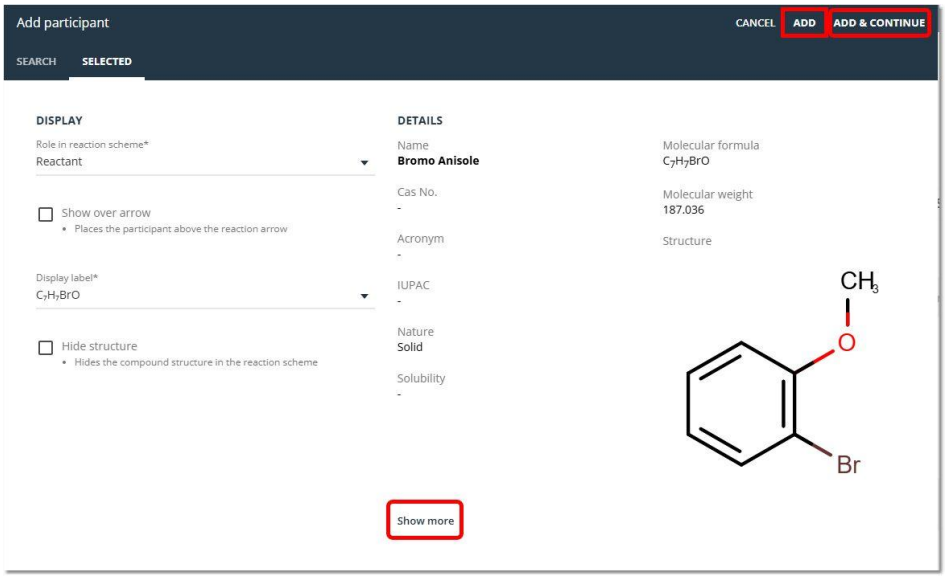
Clicking on the 'Add Participant' button  will allow you to add a participant to the experiment.



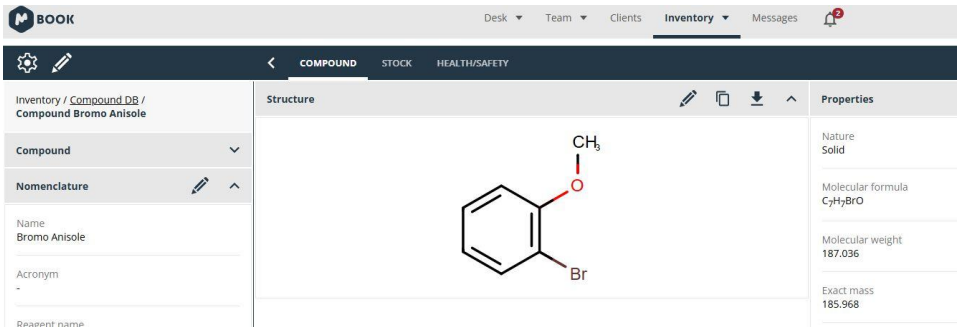
You can type the name (or at least three letters) of the desired compound (acronym, molecular formula, CAS Number, stock reference, supplier etc.) in order to search the database for that substance (this will be faster than drawing the molecule in the molecular sketcher, so we recommend you to attempt to find your reactants in the database in the first instance).



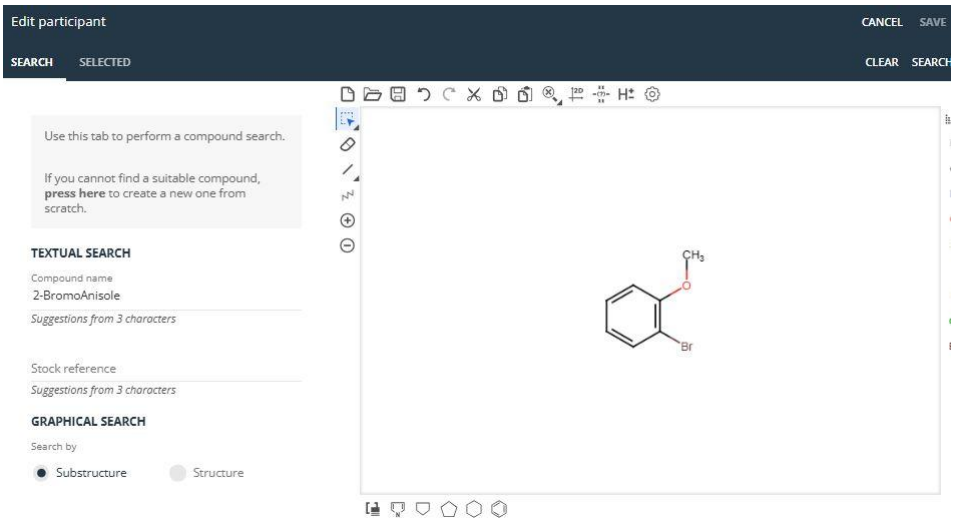
If the compound is included in the Database, a new dialog will be displayed to confirm the structure and select the label displayed in the reaction scheme. Clicking on the 'Role' scroll down menu will allow you to select the role of the new participant (reactant, solvent, or product). Check boxes will be available to include the new participant in the graphical reaction or in the arrow section.



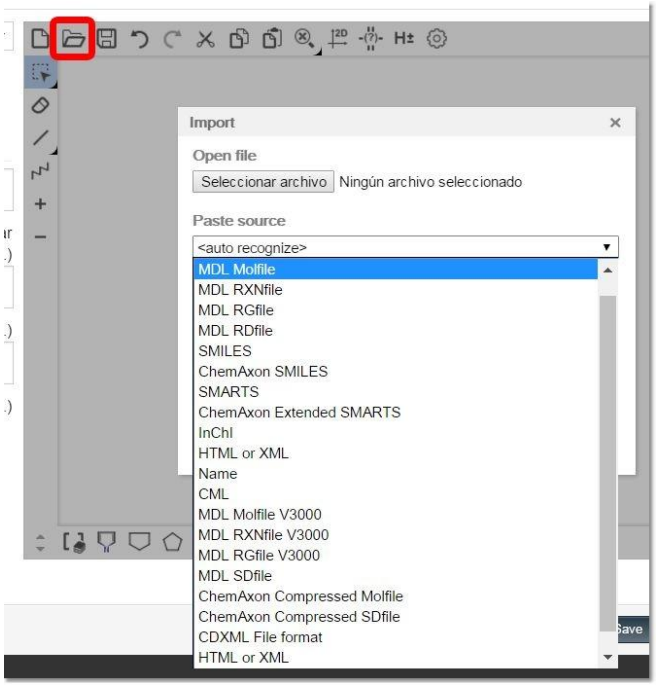
Clicking on the 'Show more' hyperlink (at the bottom) will display the record in the compound Database:



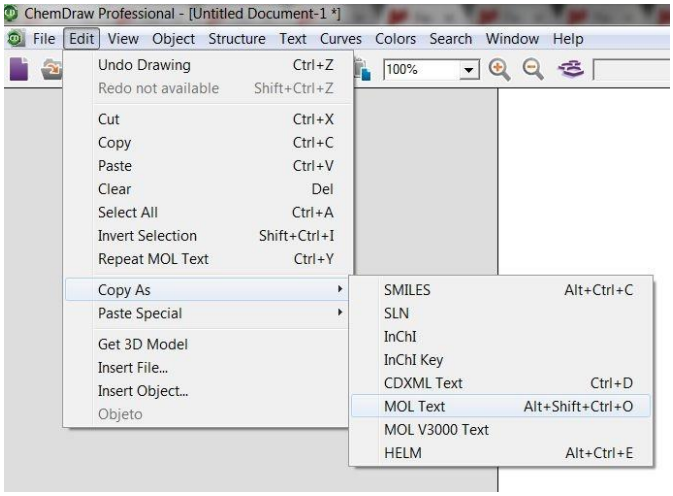
Clicking on the Add button (top left corner) will add the participant to the experiment. Clicking on 'Add&Continue' will add the participant to the reaction scheme and will allow you to continue adding other participants:



You can load molecules in the .mol, .cdx, smile, etc., formats by following the menu 'File/Import File (or even drag & drop .mol and .cdx files directly into the sketcher window):



You can also copy and paste structures directly from ChemDraw to Mbook using the 'Copy As: MOL Text' (shortcut Alt+Shift+Ctrl+O) option.

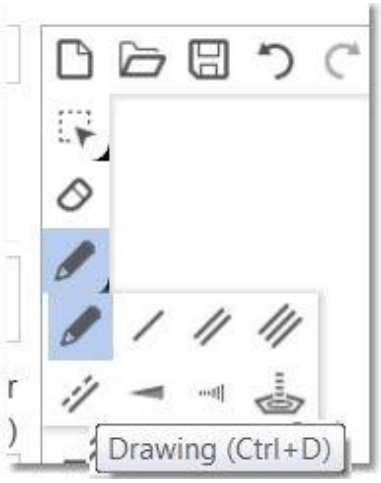


Of course, you can draw molecular structures using the sketcher itself (useful if your compound is not present in the database) or just drag and drop .mol files into the sketcher window.

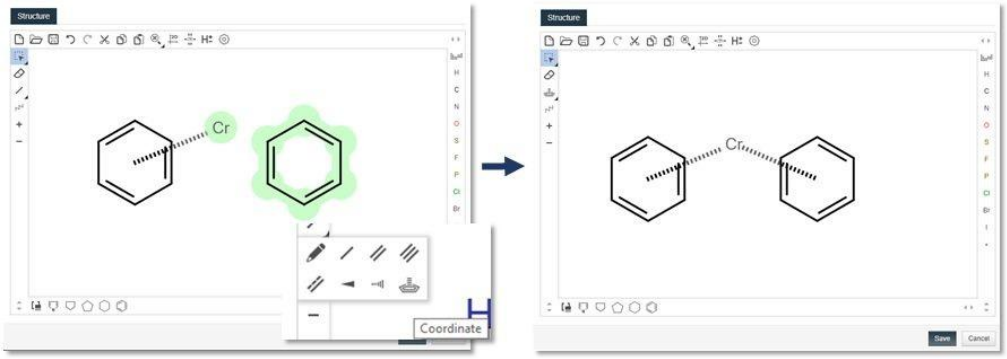
The 'Move' mode will allow you to move an atom or a bond just by clicking and dragging.

The Drawing mode (shortcut: Ctrl+D) will allow you to draw a carbon on your spectral window just by clicking and dragging on any empty field. Clicking on any existing atom will add an additional carbon. If

you click on a single bond, you will get a double bond (clicking on a double bond will convert to a triple bond).

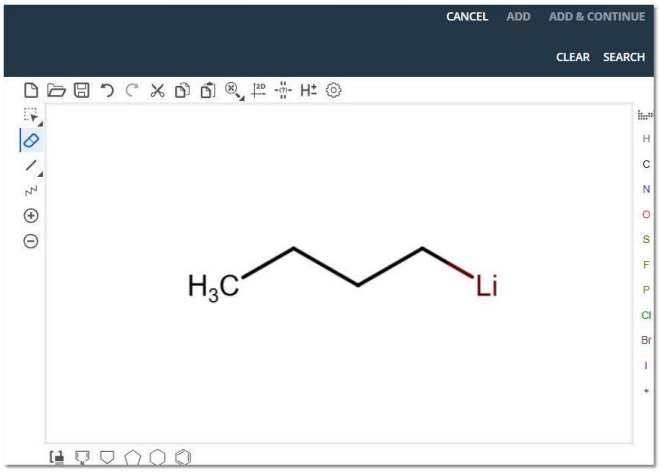


You can change the atom just by hovering the mouse over the atom and typing the applicable letter(s).

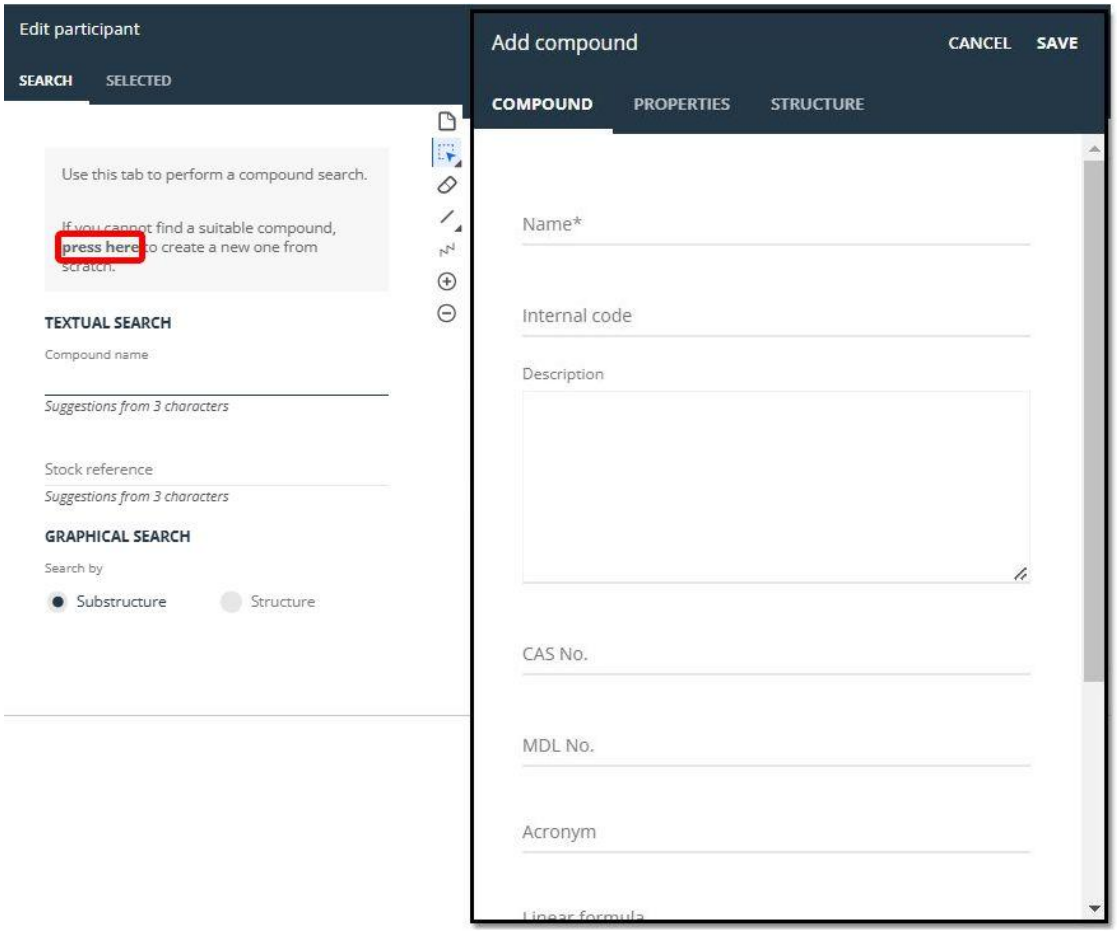


Mbook incorporates Marvin JS Sketcher. For further information about this program, please follow this link.

Once you have drawn the molecule, you can click on the 'Add' button to add the structure to the experiment graphic. You can also click on the 'Search' button to look for the molecular structure (or substructure) in the database.

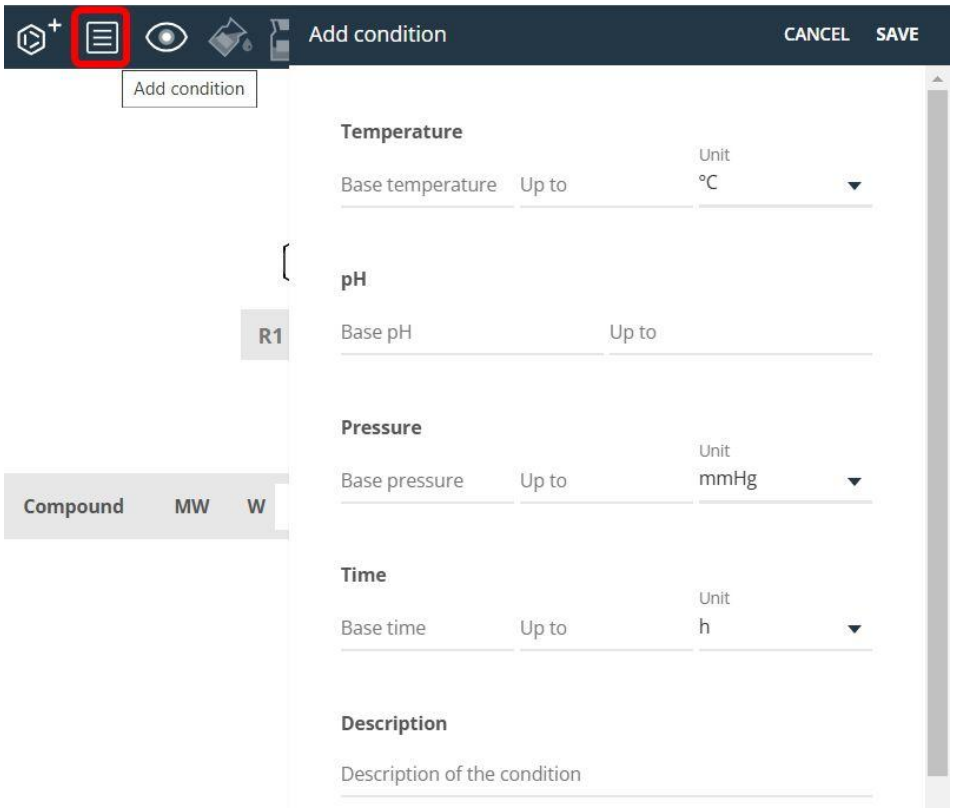


If the compound is not in the Database, you can select the option to **'press here'** to create a new compound:

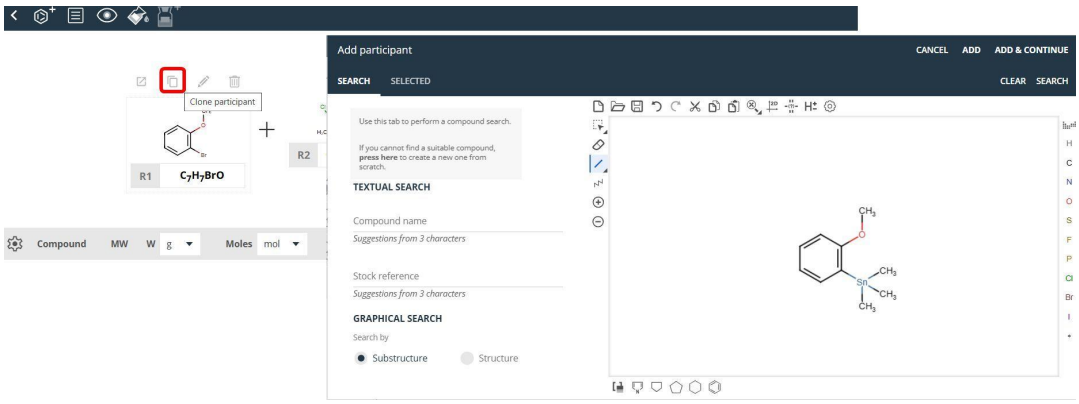


The next step is to add the remaining reactants and solvent (THF) in the same way.

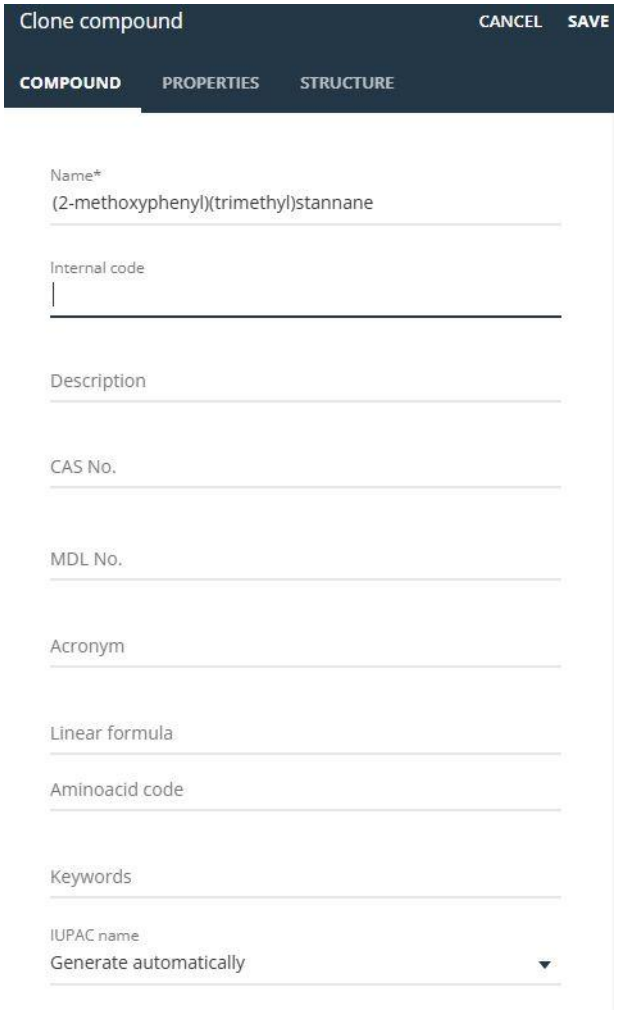
Clicking on the 'Add Conditions' button, will allow you to add the experimental conditions (after clicking the 'Save' button):



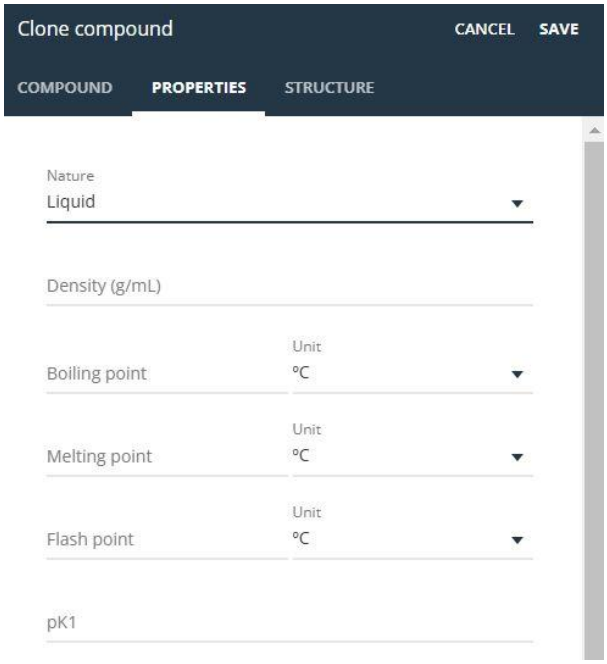
The next step is to add the product. If the structure of the compound is similar to any of the reagents, you can just select the 'Clone Participant' feature. The sketcher will then be launched with the structure of your reagent, so you will only need to add the necessary changes (a -$SnMe_3$ instead of the -Br, in this case) and click on the search button. If the compound is present in the database, just select the product role and click on the 'Add' button to continue:



If the compound is not in the database, it will be added (you can include the IUPAC name) after having filled in the desired fields (internal code, description, acronym, etc.) and clicking on the 'Save button':

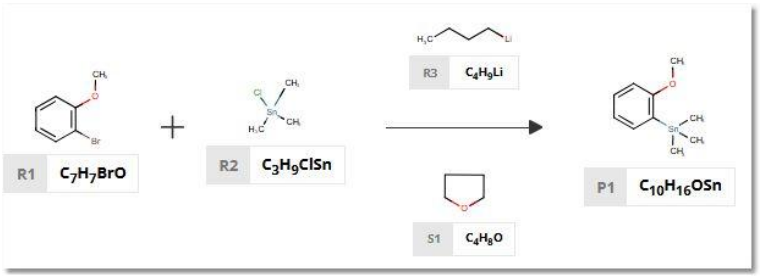


Clicking on the 'Properties' tab, will allow you to define different types of compounds (Resin, Enzyme, Solution and Supported reagent).



- Resin: If a compound checked as a Resin is added to an experiment, a column labelled 'Loading (mmol/g)' is added to the stoichiometric table.
- Enzyme: If a compound checked as an Enzyme is added to an experiment, a column labelled 'Activity (U/g)' is added to the stoichiometric table. No automatic calculations are performed for this participant (the amount used in the experiment must be manually added by the user).
- Supported reagent: If a compound checked as a Supported reagent is added to an experiment, a column labelled 'Loading (wt%)' is added to the stoichiometric table. No automatic calculations are performed for this participant (the amount used in the experiment must be added manually by the user).
- Solution: If a compound checked as a Solution is added to an experiment, the concentration column is automatically populated from the defined value in the compound.

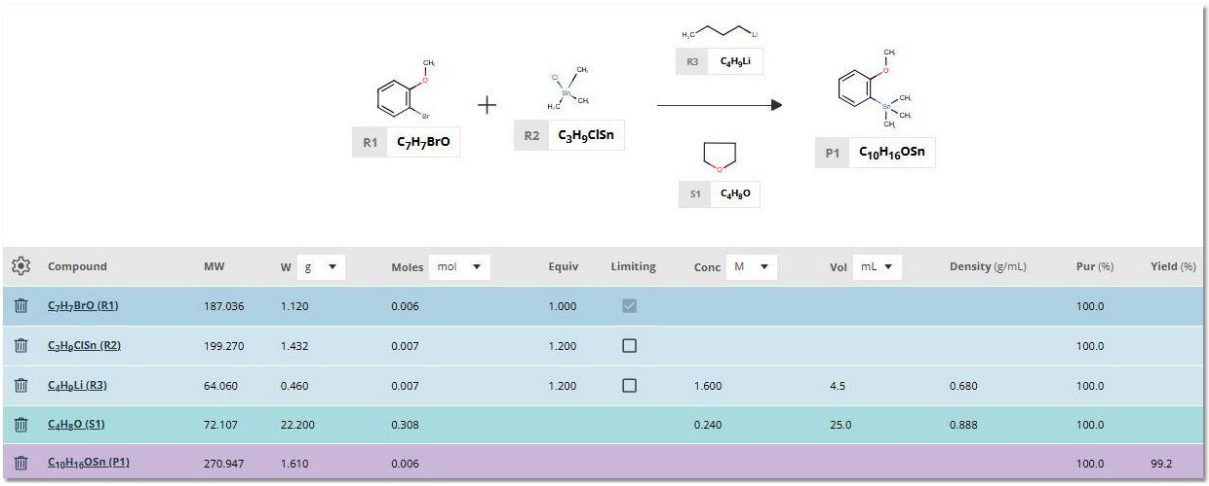
The resulting structure will be added to the Products:



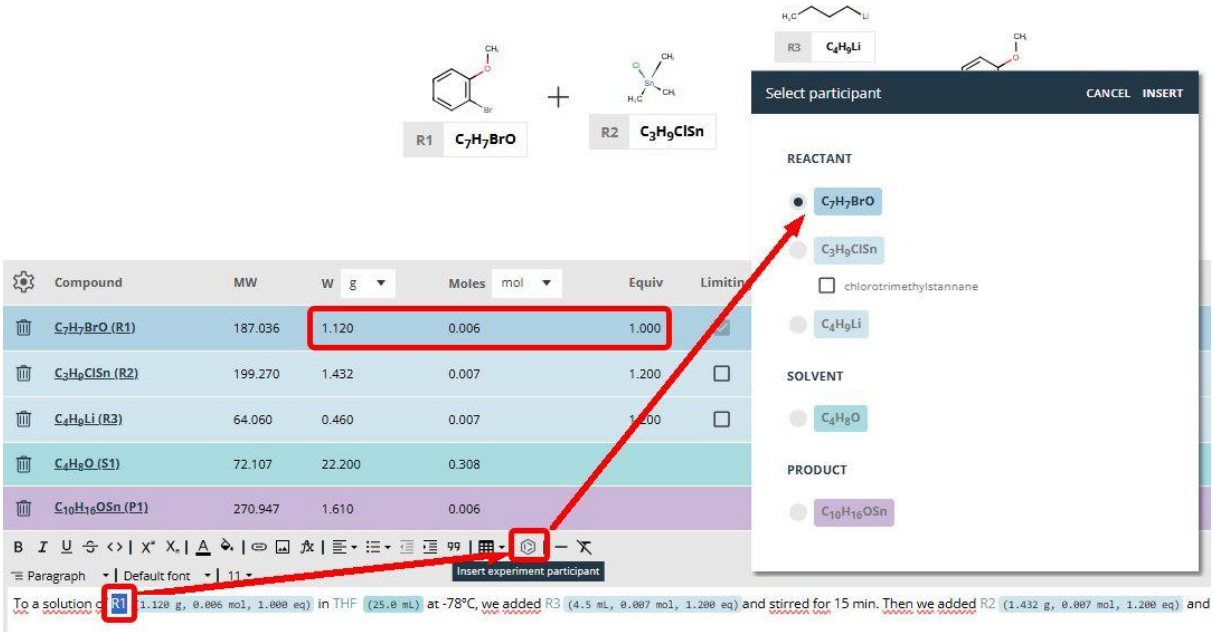
You can move the reactants from the arrow to the reaction section (and vice versa), just by dragging and dropping.

Once you have drawn the experiment reaction with all the relevant participants, you can select the applicable amounts of reagents and solvents in the stoichiometry table.

After inputting all the necessary information and formatting all the experimental procedures, the changes will be automatically saved:

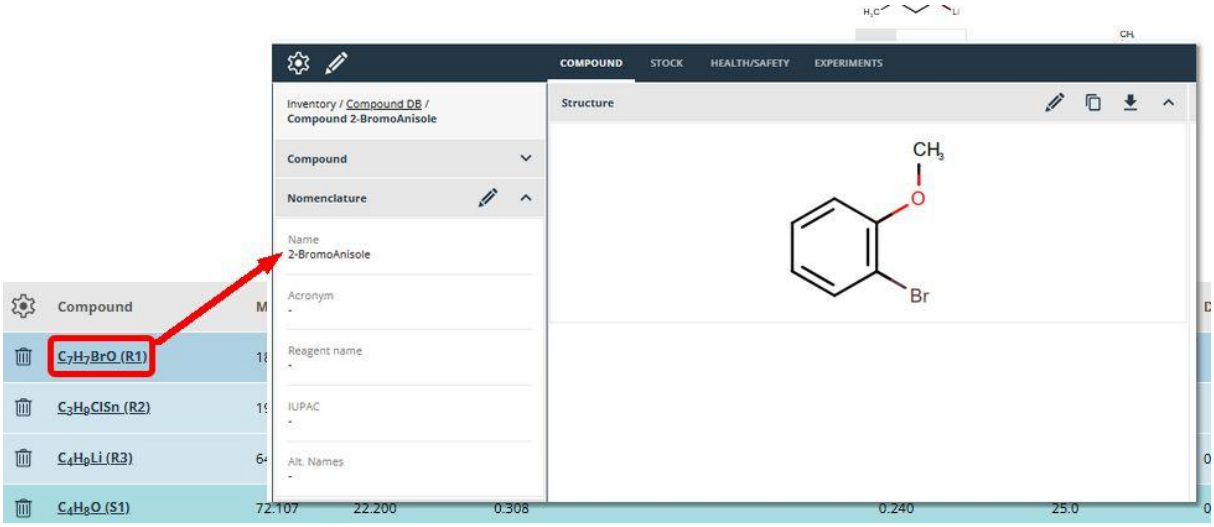


You can create links in the experimental section to the participants (to parse information about weight/volume, mols and number of equivalents): just by highlighting the applicable text in the description and clicking on the 'Insert experiment participant' button:

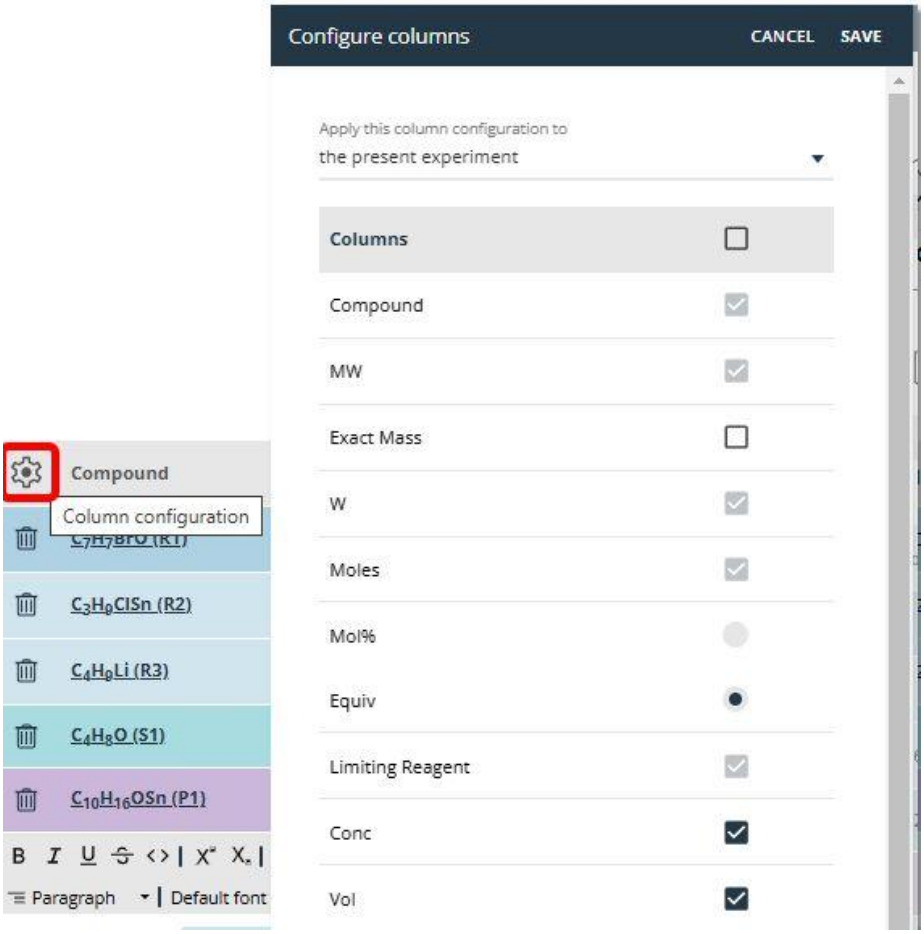


In the case of reactants, the amount and number of moles will be synchronized in both the table and the description. The same is true for the volume of solvents and for the amount, number of moles, and yield of the products:

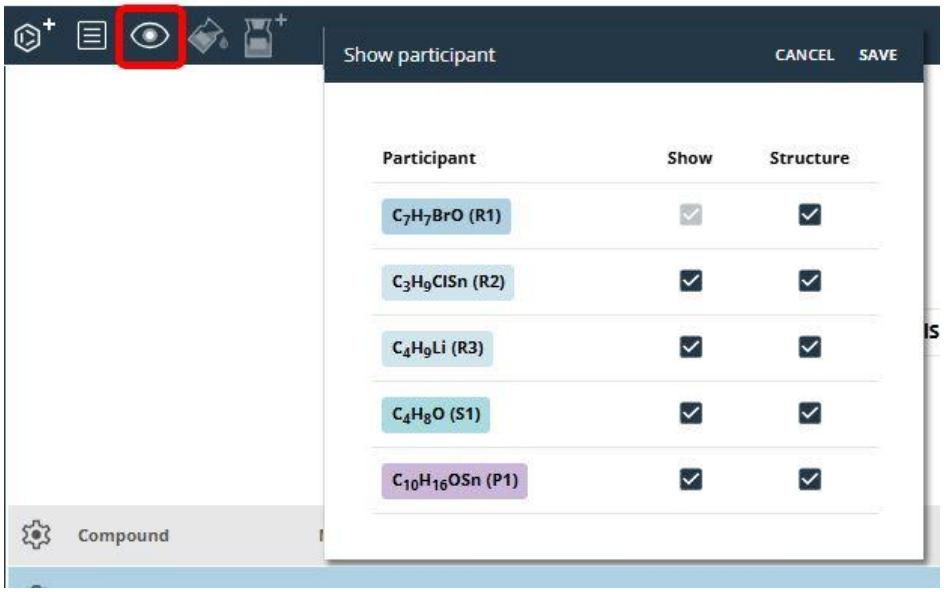
The compound names in the stoichiometric table include links to the inventory entries:



You can [configure the desired columns](#) that will be displayed in the stoichiometric table by clicking on the button highlighted in the figure below:

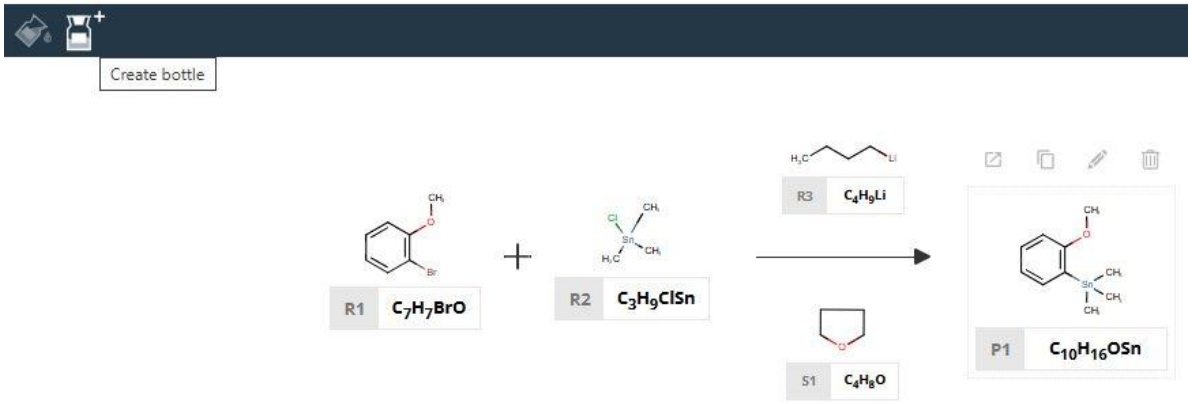


Clicking on the 'Show Participant' button  , will allow you to show/hide the molecular structure in the graph experiment, and to display the participant as a structure, name, or both:

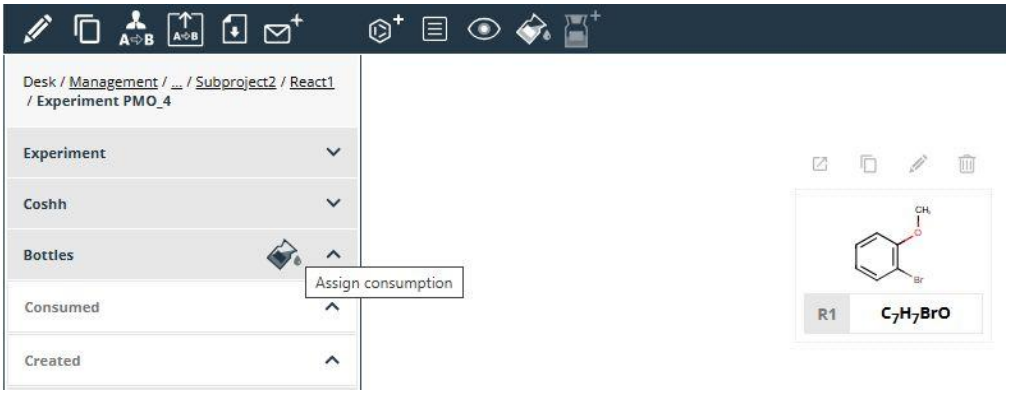


To edit or delete participants, highlight them and click on the applicable buttons (from the toolbar or from the table).

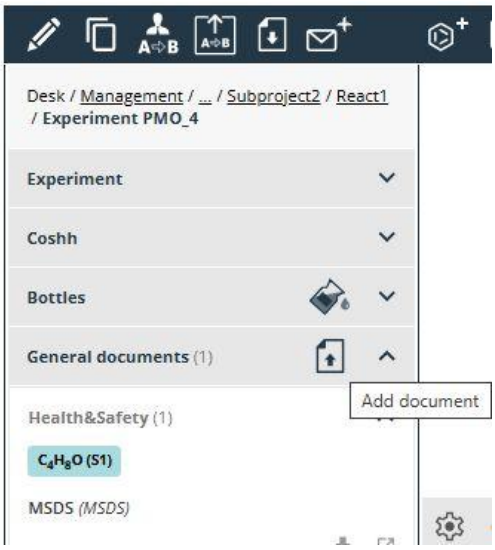
To create bottles for products and assign co for reactants and solvents, highlight the participant and click on the applicable button  .



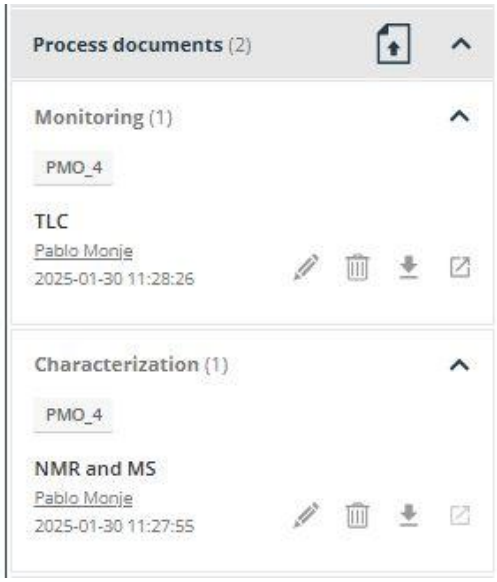
You can assign consumptions also by clicking on this button:



From the panel, you will be able to 'add/edit or download in PDF format' the 'Material Safety Data Sheet' of any of the participants:



Selecting the 'Process documents' tab, will allow you to add other relevant documentation such as Mnova documents, the raw NMR/MS spectra in .zip or .mnova format, images, etc.:

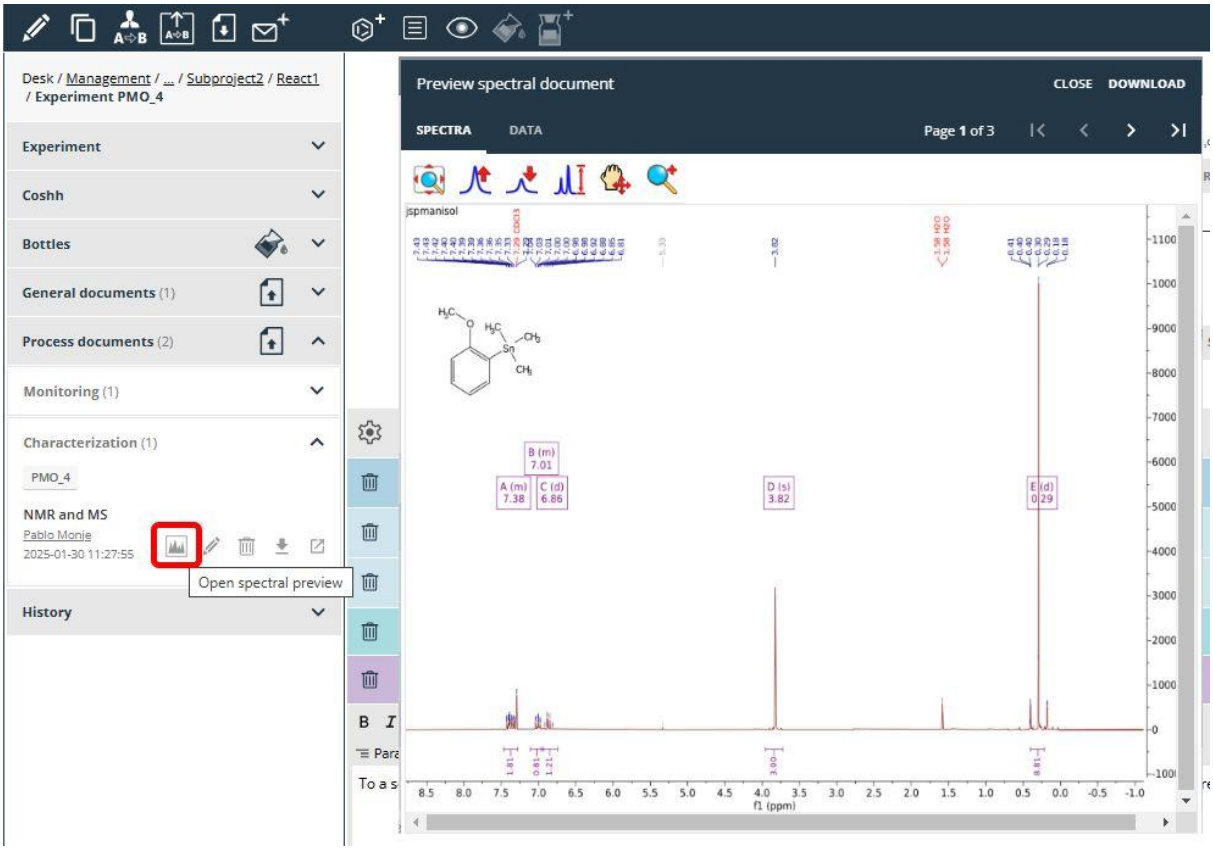


Once you have added the attachments, they will be listed in the appropriate panel.

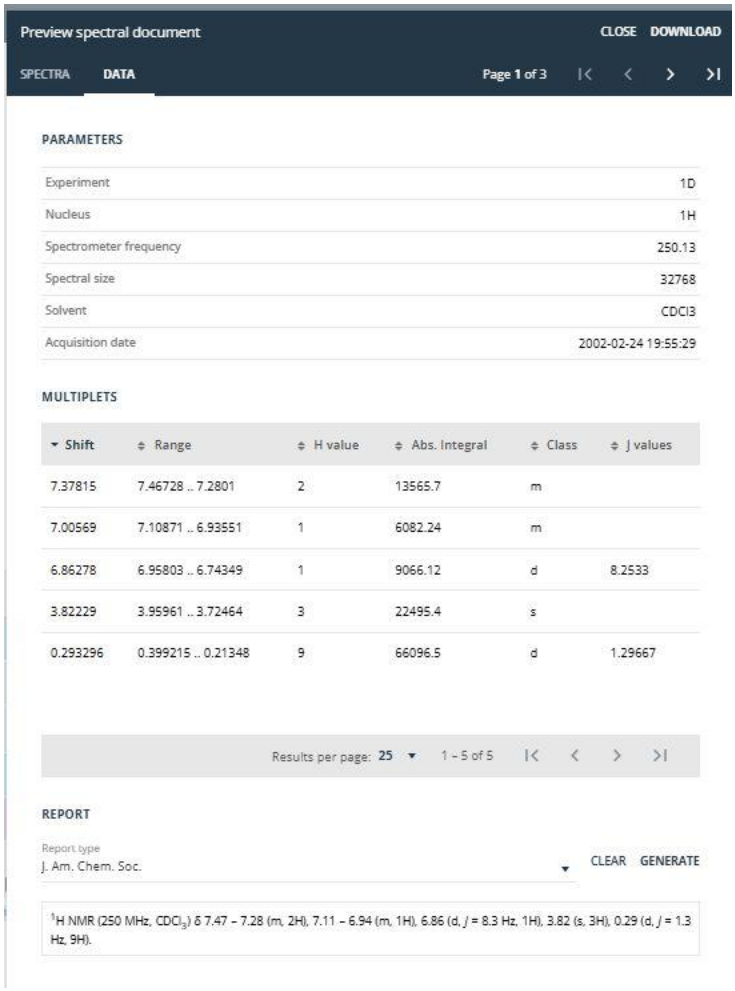
NMR, MS, or ElViS datasets can be uploaded as Mnova documents or as raw data in zip files.

If you load a Mnova document, you will be able to see a small preview just by clicking on the 'Open Document' button.

Clicking on the 'Open Spectral preview' will display the viewer which will allow you to increase the intensity of your NMR spectrum, panning or zoom in:



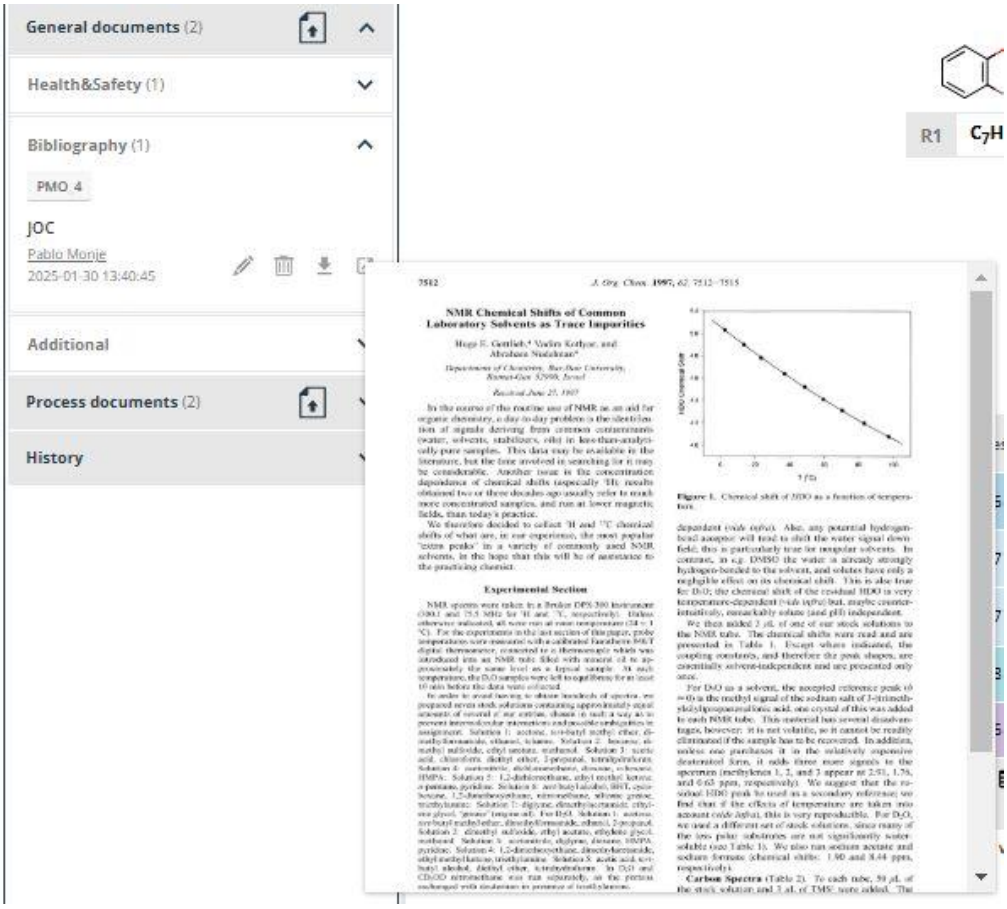
Selecting the 'Data' tab will allow you to display the ‘Multiplets Table’ or generate a ‘Mutiplet Report’ in the journal format selected in the combobox (JACS, in the example below):



The original raw file can also be downloaded by clicking Edit and selecting the raw file from the same window.

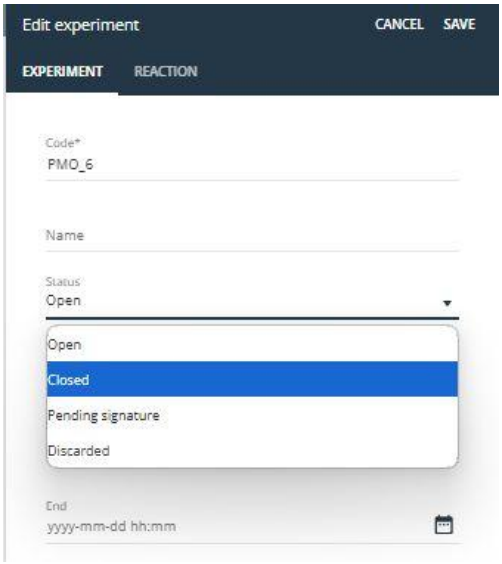
You can also add images (very useful, for example, when adding TLCs) to your experiments. Clicking on the 'Open document' button will display a preview. These images can be included at the end of the report (with the description added).

You can also add PDF files in the bibliography section. Hovering the mouse over the PDF link will display a preview of the first page of the document:

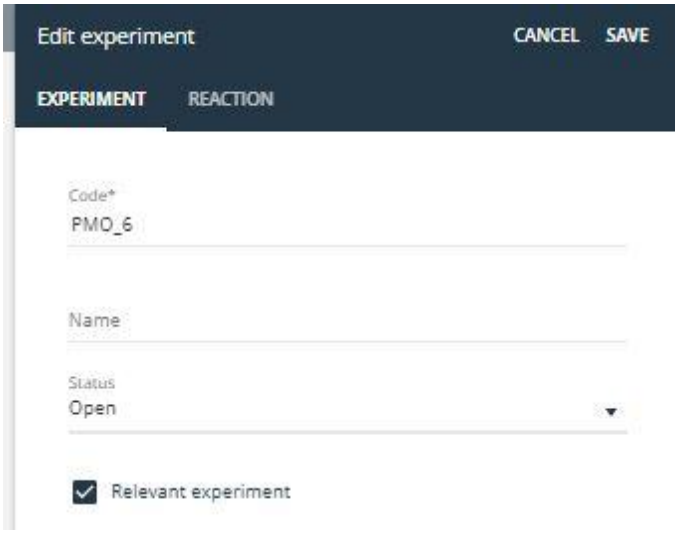


From the experiment panel, you can edit the description of the experiment, clone, assign the experiment to another user, generate a report as a PDF, import a reaction scheme from Chemdraw, and send a message with the report (to any member of the same group):

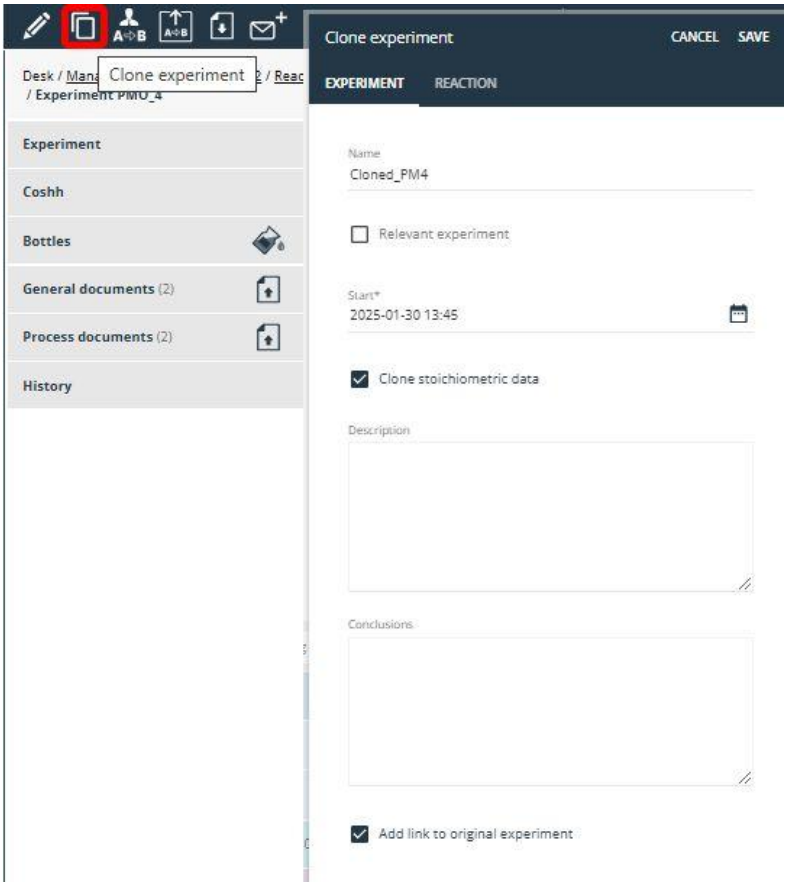
For reasons of integrity, it is not possible to delete experiments. However, clicking on the 'Edit Experiment' button will allow you change the status (from **open** to **closed** or **discarded**). From here, you can also rename the experiment code, modify the start and end dates, and type 'descriptions' and conclusions':



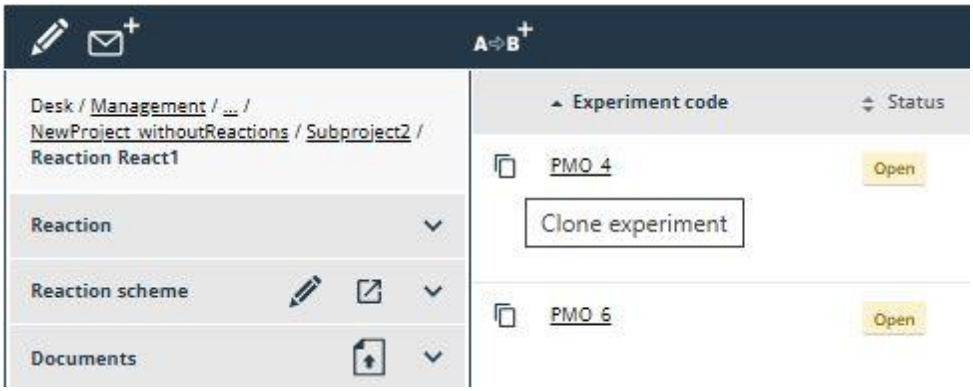
From the experiment tab, you can check the 'Relevant experiment' box. This type of experiment will be highlighted in blue in the desk, allowing the users to easily select the important experiments in a reaction (for cloning, reporting, etc.). You can also filter your searches using the relevant experiments:



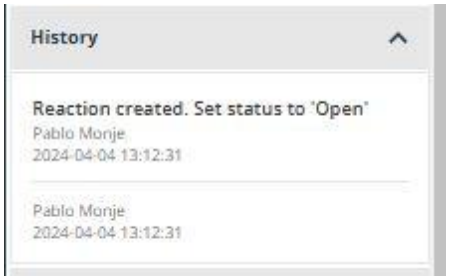
In the ‘Experiment panel’, you will also find a button that allows you to ‘Clone’ any experiment, a very useful feature for the creation of new experiments using existing ones as starting points (for instance, if you run the same experiment again under different conditions, or if you run a new experiment that is a modified version of an existing one).



When the 'Clone stoichiometric data' box is checked, the weight, volume, and number of moles will be automatically completed in the table for the cloned experiment. Please bear in mind that when you modify the amount of the limiting reagent, all the amounts of the remaining reactants will be automatically calculated according to the number of equivalents. The same button will appear in the list of existing experiments:

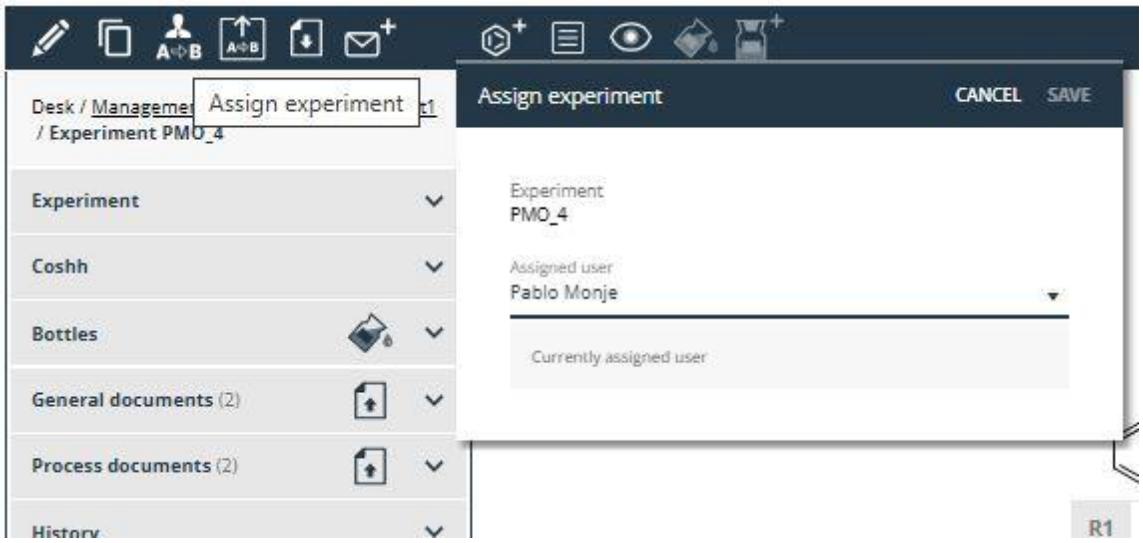


Clicking on the History field will display the relevant status information:

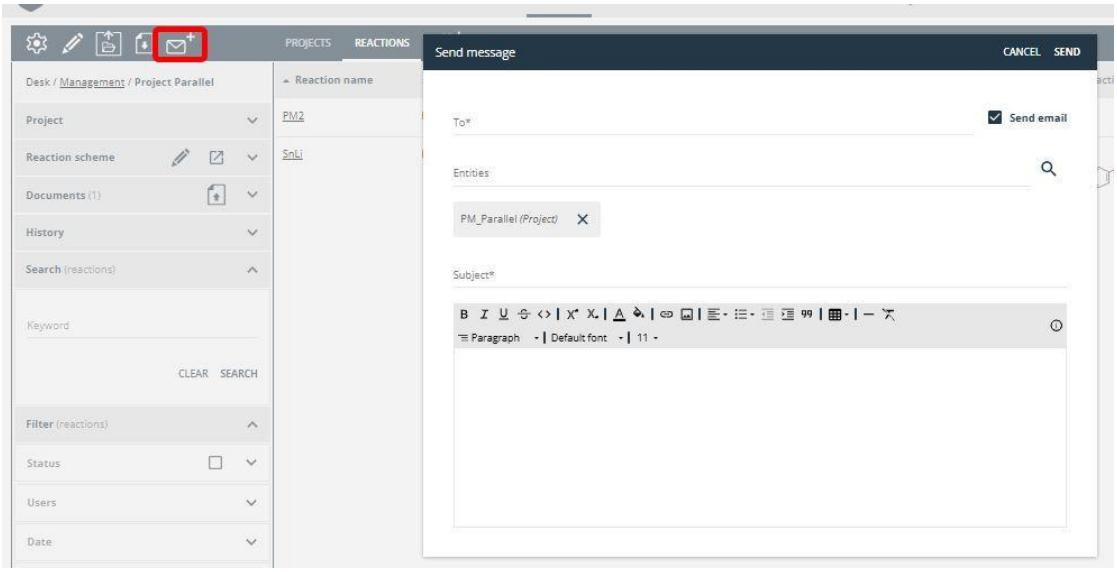


You can also navigate through the experiments by using the arrow buttons in the reaction scheme header:

You can assign experiments to other group members by clicking on the applicable button:

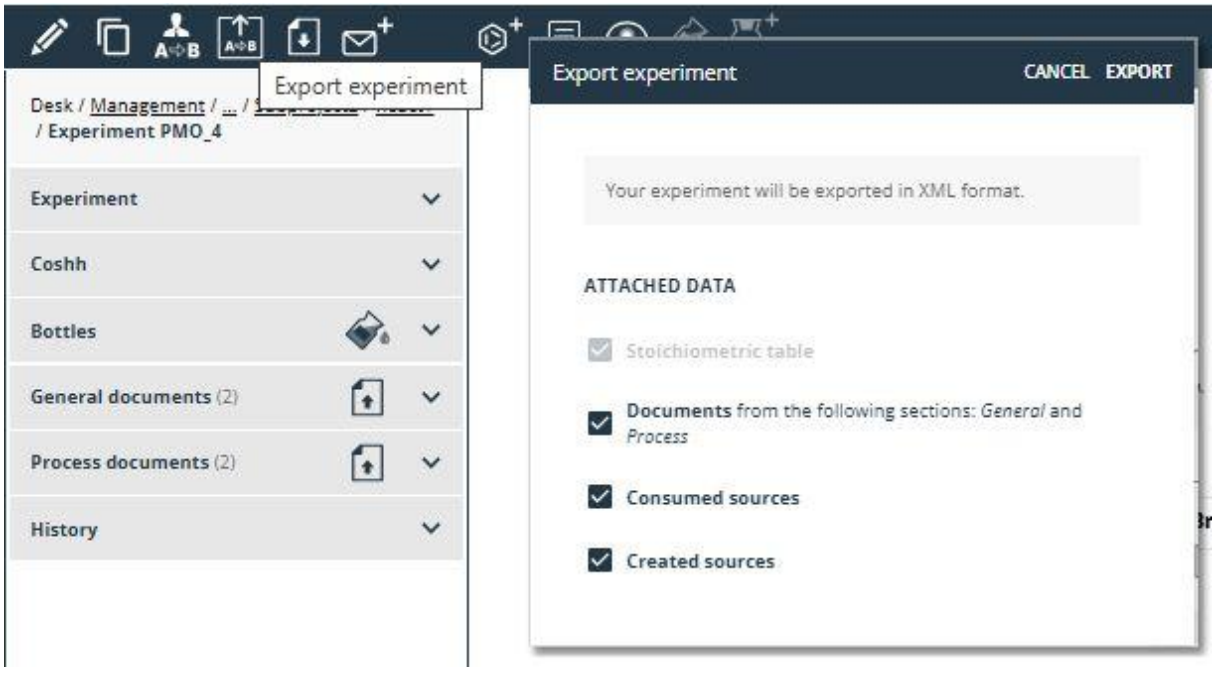


You can send messages from the reaction page, by clicking on the button 'Send message'. By doing this, the Send message dialog will opened, and the reaction will be displayed in the entities section:



5.1 Export Experiments

You can export any existing experiment just by clicking on the 'Export Experiment' button and selecting the desired attachment boxes:



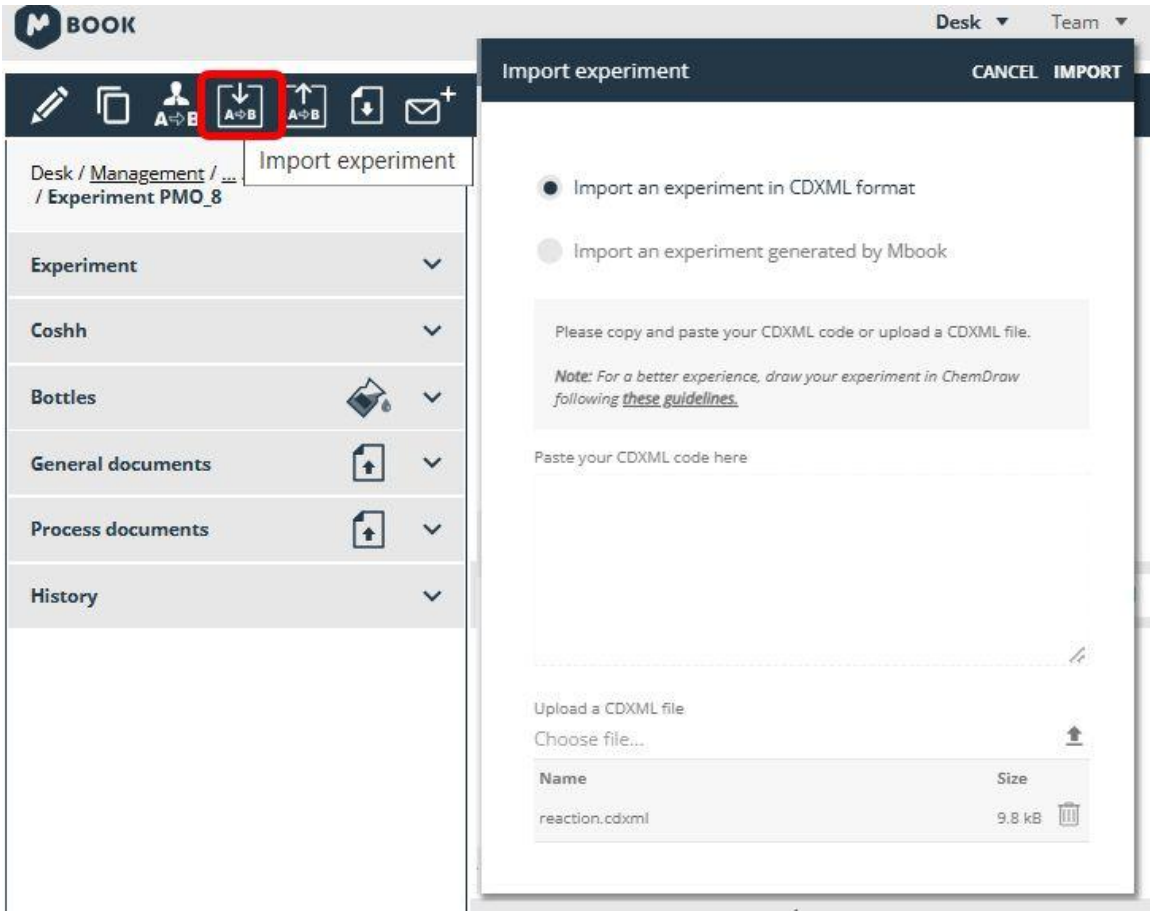
After clicking the “Export” button, a zip file with the name of the experiment code will be created. The zip file will contain several folders and files depending on the options checked in the export dialog:

a) It will always contain an .sdf file containing the structures of all the participants (reactants, solvents, and products).
b) An .xml file will be always present with the description, history of the experiment (project, reaction, and owner) and consumed/created sources if the applicable options were checked.

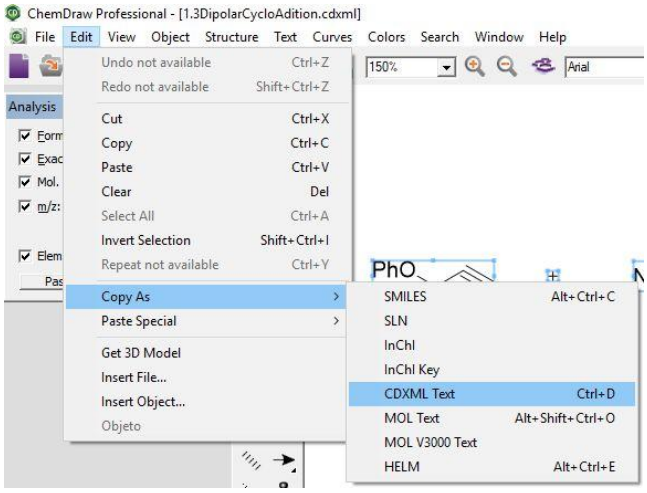
c) If the option to include documents is checked, besides the .xml and .sdf files, one folder for each section which has documents attached in the experiment will be included in the zip file and will have the name of the section and the type (Bibliography, Monitoring, Characterization). Insides these folders there will be subfolders for each participant with the applicable documents.
c.1) If you uploaded a raw dataset, the folder in the zip file will contain: the original file, the Mnova document automatically generated when uploading the file to Mbook, and a bunch of .txt files with the parameters, peaks and multiplets of the different pages.
c.2) If you uploaded a Mnova document, the folder in the zip file contains: the original Mnova document and a bunch of .txt files with the parameters, peaks and multiplets of the different pages.
c.3) If you uploaded a PDF, image or any other format, the folder will only contain the original document attached to the experiment with its native format.

5.2 Import experiments

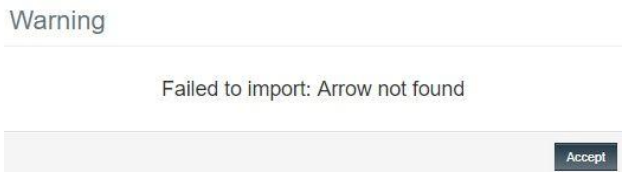
You can import experiments from Mbook (as zip archives) or from ChemDraw (in CDXML format) just by clicking on the applicable button (highlighted in red in the screenshot below):



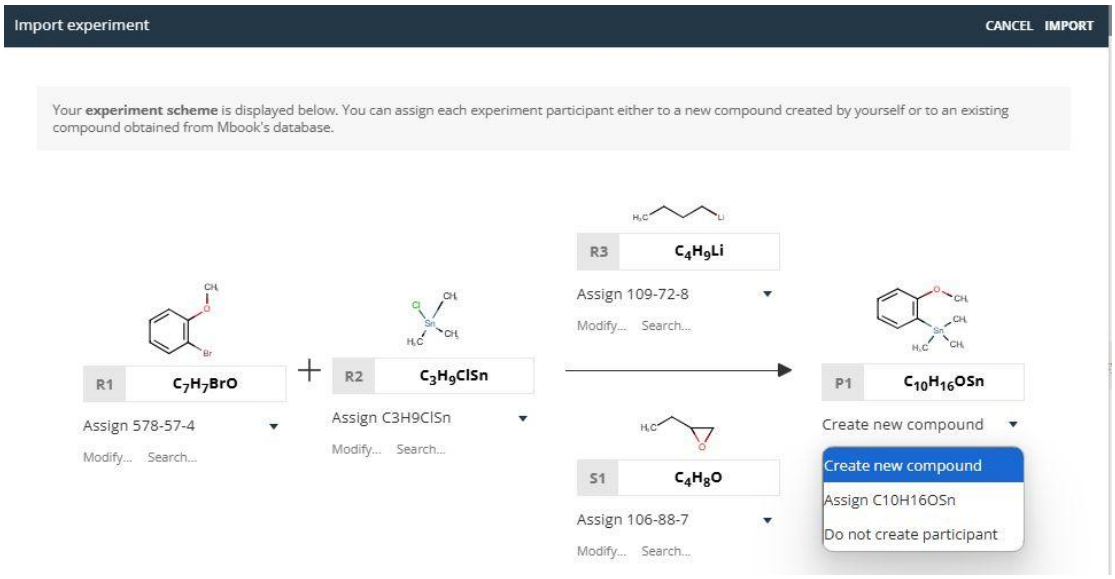
Another option would be to copy and paste the experiment from ChemDraw using the 'Edit/Copy As: CDMXL Text' (Ctrl+D) command.



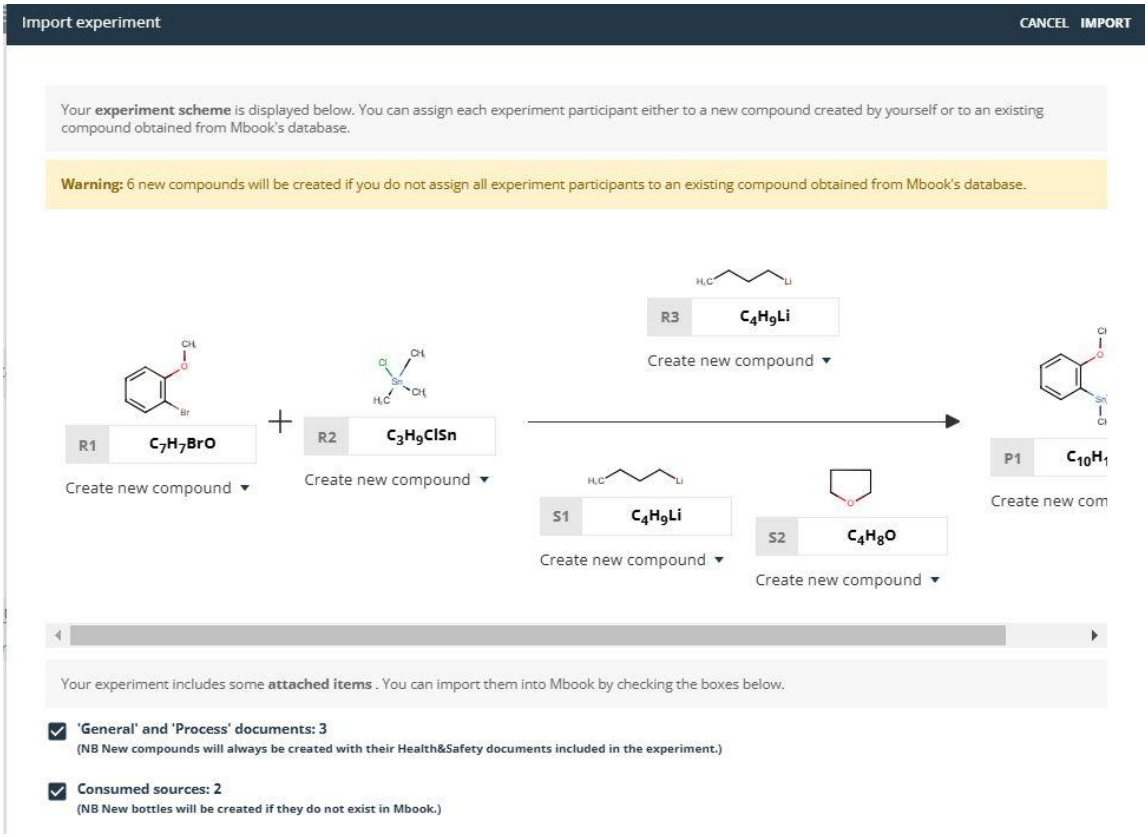
If the file is in another format or it does not have a reaction or a recognizable structure, a warning will be shown.



The compounds detected will be searchable in the compound database. If they do not exist, the user can make the decision to create them.



If you are loading a zip file containing an experiment created with Mbook, you will get a dialog box like the one below (also with the ability to import attached documents and consumed sources):



5.3 Column Configuration

Mbook includes column configuration capabilities in the stoichiometric table. The user can:

- Choose between equivalents and mol% (default value: equivalents) for relevant columns.
- Display a column to select the Limiting Reagent.
- Remove the Concentration, Volume, Density, and Purity columns.
- Show the CAS Number of each compound.
- Add customized text columns.

The Compound, Molecular Weight, Weight, Moles, and Yield columns will always be shown in the stoichiometric table. If no configuration is performed, the column structure will be the identical to those in previous Mbook versions.

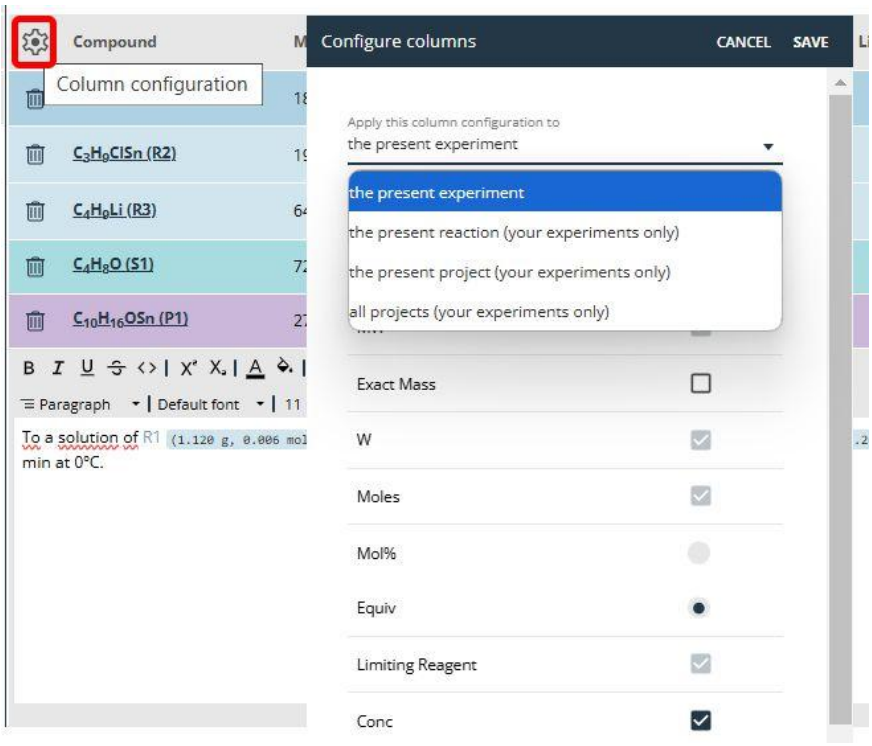
Column configuration can be completed via the Group Manager, each Project Manager, or each experiment's owner:

- If the Group Manager defines the column setup in the stoichiometric table for the entire Group; this configuration will apply to all the Group's projects.
- If a Project Manager defines the column setup of the stoichiometric table for a project, this configuration will apply to every subproject and experiment.
- If no column configuration has been completed by the Group Manager or the Project Manager, chemists can define the column setup of the stoichiometric table for their own experiments.

Column configuration will also apply to experiment reports.

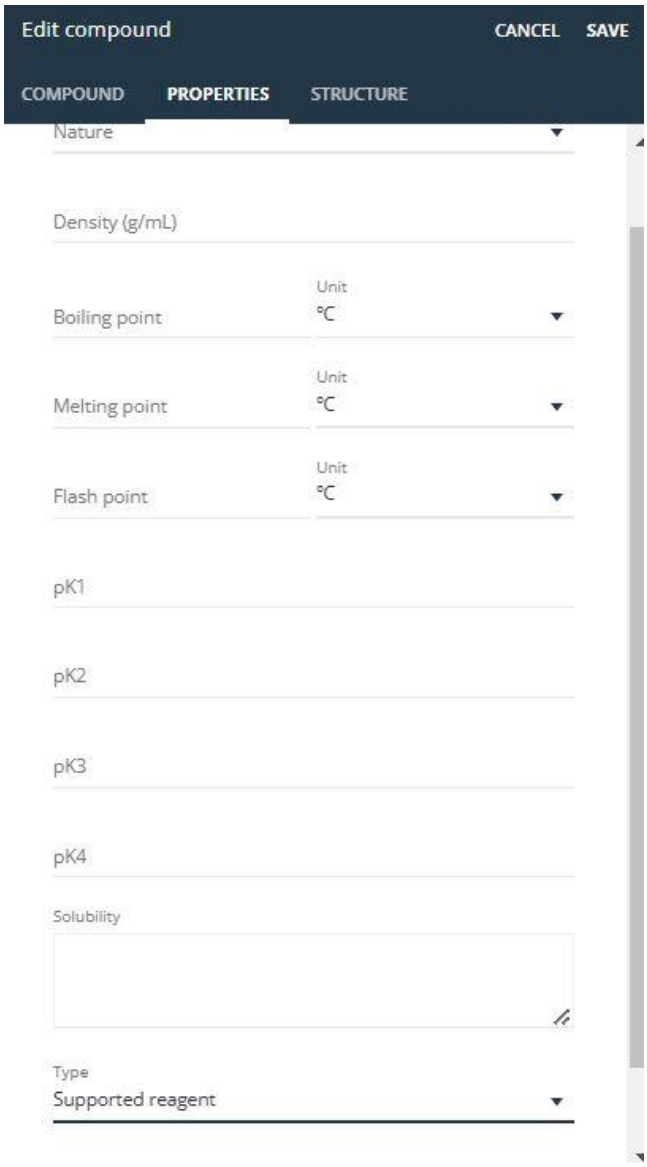
Column configuration by the Experiment owner

Users can define the column setup of the stoichiometric table in their own experiments just by clicking on the Configuration icon, as shown below.

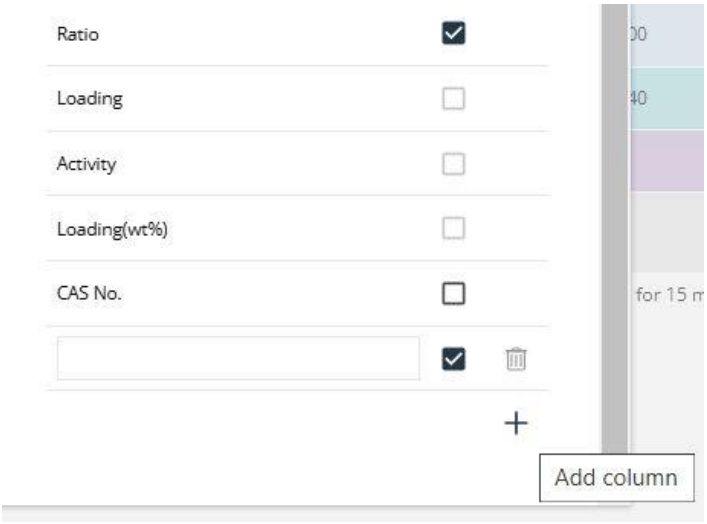


There are three types of available columns:

- Fixed columns that cannot be removed from the stoichiometric table (Compound, Molecular Weight, Weight, Moles, Limiting Reagent and Yield).
- Default columns that will initially be shown in the stoichiometric table but that can be removed by the user at any time (Equiv, Concentration, Volume, Density, Purity and ratio).
- New columns that are not shown in the stoichiometric table by default but can be displayed by the user at any time (Exact Mass and CAS Number). Other columns such as 'Loading(wt%)' can only be checked for supported reagents (after having checked the box below under the 'Edit Compound' dialog):

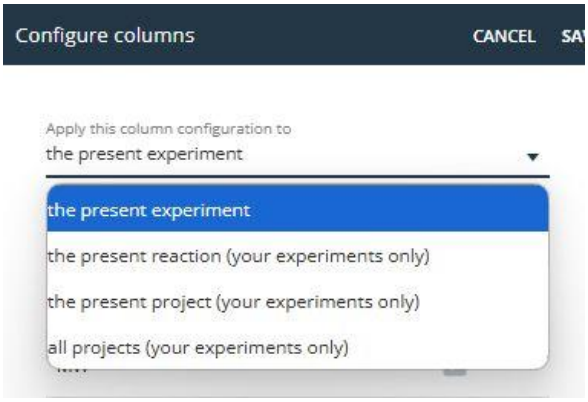


Users can also add their own custom columns to the stoichiometric table by clicking on the 'Plus' icon, specifying a name for each column header and ticking each column's checkbox:



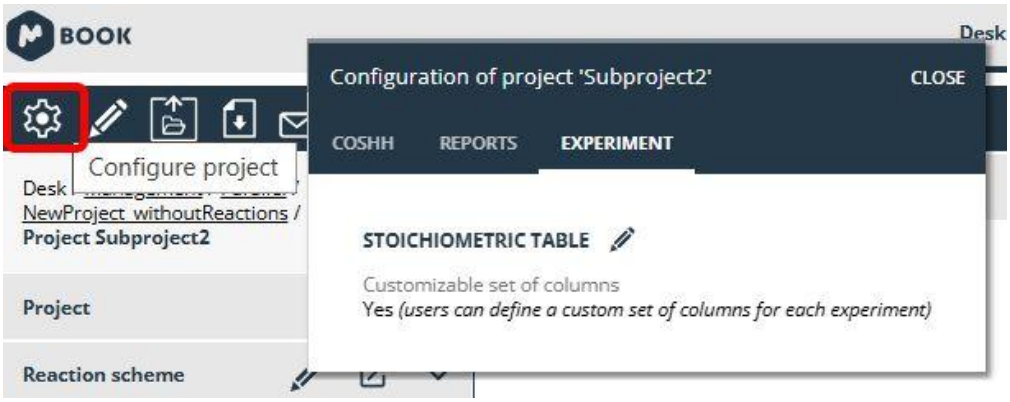
Custom columns can be removed at any time by clicking on the 'Delete column' button.

Finally, the column setup that a user defines for a particular experiment can be extended to every user's experiment in the current reaction or project or even to all the experiments owned by the user:



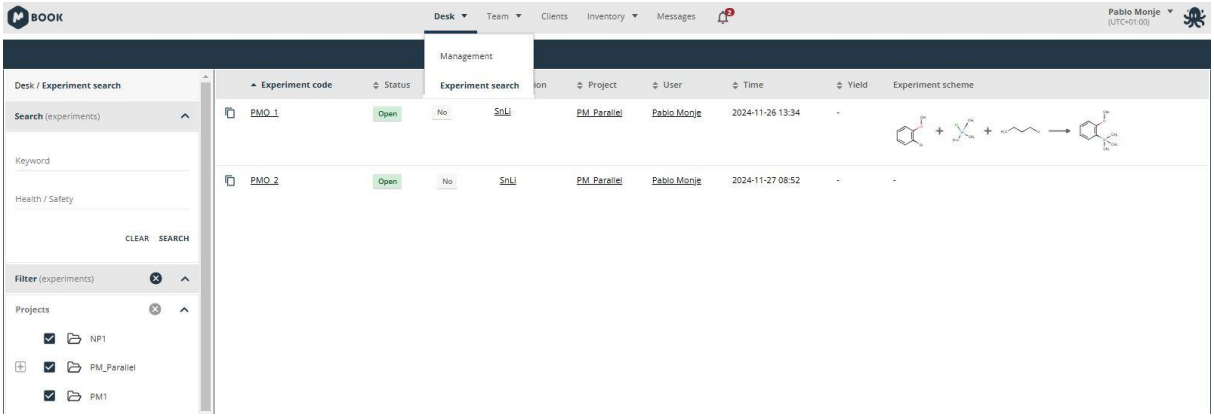
Column configuration by the Project Manager

To open the column configuration section, the Project Manager should navigate, respectively, to the Group's management panel or to the project's management panel, and then click on the icon below.

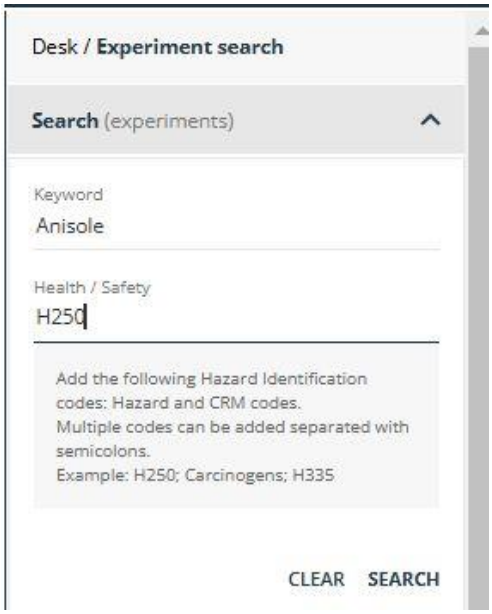


5.4 Searching

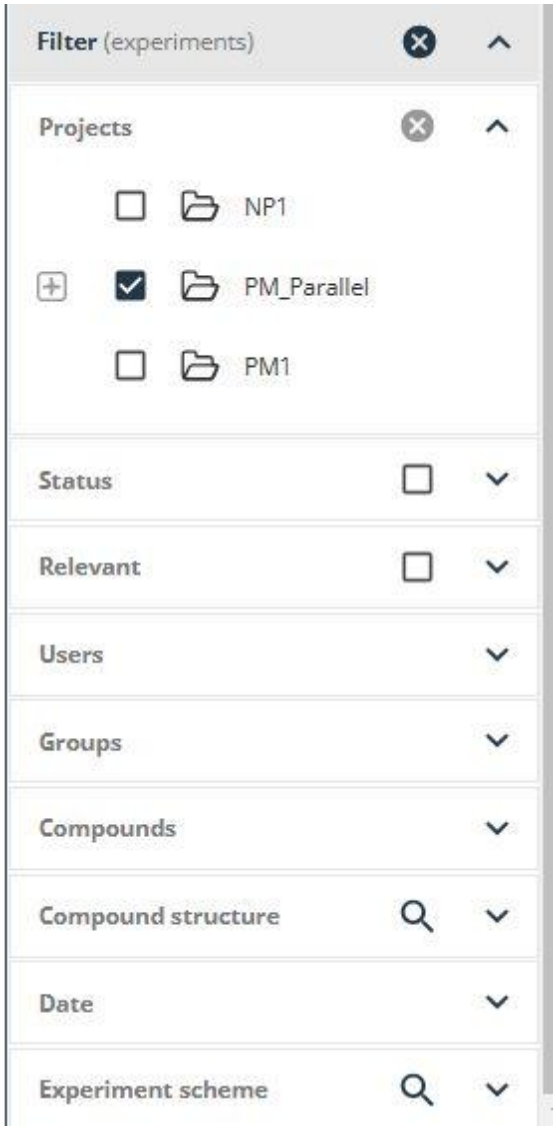
You can get the list of experiments just by selecting 'Experiment Search' from the Desk scroll down menu:



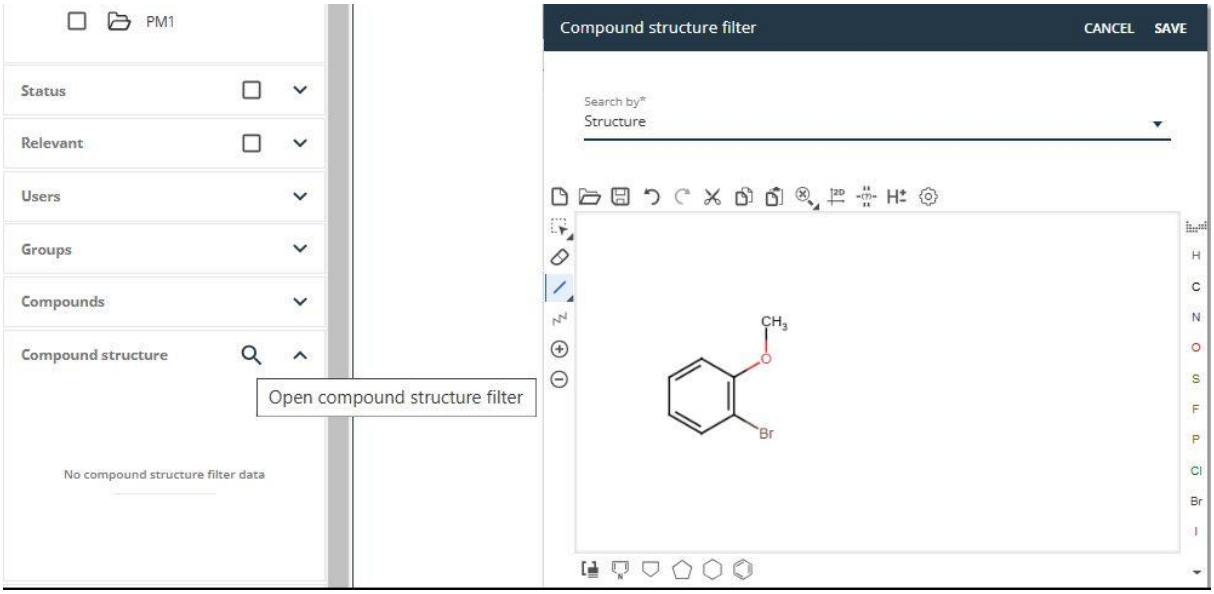
You can search by keywords, Hazard and CMR codes by using the left panel, and use the filters to restrict your results by project, status, users, groups, compounds, dates, experiments, etc.



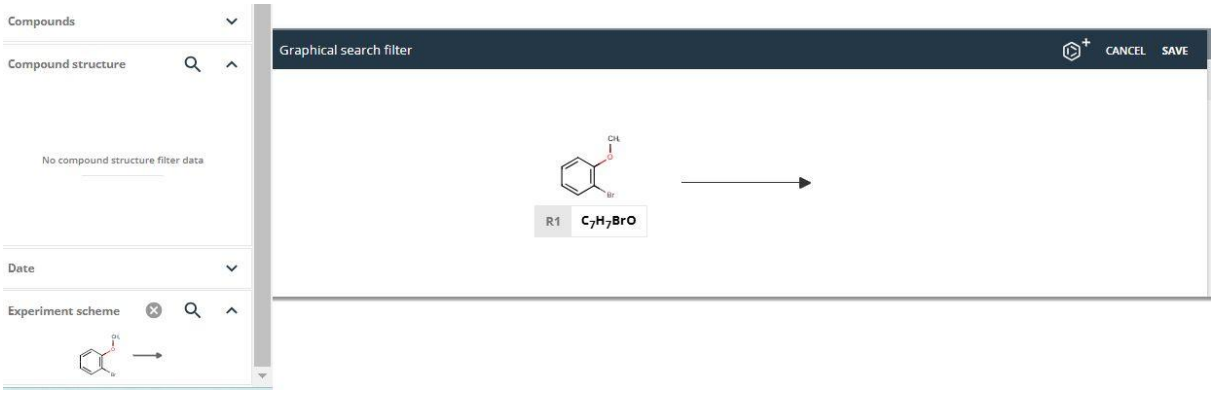
The experiment search menu can be un/collapsed by clicking on the arrow (located in the right upside corner). This collapsible contains a breadcrumb. The sections 'Search' and 'Filter' (can be also un/collapsed by clicking on the arrows next to each header):



Search for any existing compound can be done just by clicking on the 'compound Structure' button and drawing the desired molecular structures of the participants:

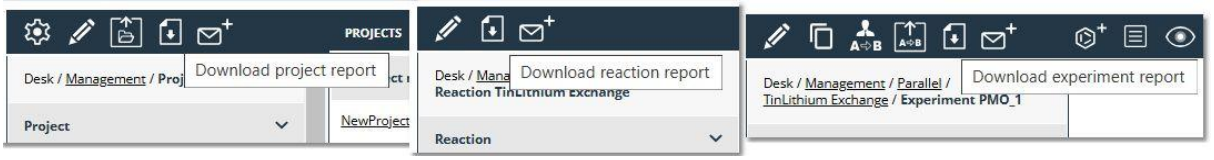


Filtering the search by experiments schemes is also possible:

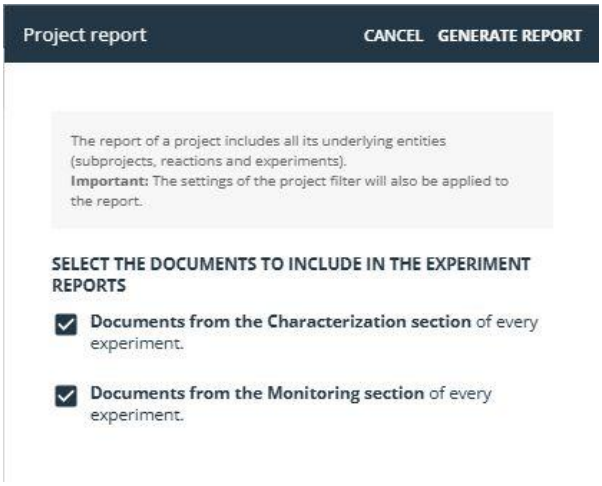


5.5 Generating Reports

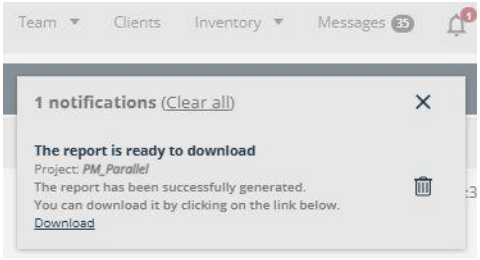
You can generate project, reactions and experiments just by clicking on the applicable button



When exporting a project report, you will have the capability to export the documents used for the characterization and monitoring for every experiment:



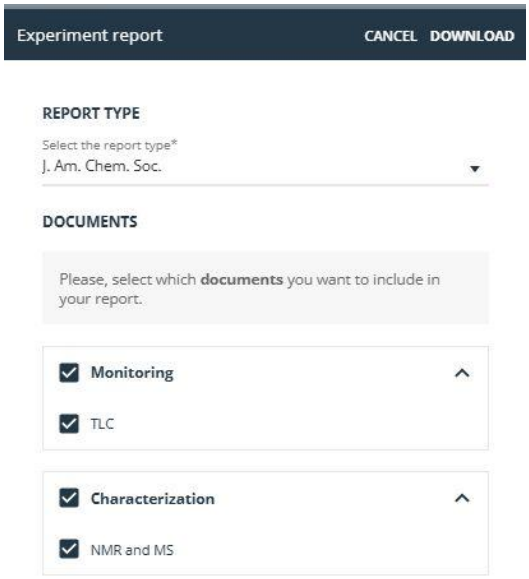
Once the report will be ready to be downloaded, you will get a notification in the Mbook toolbar:



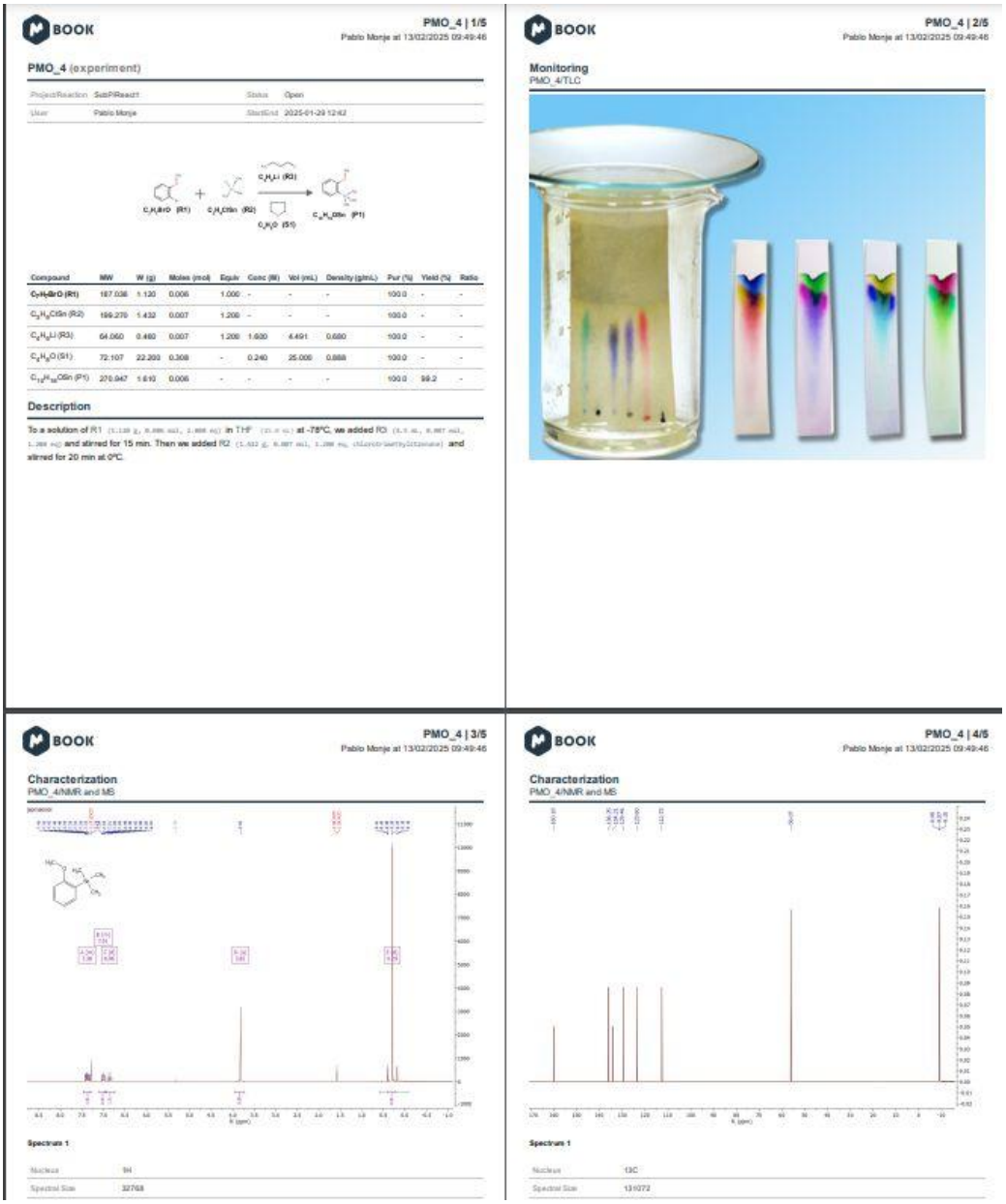
Clicking on the Download button will create a zip file with a subfolder per each reaction and with information about each experiment.

When reporting a reaction, you will get a PDF with a summary of the experiments included in the reaction.

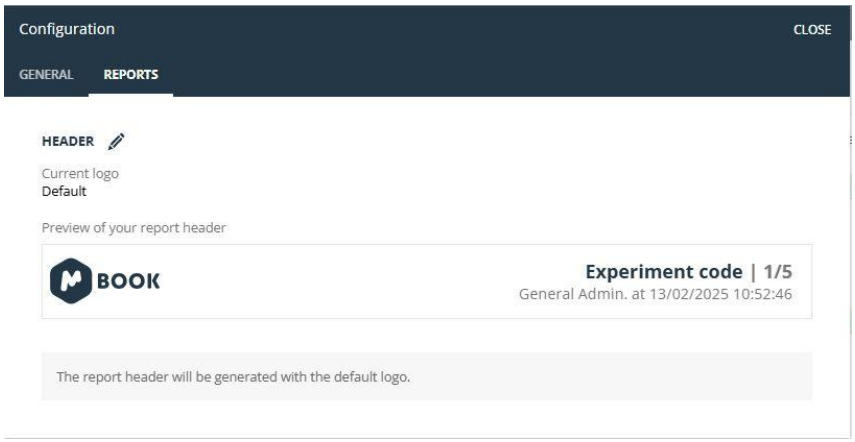
When reporting an experiment, you will be able to select the multiplet report format and to include the documents of the monitoring and characterization sections:



By clicking on the ‘download' button, a PDF will be generated for the current experiment:



From the 'Configuration panel', the administrator can upload a corporate logo that will be displayed on the header of all Mbook reports:

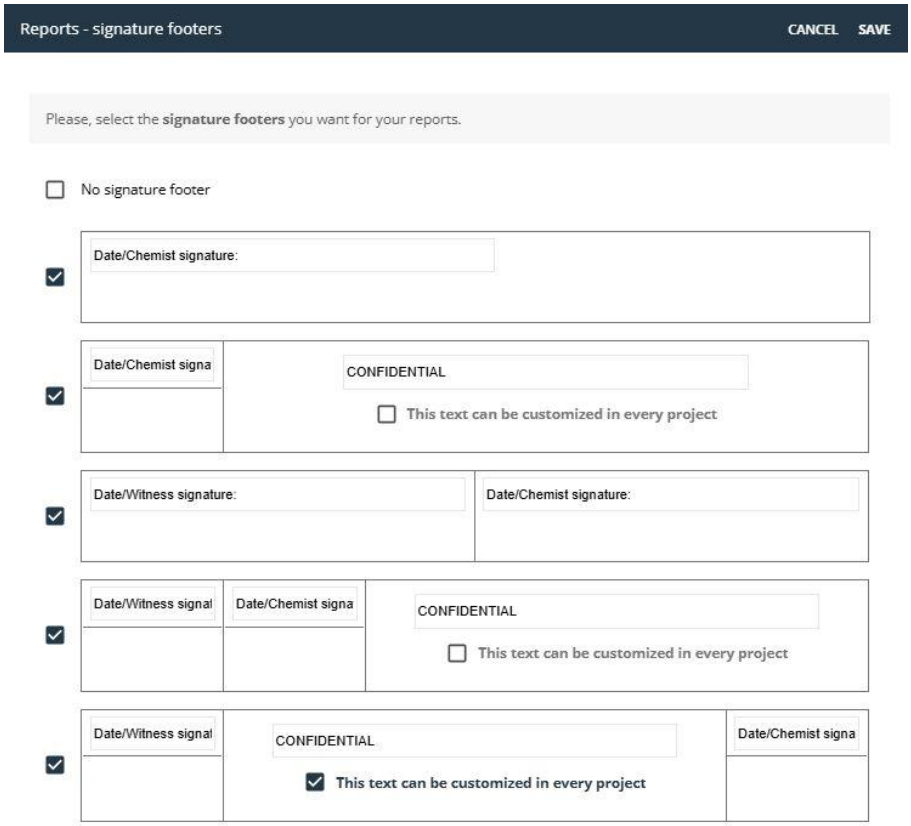


5.6 Report Footer

Footers can be added to the PDF reports generated for each experiment. Footers may contain one or two signature sections, as well as a text area where warnings or informative messages are displayed. Mbook provides each Group with five configurable footer templates. The Group Manager can customize each template, and then select which of those customized templates are available to the Groups' Project Managers. Each Project Manager can select the specific footer that will be added to all the project's experiment reports (and its eventual subprojects) from the customized templates made available by the Group Manager. Finally, each experiment owner can decide whether to include a report footer when generating a PDF report.

Report footer Templates

Report footers in Mbook contain one or two signature sections, as well as a text area where warning or informative messages are displayed. The picture below shows the five footer templates available in Mbook.

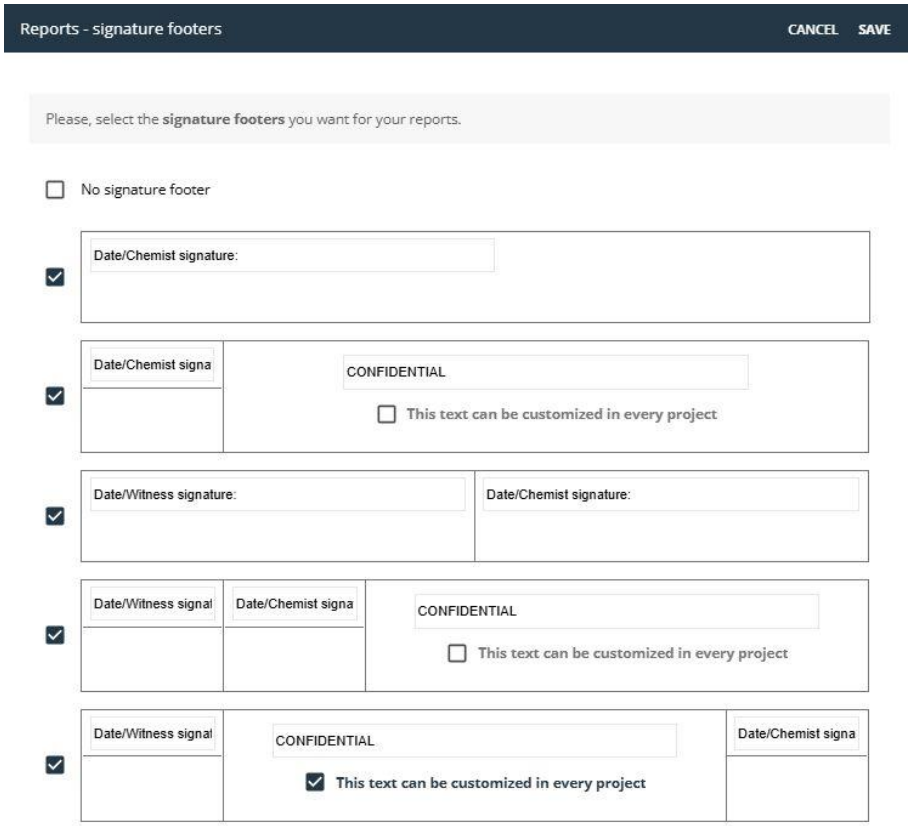


Group Manager

The Group Manager can customize each report footer template, and then select which of those customized templates are available to the Group's Project Managers.

To open the report configuration window, the Group Manager should navigate to the Group's management panel and click on the setup icon highlighted below.

The report configuration window will pop up:



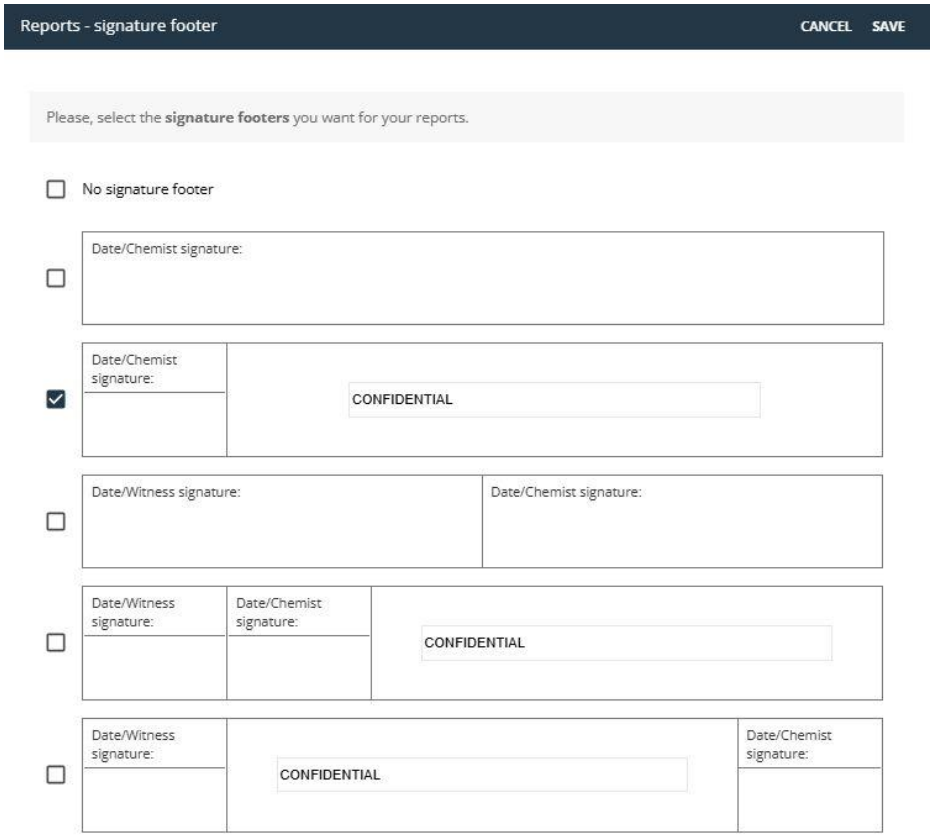
During the customization of a footer template, the Group Manager can check the **"This text can be customized in every project"** option (see picture above). In this way, the Group Manager allows the Project Manager to customize the content of the text area on a per-project basis. In the report footer below, the Group Manager has defined the message "PROPERTY of XXX" so that each Project Manager can modify the "XXX" part at some later point.

If no footer is needed for the Group's experiment reports, the Group Manager should check the "**No signature footer"** option.

Project Manager

Each Project Manager can select the specific footer that will be added to all the project's experiment reports (and its eventual subprojects) from the customized templates made available by the Group Manager. To open the report configuration window, the Project Manager should navigate to the project's management panel and click on the icon below.

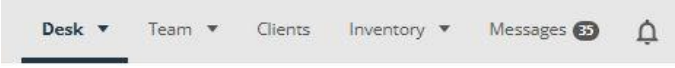
The report configuration window will open. Only the report footers previously selected by the Group Manager will be available to the Project Manager, who can then decide which one, if any, will be included in the project's experiment reports.



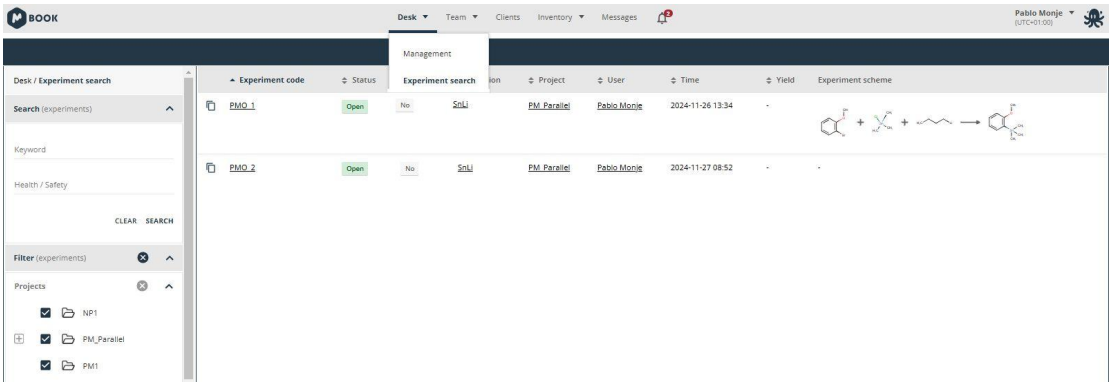
Part

6 Main Toolbar

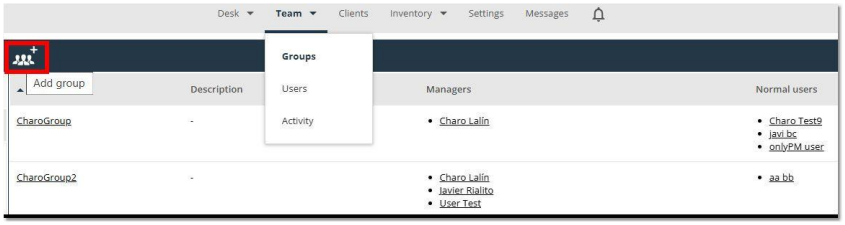
The user will find a toolbar on the upper left corner to go to the desk, to work with the database of compounds and suppliers, and to send messages to other members of the same group. Group managers will also find a button (Team) to manage the groups and the users.



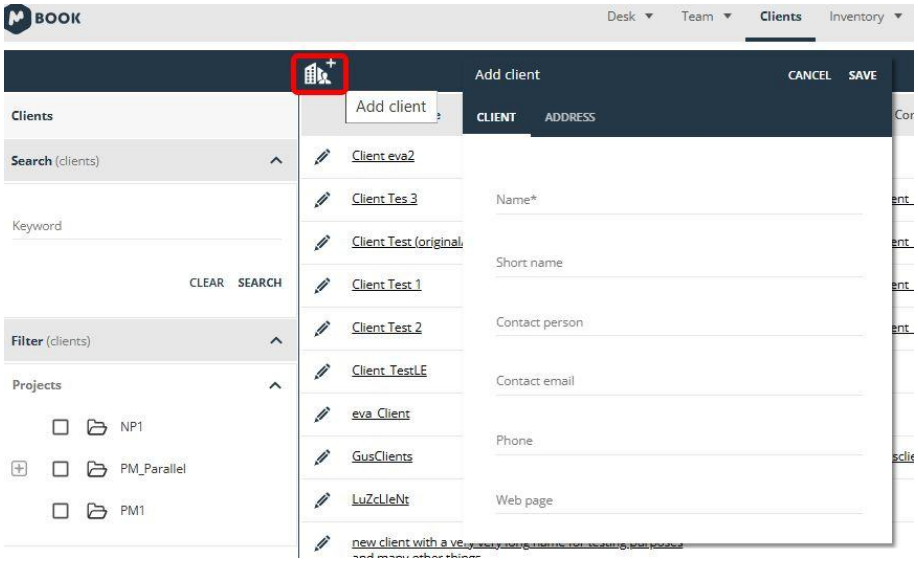
From the desk, you can search for experiments by molecular structure or by typing any free text just by selecting the 'Search' option:



From the Team scroll down menu, group managers can configure groups, users and activity:

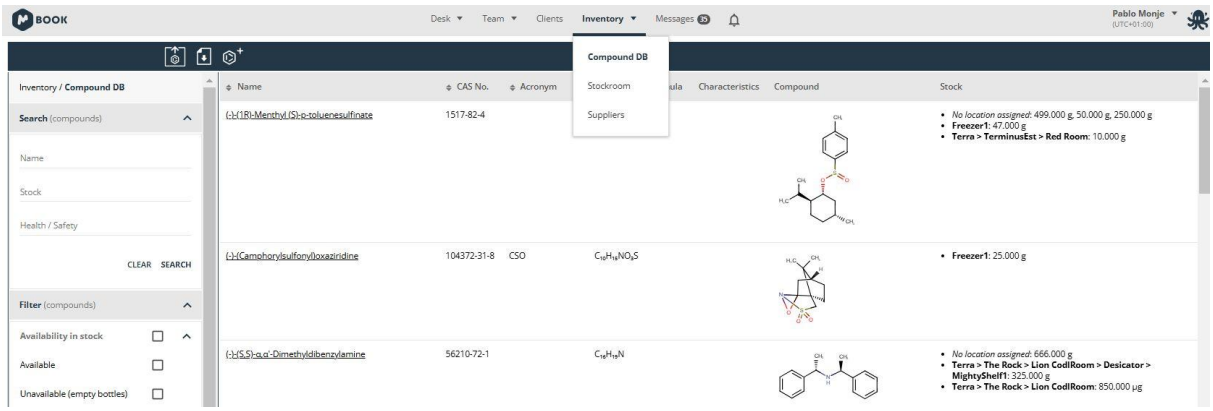


From the clients menu, you can add clients and filter them by projects:

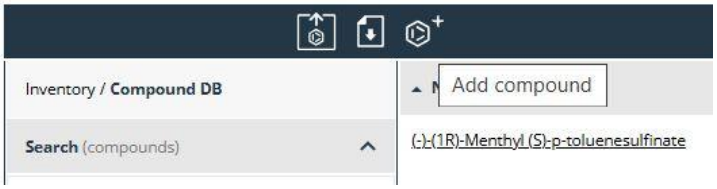


Inventory

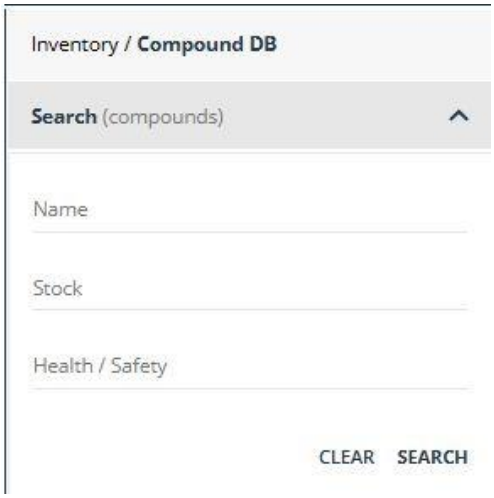
Selecting the 'Compound DB' from the Inventory scroll down menu will display the compound list:



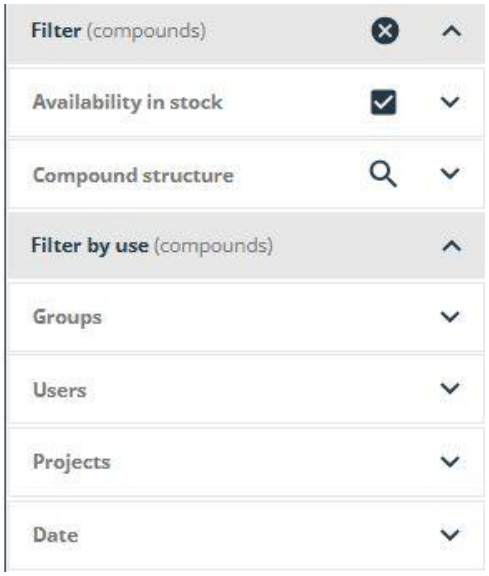
New compounds can be added to the database just by clicking on the appropriate button:



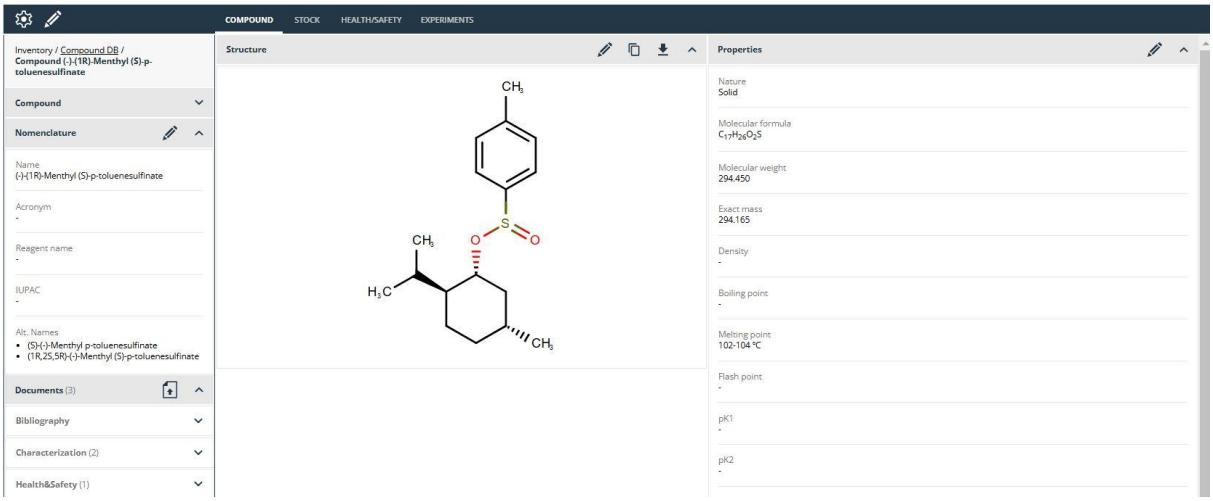
From the left panel, you will be able to search by name (including CAS Number), stock number, hazard and CMR codes.



You can apply several filters to your searches (availability in stock, by structure, groups, users, projects and dates)

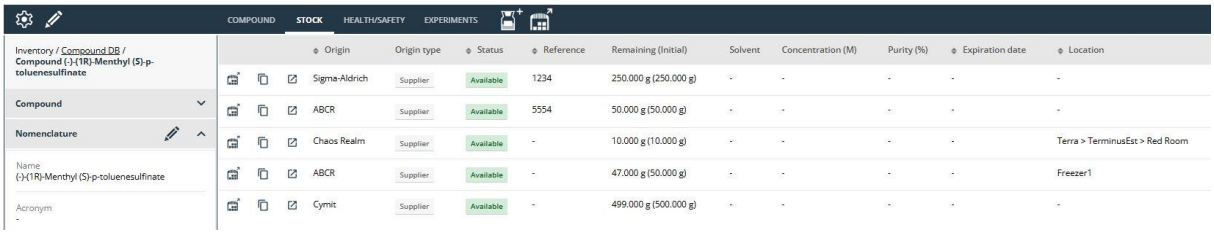


Left clicking on any existing record will display a dialog to add or edit the existing information (Name, Acronym, Molecular Formula, Melting and Boiling Points, Density, etc.):

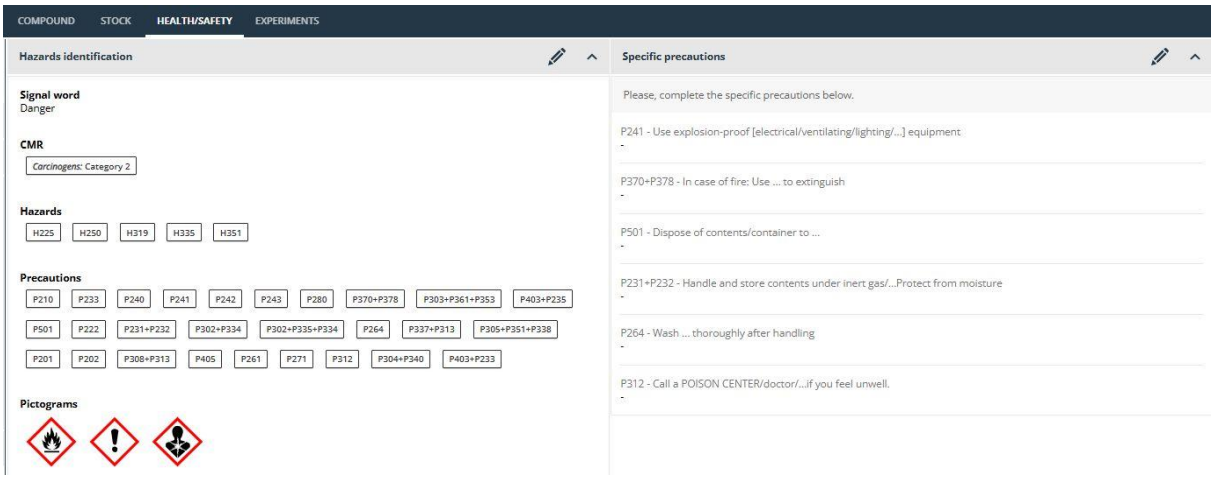


From here, you can get the MSDS document and download the molecular structure as .mol, .sdf or smile.

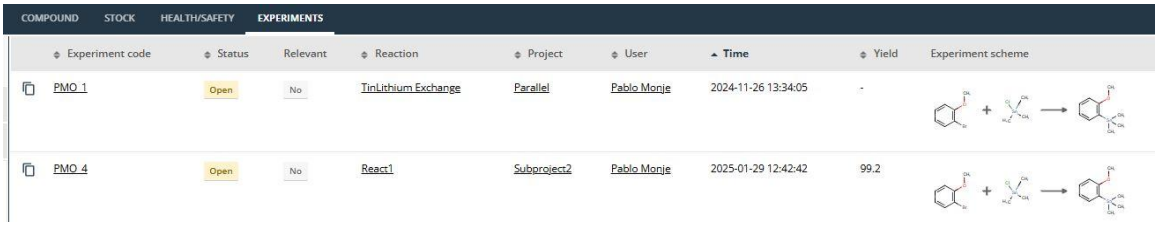
Clicking on the 'Stock' tab will display the location and the number of available bottles of the compound:



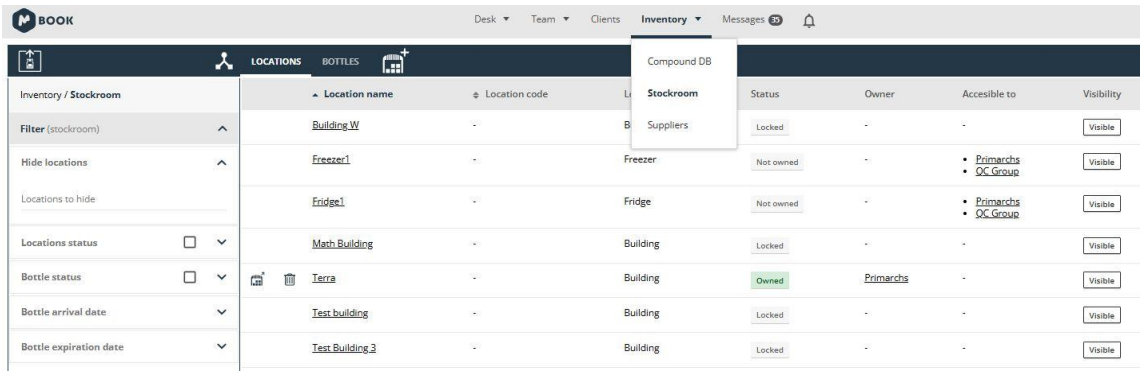
The 'Health/Safety' panel will allow you to check and modify the hazards and precautions assigned to the compound:



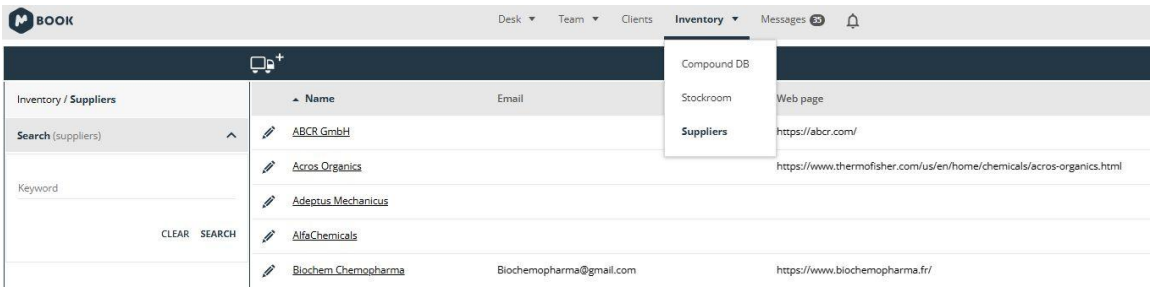
Clicking on the 'Experiment' button will display the list of experiments where the compound has previously been used:



The new Stockroom section is available by selecting the 'Stockroom' icon from the Inventory scroll down menu:

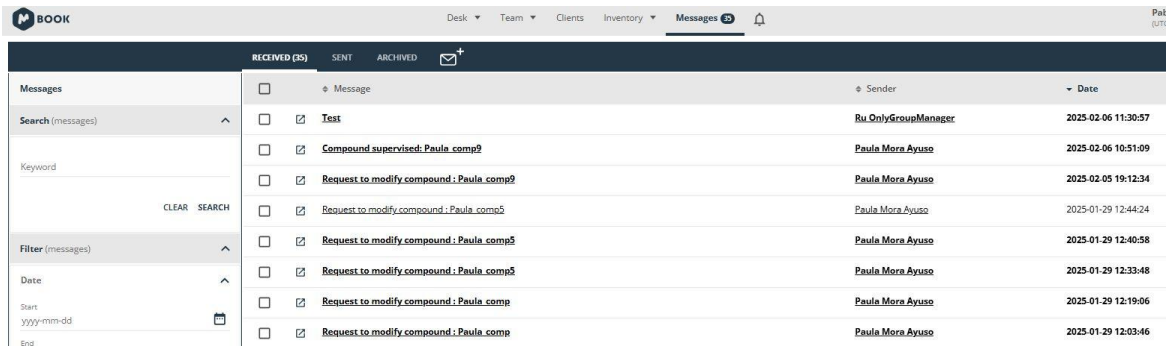


The Suppliers option in the toolbar will allow you to search/edit/add suppliers to your database:



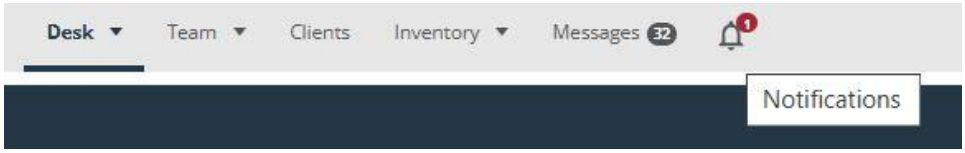
Message

The message button will display all the messages (sent, received, or archived) associated with your inbox:

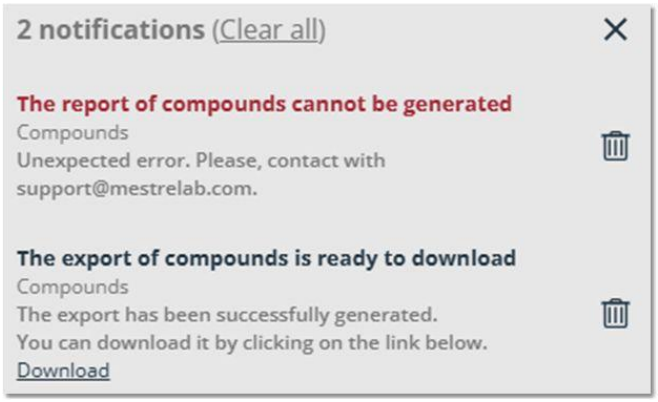


Notifications

The notification button is displayed in the navigation bar (Bell button) with the corresponding number of messages:



Each notification is shown with blue color and will be removed after clicking on the 'Delete Notification' or 'Clear All' button (or after having accepted the action). When the process failed, the notification will appear in red:



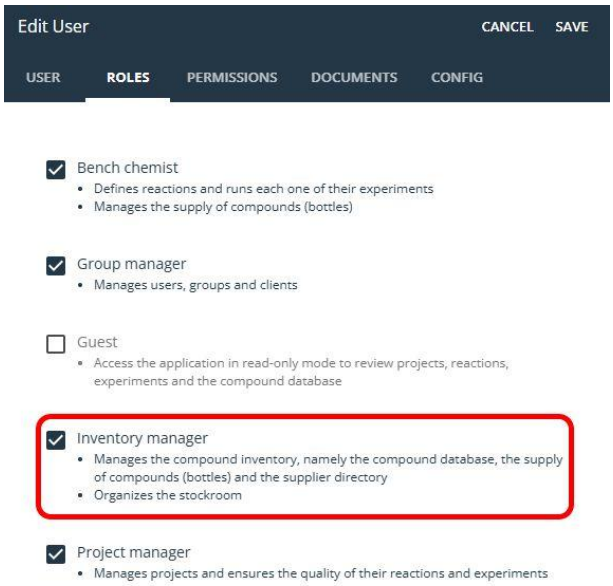
Part

7 Inventory

Many organizations choose an ELN, deploy it, get it adopted, train their users in it, etc., and at the end of this effort they start again with an inventory solution. Mbook comes with inventory integrated, so you deploy and adopt a single application that fulfils both functions with no additional effort and no integration concerns.

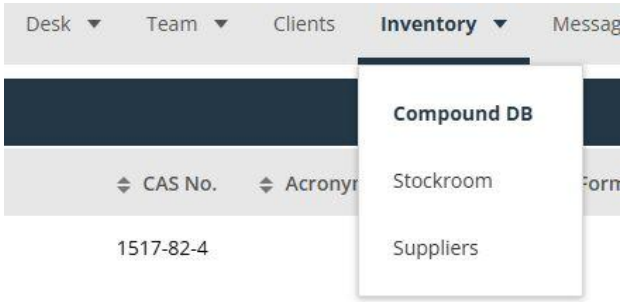
Preliminary step: Become an inventory manager!

Any user in your group can read the information available in the inventory section. In order to add or edit entries, you will need access as an inventory manager. For this, a user assigned as a group manager can go to the user options and select “edit user” to enable or disable the inventory manager privileges.

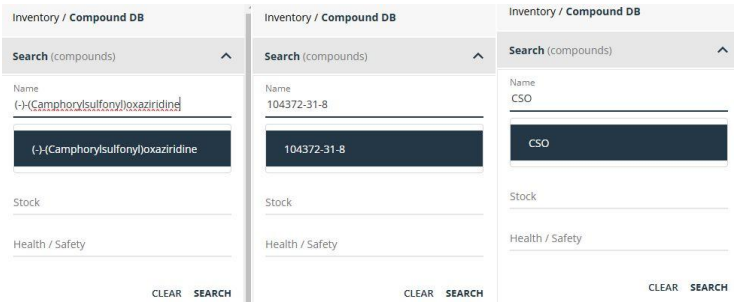


The inventory menu

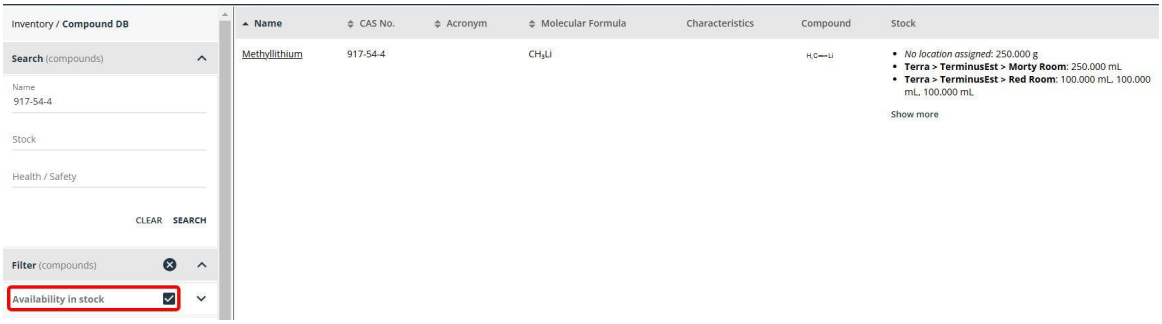
The inventory tool can be found on the top bar menu and is linked to the compound database entries. You can enter or edit new suppliers as well as searching for any compound in your Mbook database.



You can search by name (CAS Number or Acronym), code, stock or Health/Safety: by the H phrases or CMR categories, or even by searching by keywords as Lactancy, Lactation, Carcinogens, Mutagens, Reprotoxics is available using this field.

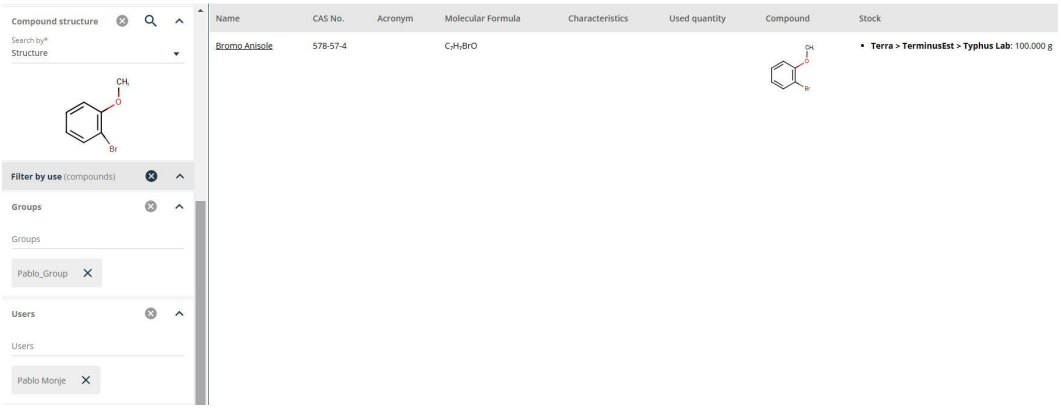


You can search by compounds available in stock, just by checking the applicable box:

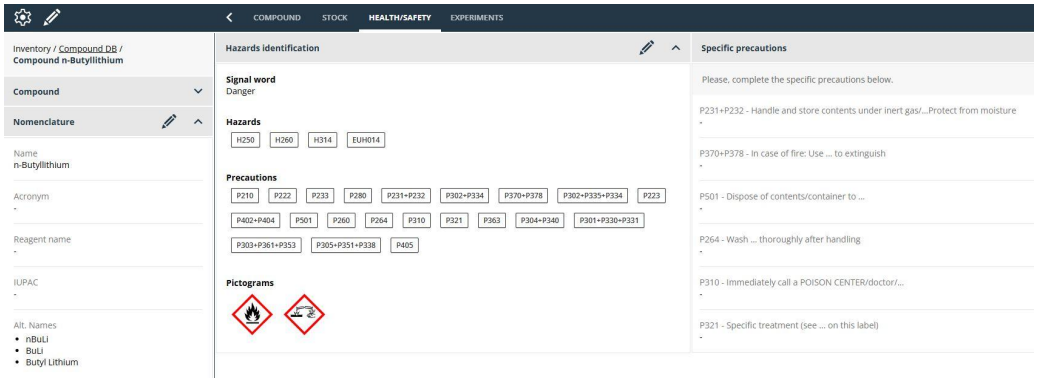


Use the option to search by compound Structure to load or draw a molecule and search for it.

The search mode “By Use” allows you to search by compounds used by a group, project and/or user. Once you run the search with the 'By Use' option, you will get a new 'Used quantity' column, showing the amount used for each compound.



The inventory manager will be able to add hazards and the applicable pictograms to any existing compound from the 'Health/Safety' tab:



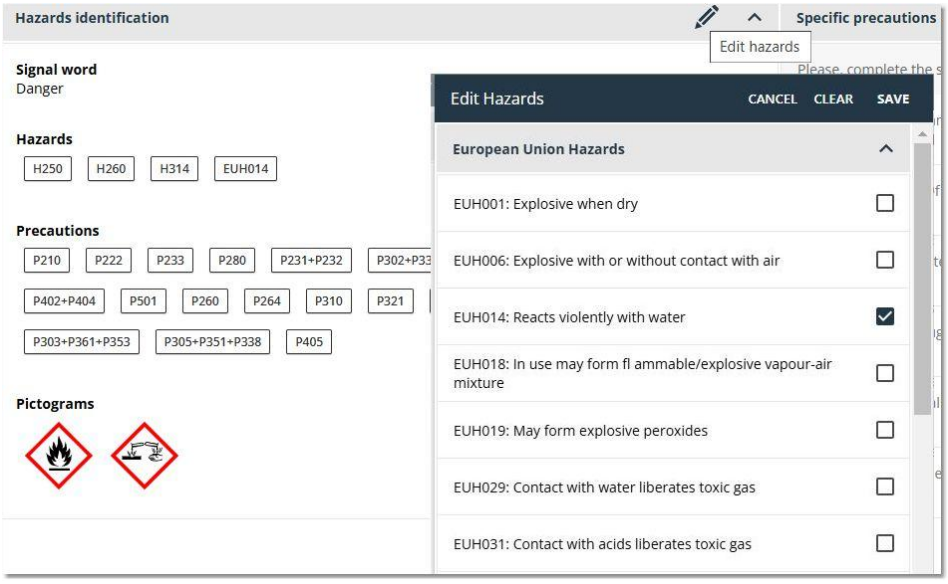
You can categorize compounds using the CMR (carcinogenic, mutagenic or reprotoxic) categories. The CMR categories are related with the H phrases according to the table below:

Table 2: Hazard statements for CMR categories

Hazard statements	Category 1A or 1B	Category 2	Effects on or via lactation
Carcinogens	H350: May cause cancer	H351: Suspected of causing cancer	
Mutagens	H340: May cause genetic defects	H341: Suspected of causing genetic defects	
Reprotoxics	H360: May damage fertility or the unborn child	H361: Suspected of damaging fertility or the unborn child	H362: May cause harm to breast-fed children.

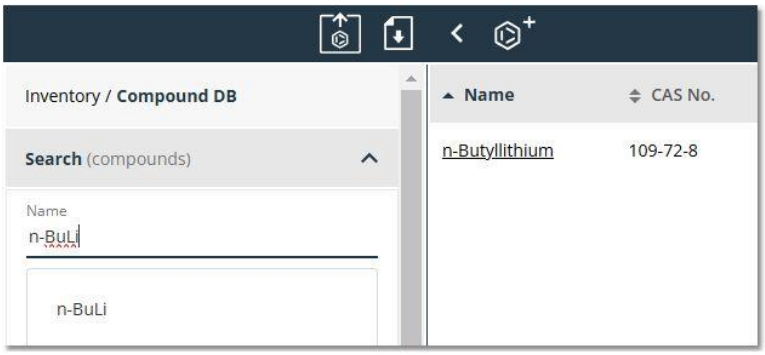
Source: Regulation (EC) No 1272/2008[2]

The CMR categories are automatically added to the compounds when the corresponding H phrases are added, after having clicked on the 'Edit Hazards' button:



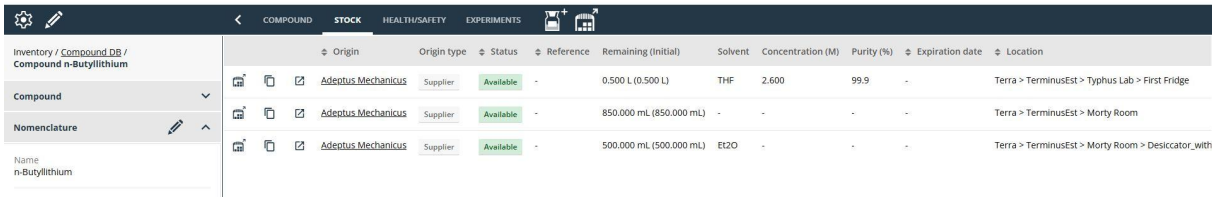
A practical example

Let´s go to the main menu and select Inventory/Compound DB and search “n-BuLi” as an example:



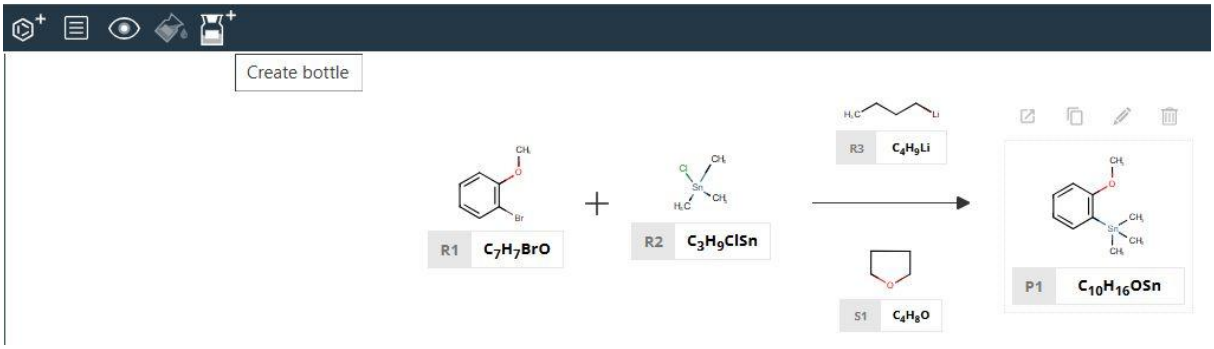
(You can also search by code, stock or Health/Safety: by the H phrases or CMR categories, or even by searching by keywords as Lactancy, Lactation, Carcinogens, Mutagens, Reprotoxics is available using this field.)

Click on “n-Butyllitium” in the list and go to the “Stock” tab for this compound. Here you can see we have three different bottles. This window also displays details such as status, batch number, and remaining number for each of the bottles.

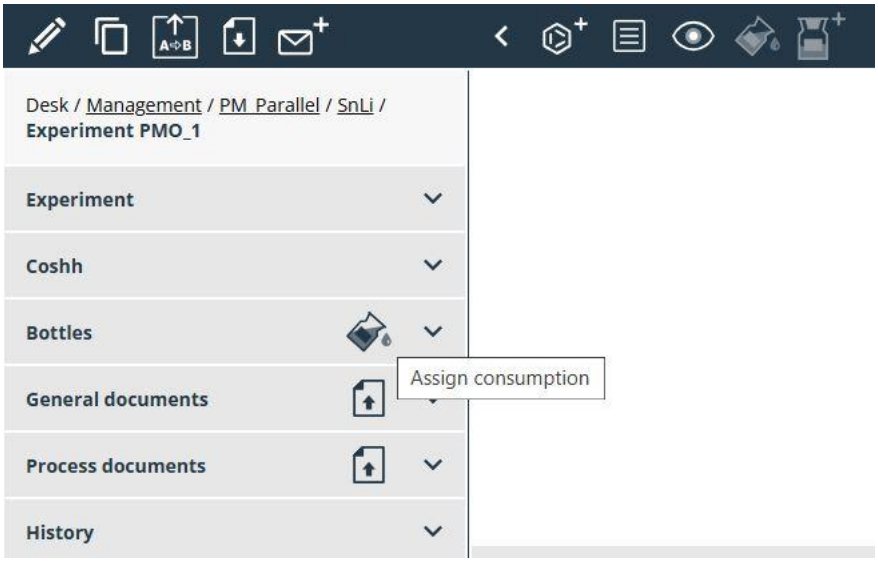


As an inventory manager you can add a new entry or edit the information relating to any of these bottles, such as the description, quantity, purity, order date, who ordered it, etc., and then just save any changes made.

You can also add bottles to the inventory from the reaction scheme just by highlighting the appropriate product and clicking on the 'Create bottle' button:



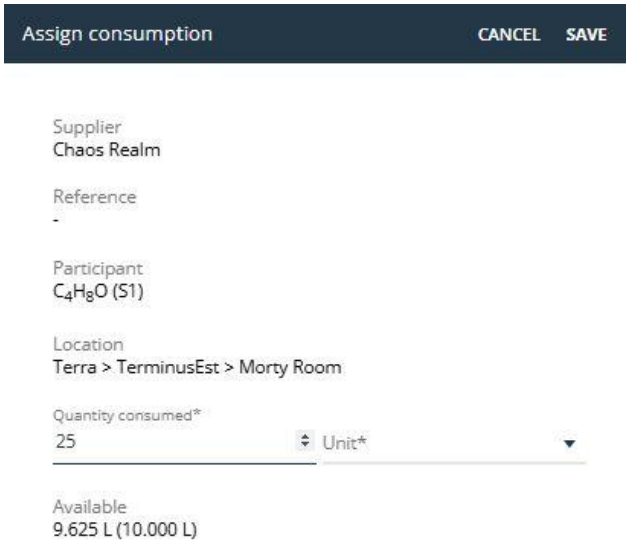
Any user can go to Mbook’s desk panel and use the inventory entries to link to an experiment. Let’s click on a recorded experiment and check the entries for n-BuLi (or your preferred reaction participant) by clicking on the “Assign consumption” icon.



You can now set the amount you have used of each chemical for any of the source entries.

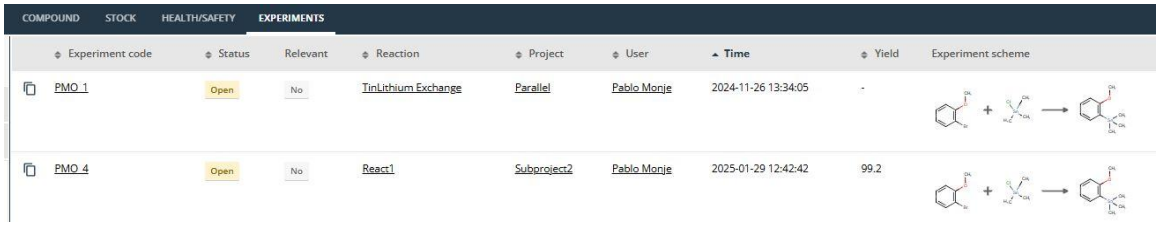
Besides the available number of each of the source bottles, it also displays the “quantity deficit”. This shows you the amount of participant required for the reaction as per the stoichiometric table.

You can register a value on the “quantity consumed” box to keep track of your chemicals as shown below.



Note: If you use a bottle with a different purity than the one recorded in the experiment table, then this new purity value will be automatically updated. In this way, you can keep track of your chemicals in the lab in a straightforward manner with everything you require integrated into your electronic laboratory notebook.

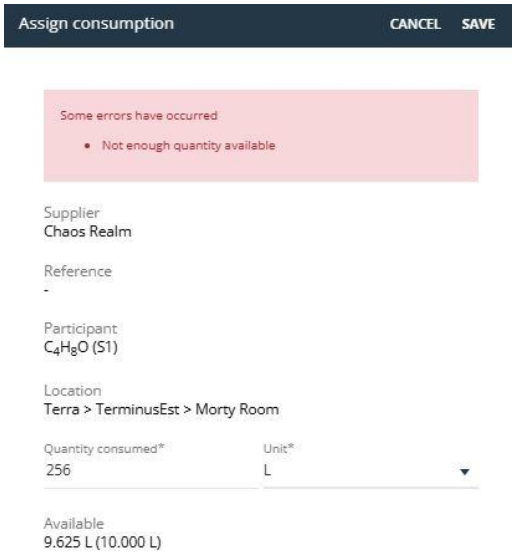
When selecting a compound from the Inventory/Compound DB, the experiment tab displays the list of experiments where this compound has been used:



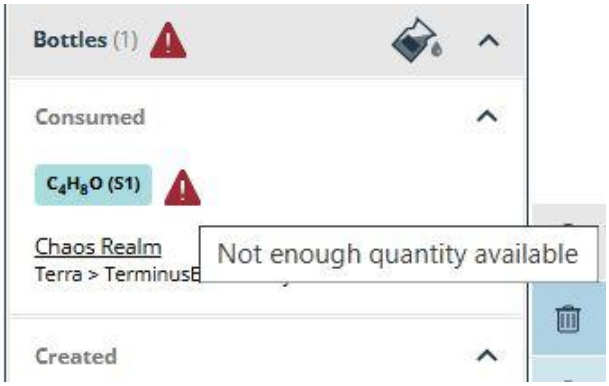
Warning messages

The inventory tool will also try to help you avoid mistakes when recording your entries.

- If the value of the quantity consumed is greater than the number of bottles you have available, you will see the following error message:

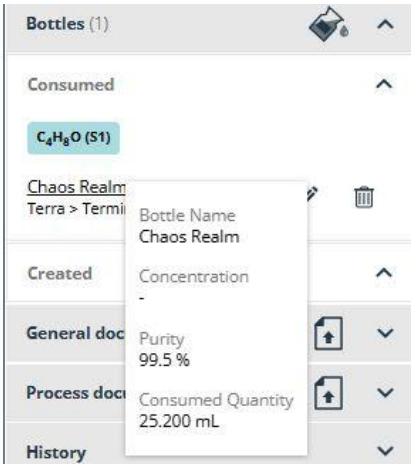


- If the quantity consumed is less than that required according to the stoichiometric table, the warning message below will be displayed on your source panel with an exclamation mark symbol.



If this is the case, you will just need to edit the value to a suitable one and the warning message will disappear.

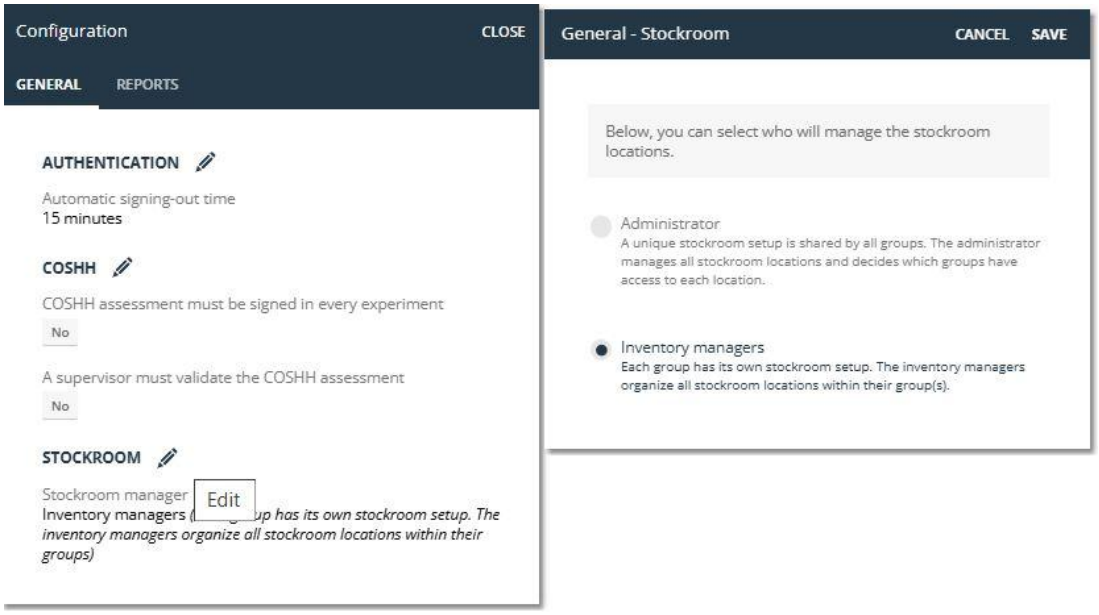
Hovering the mouse over the source entry will display information about it:



7.1 Stockroom

Preliminary step: Become an Inventory Manager!

In order to add or edit any entries in the stockroom, you will need administrator privileges (or the administrator's permission if you are an Inventory Manager). To do this, the administrator will need to go to 'configuration' to select the desired privileges.



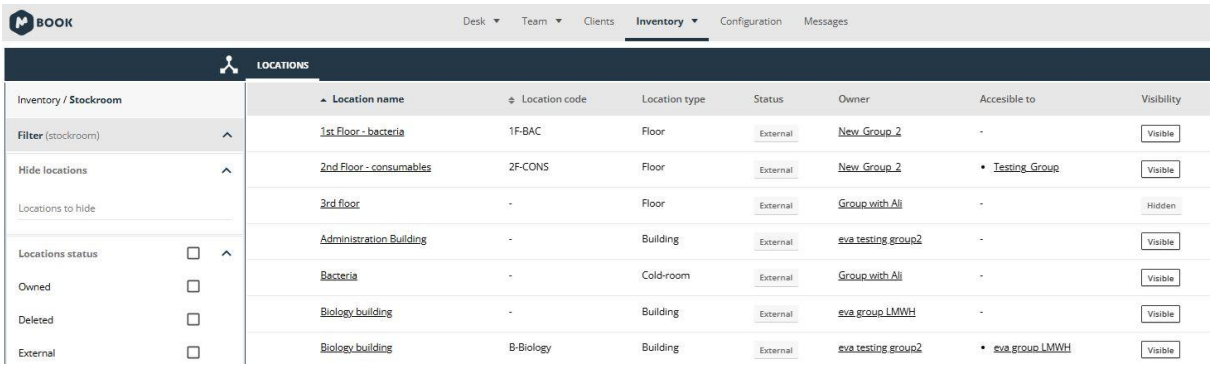
'The Administrator' option is the default configuration.

A unique stockroom setup is shared by all groups. The administrator manages all stockroom locations and decides which groups have access to each location.

The administrator is allowed to add locations, as explained below.

In this mode, the administrator can only see the locations, but not the information about the assigned bottles.

This mode will typically be used in organizations where the stores department manages all locations.



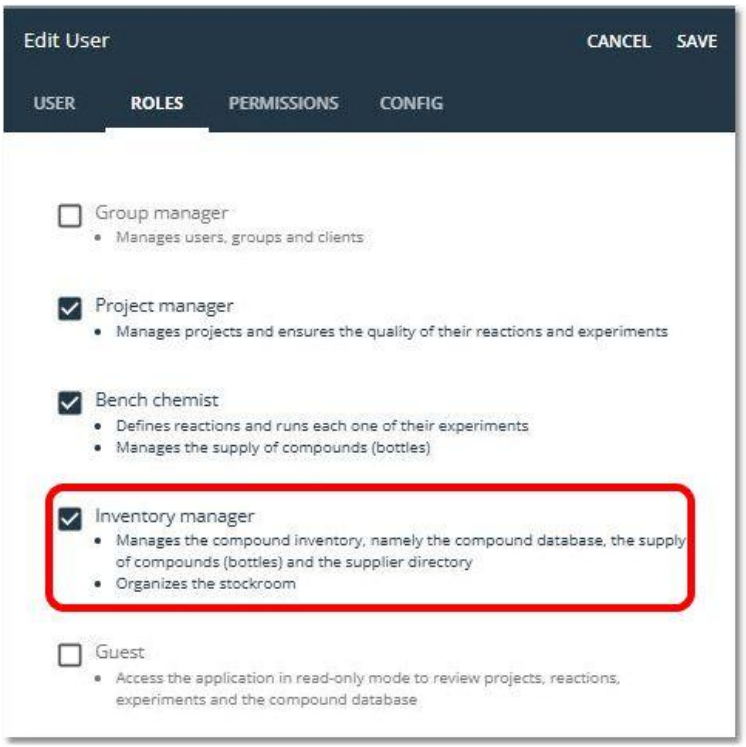
Inventory Managers can assign bottles to the existing locations created by the administrator but cannot create new locations.

When **the Inventory Manager** option is selected, each group has its own stockroom setup. The Inventory Managers organize all stockroom locations within their group(s).

The administrator cannot change locations in this mode and the menu bar will not display the Inventory/Stockroom tool.

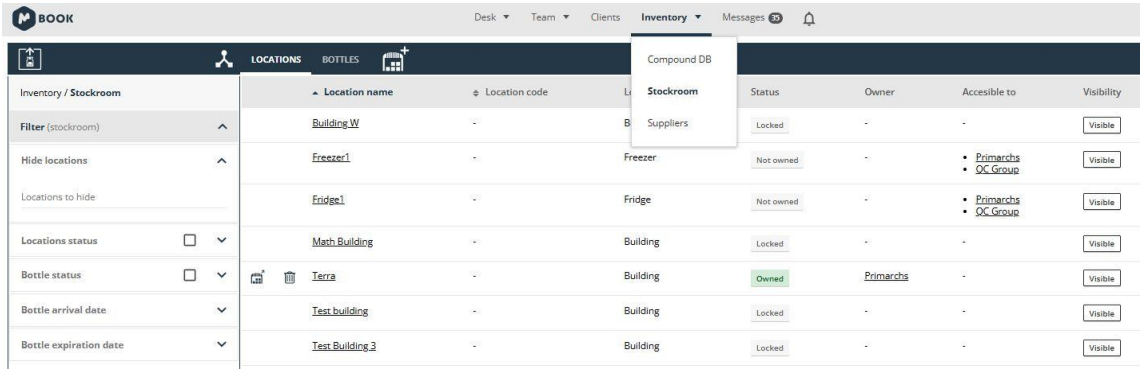
This stockroom mode will typically suit environments where chemists prefer to handle bottle locations around the lab and building(s) themselves.

The Group Managers will be able to give 'Inventory Manager' permissions to any existing user:

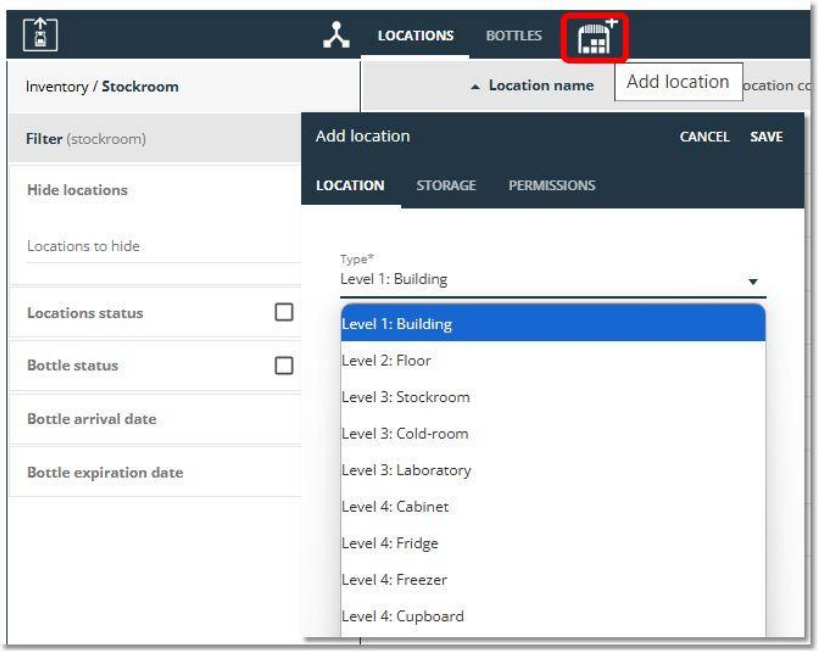


The stockroom menu

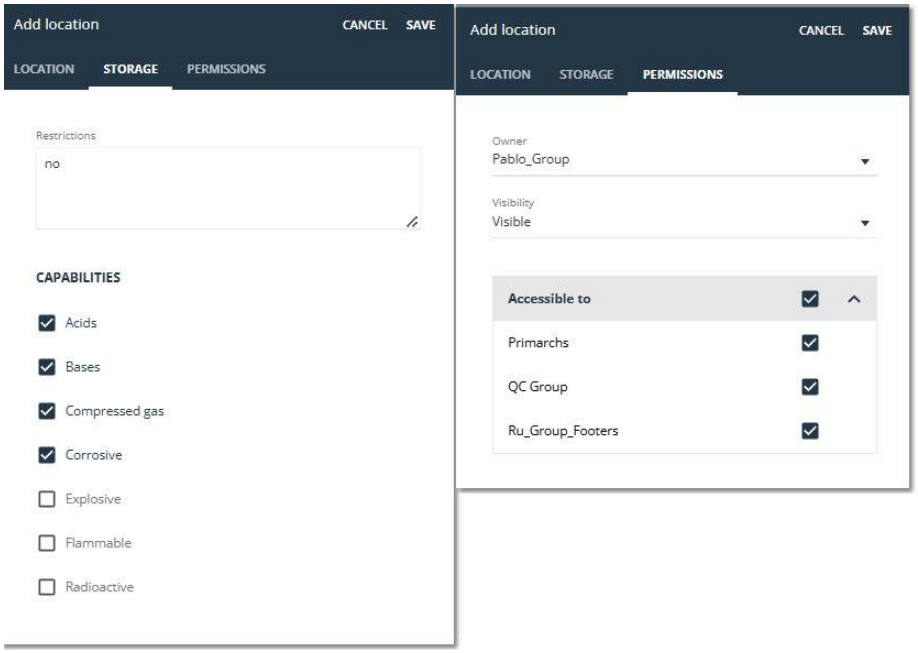
The stockroom tool can be found under the 'Inventory' scroll down menu:



The first step is to 'Add a location':

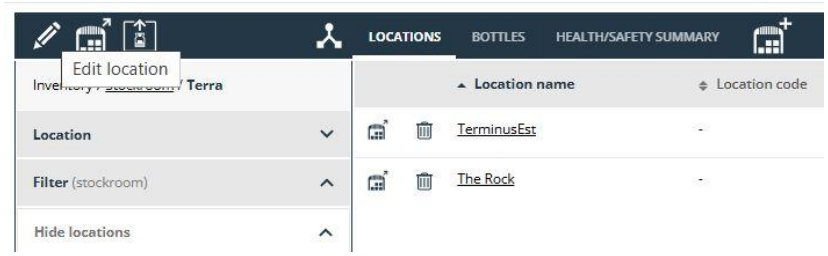


From here, you can enter the type (Level 1 in this example), location name, description, storage conditions (from level 3), and manage permissions (Group owner, visibility, and allowed groups) for the new location:

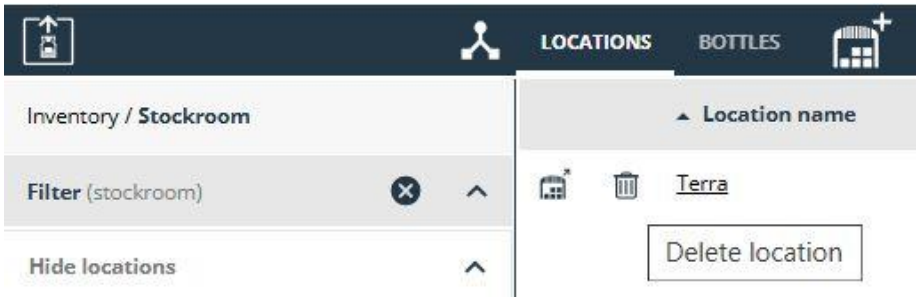


Once you have created the location in the first level, you can continue adding further levels by clicking on the 'add location' button.

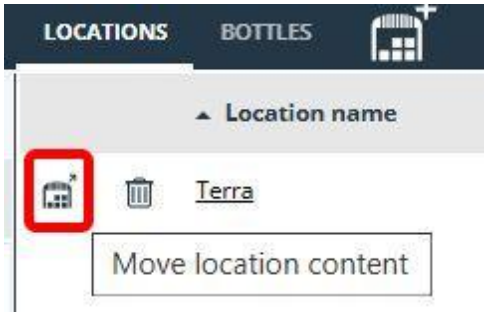
You can edit a location by clicking on it and selecting the 'Edit location' button:



You can delete any empty locations by clicking on the 'Delete location' button:

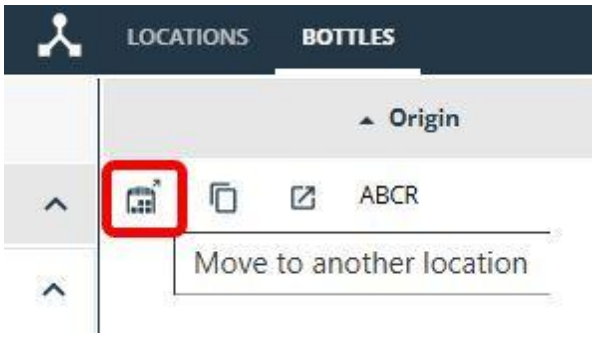


To move a location (with all the contents) to a different place, just use the applicable button:

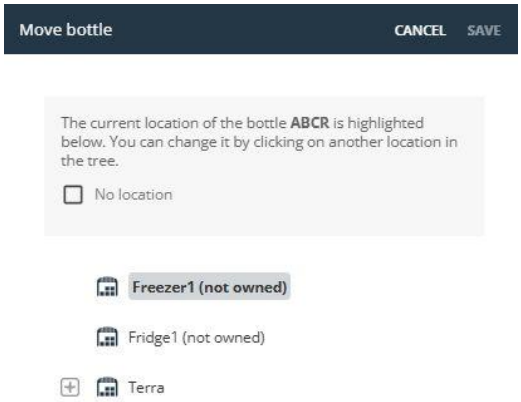


NOTE: If the bottle is not already in the inventory, you will need to add it.

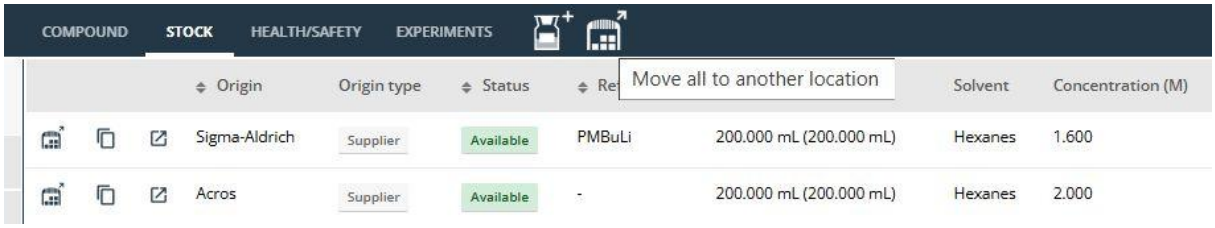
You can also move bottles to a different location:



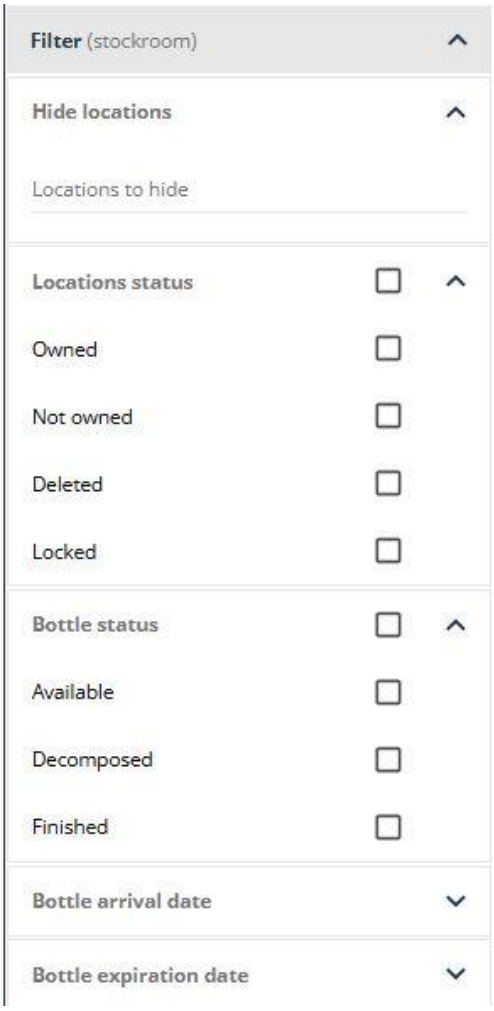
After having selected the new location and clicked on the 'Save' button, the location will be updated:



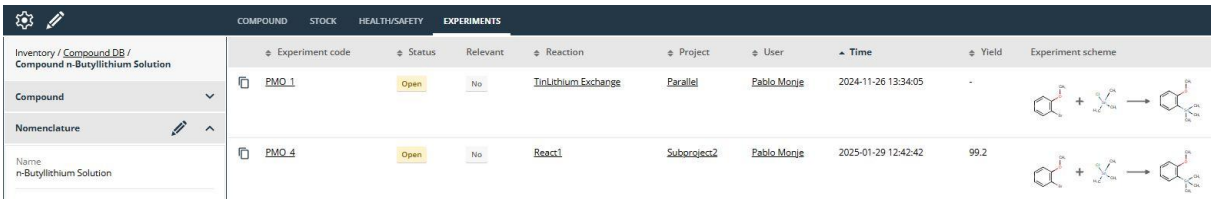
If you have several bottles of the same compound, you could move all of them together to the same location just by clicking this button (from the inventory dialog):



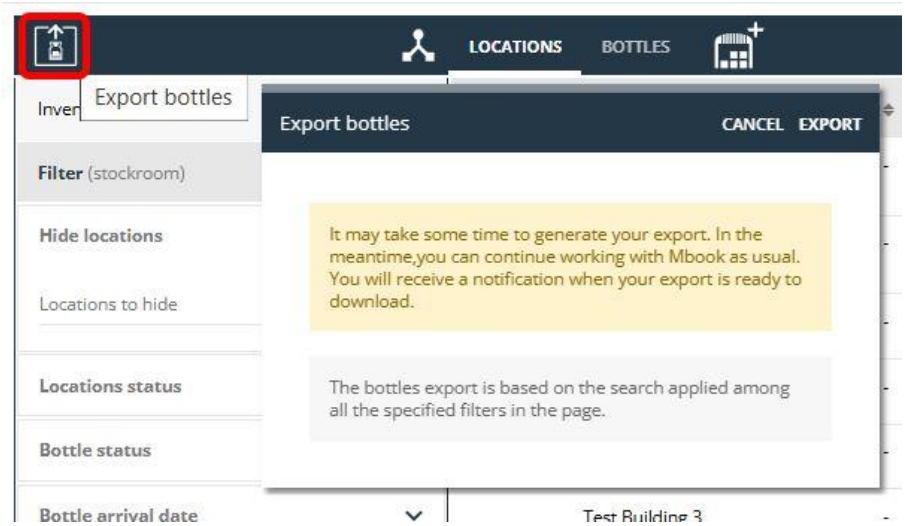
Use the filter to hide locations, display 'owned', 'deleted', 'locked, 'non editable', etc..:



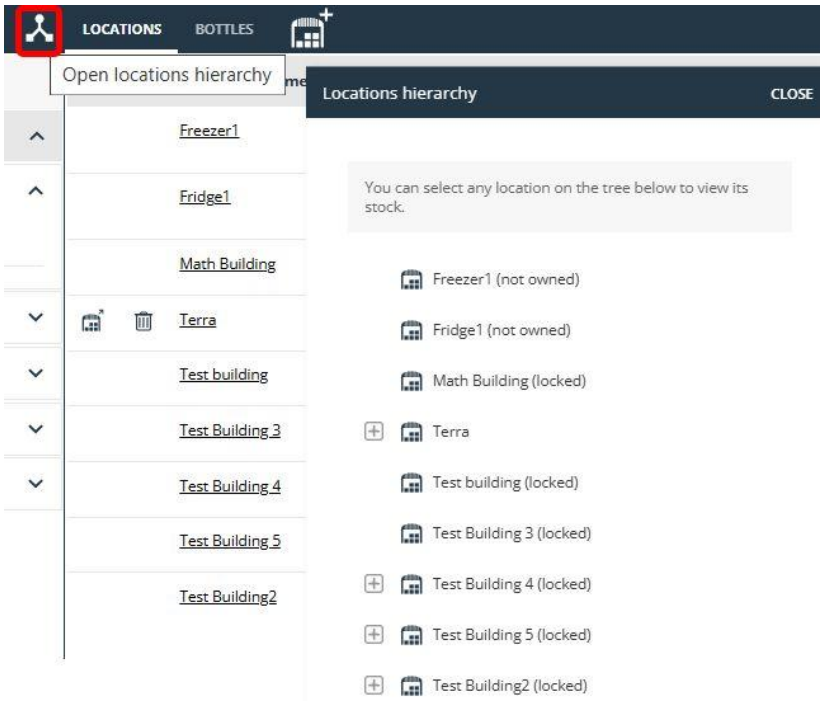
When reaching a compound from Inventory/Compound DB, the stock tab displays the list of bottles corresponding to that compound. When clicking on a specific bottle, the list of experiments where this bottle has been used is displayed. Clicking on the experiment code, that specific experiment where the bottle was used will be opened:



Click on the 'Export bottles' button to export your stockroom:



Click on the Open locations hierarchy to easily navigate through your stockroom:

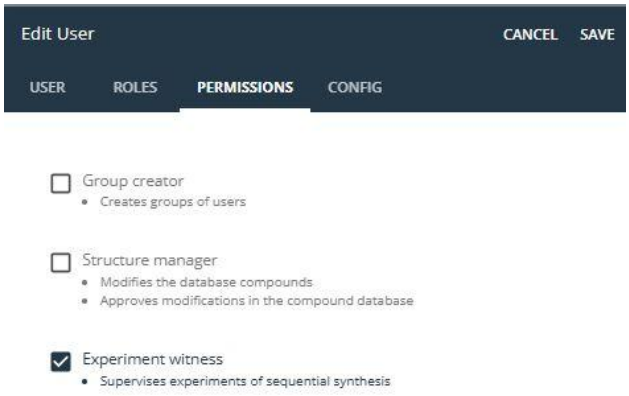


Part

8 Experiment Witnessing, Approval and Structure Managers

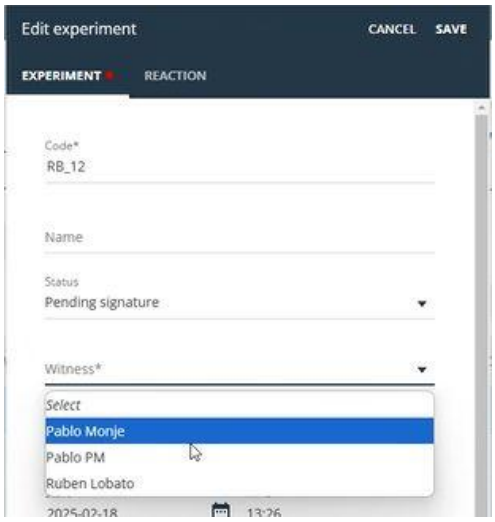
Experiment Witness

Mbook includes the ability to sign experiments as a witness. The Group Manager has the ability to create and edit users with witness power just by checking the appropriate box:



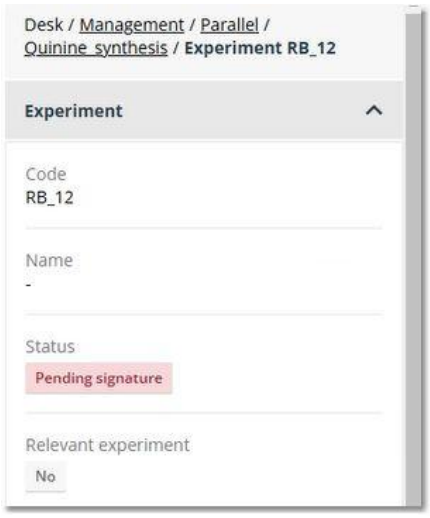
The group manager can allow any given user to be a witness to other user's experiments if those experiments are accessible by that particular user.

Once the chemist has finished the experiment, he/she will need to select 'Pending signature', from the 'Edit Experiment' dialog.

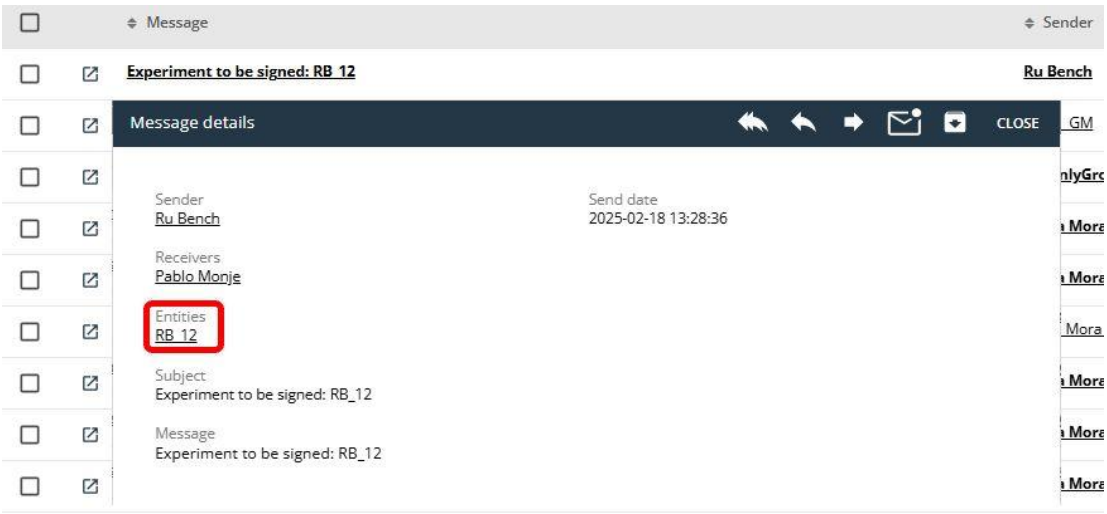


After clicking the 'Save button' and selecting the 'End Date', the user will be allowed to select the desired witness (if there is more than one).

The status experiment will change to 'Pending Signature':



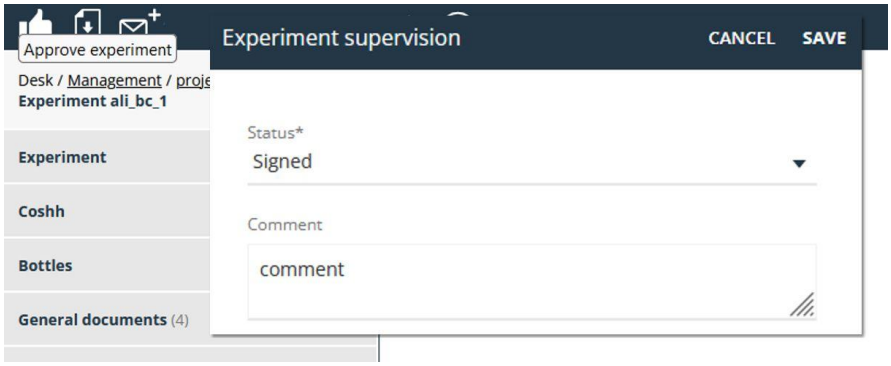
The witness will receive a notification in his/her inbox (displaying an envelope in the toolbar).



Once in the message, the witness will be allowed to display the experiment by clicking on the 'Entity' link (highlighted in red in the screenshot above).

After setting the status of an experiment as Pending Signature (or Pending Approval), the icon for Experiment Supervision will be displayed (both for the experiment owner and witness).

The witness can type any required commentary before signing the experiment (the comment is mandatory if the experiment has not been signed):



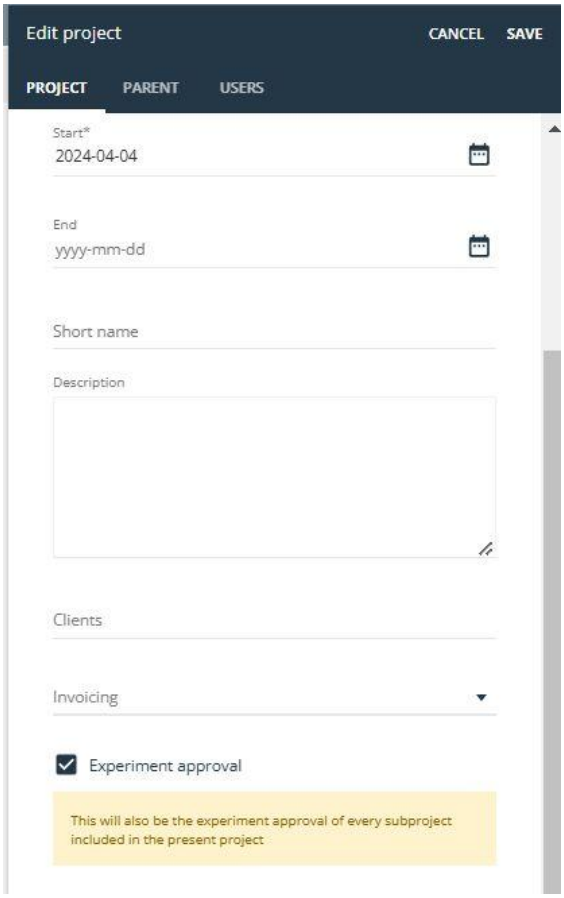
After clicking the Save button, the supervision icon will disappear and the status of the experiment will turn to 'signed'. Once the experiment has been signed, it can no longer be edited by the owner (unless the owner of the experiment is the project manager).

Experiment Approval

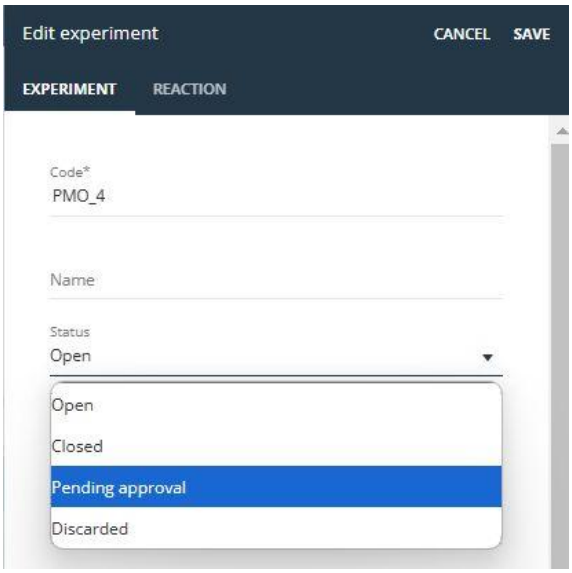
In certain companies/groups, experiments, once finished, must be **approved** by authorized users.

The group managers and project managers can be assigned privileges to approve experiments and to give approval privileges to other users.

The Project Manager has the ability to create projects with 'experiment approvals' just by checking the appropriate box in the 'Edit Project' window:

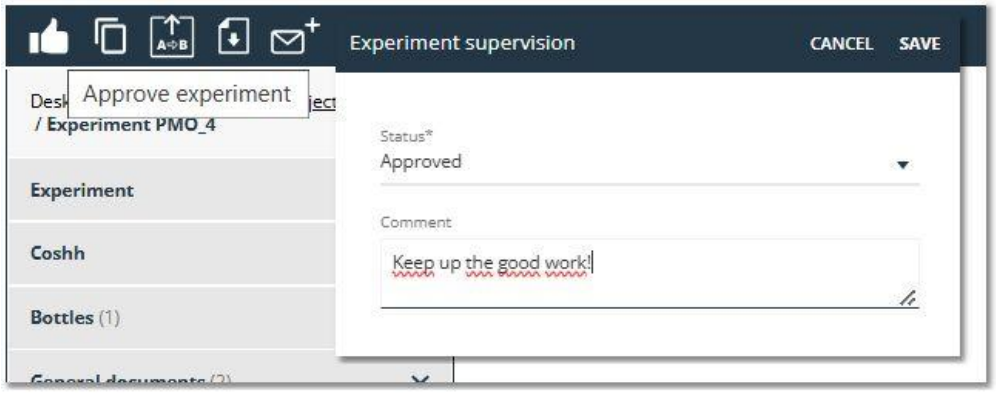


When the status of an experiment is switched to 'Pending approval', a message is sent to the group manager(s) of the project to inform them that there is an experiment that needs to be approved:



NOTE: If both witness and approval process are active, once an experiment is signed, the approval process will be launched automatically (the experiment owner does not need to trigger this action manually).

The supervisor is allowed to type any comment before approving the experiment (the comment is mandatory if the experiment has not been approved):



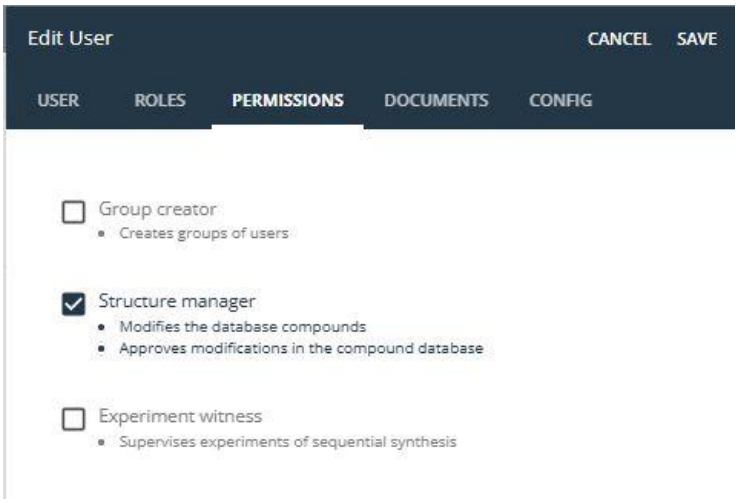
After approval, the experiment state will change to 'Approved', and the experiment owner will receive a notification of such. After the experiment is approved, it cannot be edited by the owner.

If the experiment is not approved, its state changes automatically to 'Open'.

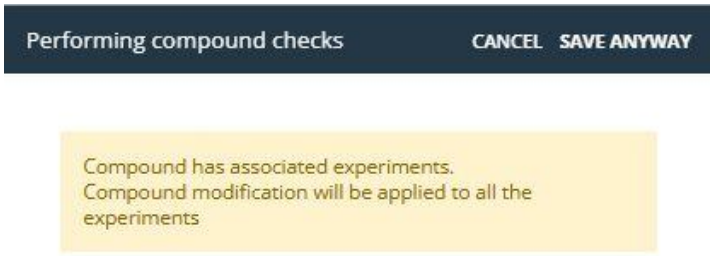
For a given experiment, you can have several associated privileged users. The experiment will be approved for the first user to check the experiment.

Structure Managers

By default, Group and Project Managers will have 'Structure manager' permissions.



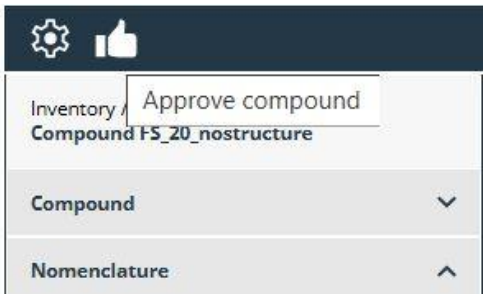
Any user can modify a compound that they have created (compounds created by other users, however, cannot be changed) that are only used in their experiments. A message informing about that change will be displayed to them:



However, if the compound is present in experiments belonging to different users, the user will need approval from the structure manager to modify it. When a user attempts to edit a compound, an approval request will be sent to all the structure managers by message. Only one approval is needed to allow the requested changes to be made:

During this step, the edition of the structure is blocked. The structure manager will see both molecules (the original and the modified):

Clicking on the 'entity' link will allow the manager to validate the changes:



If the modifications are approved, the changes will be applied immediately and a message will be sent to the users associated with the experiments and to the applicable project managers (informing them about the approval).

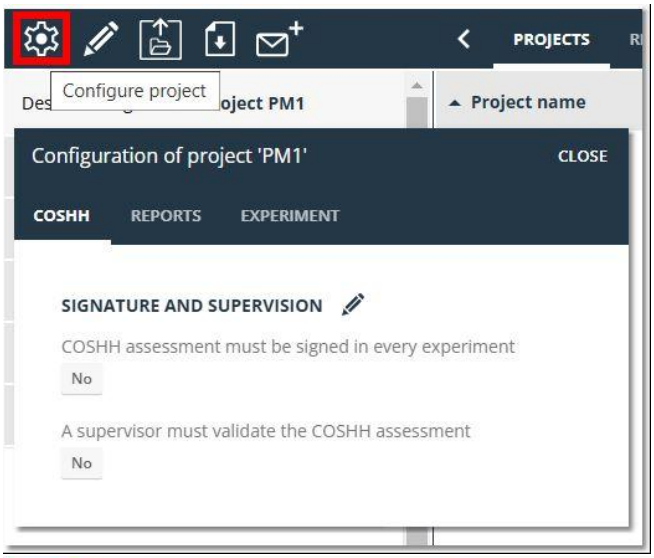
Closed experiments will be opened automatically but no modifications will be applied in the stoichiometric table.

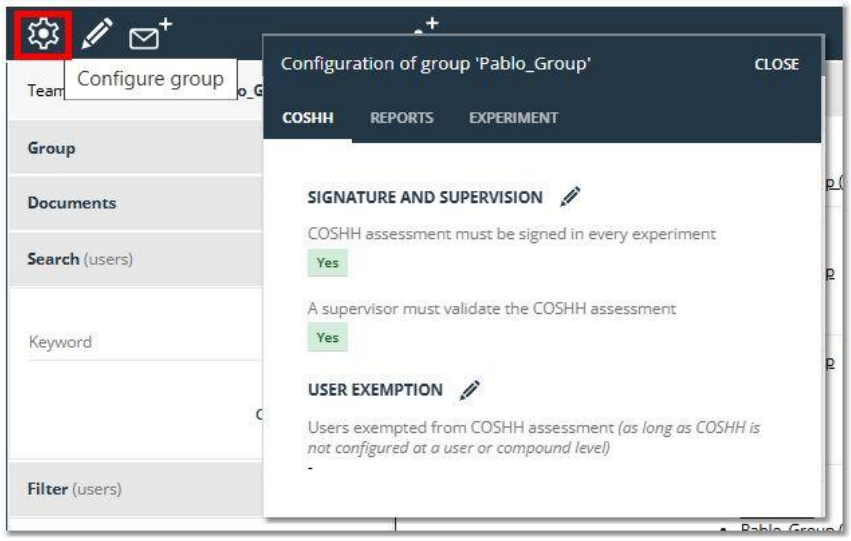
Part

9 COSHH

You can include COSHH assessments for groups, projects, users, and compounds.

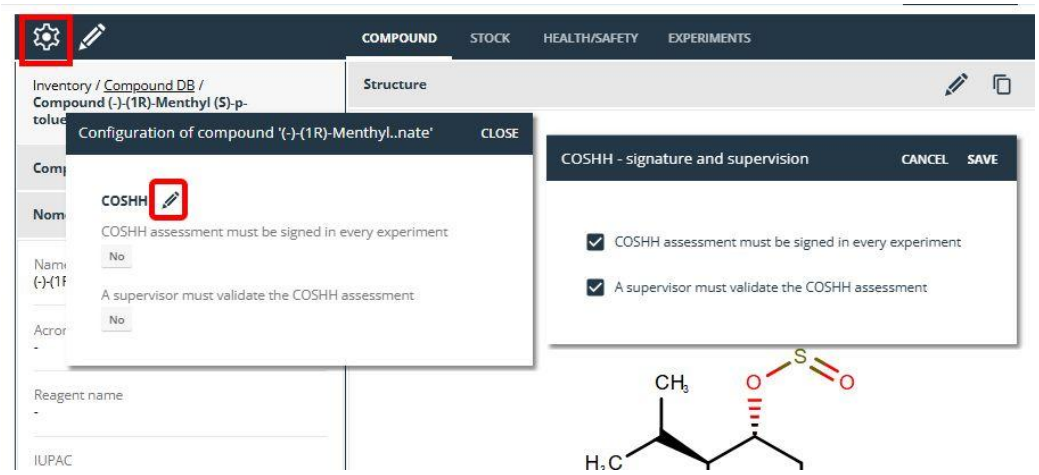
For a project or a group, you need to click the 'Configuration' button which will allow you to select the option to always require a signature for every experiment and also for a supervisor validation. You can also add user exemptions from the same panel:



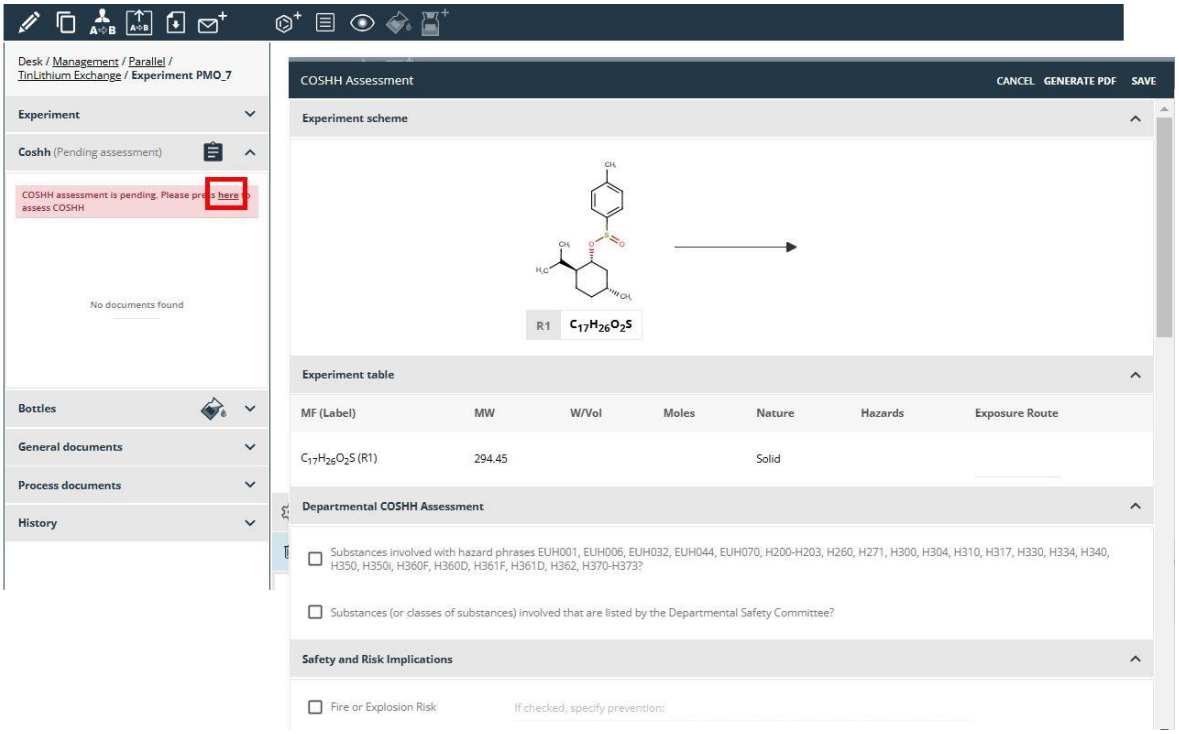


Note: parent COSHH project configurations take precedence over child project configurations.

For users and compounds configurations, the setup is somewhat similar:

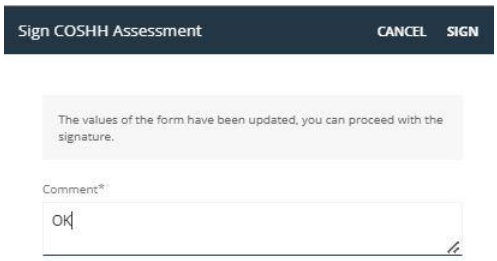


If the option to sign the COSHH assessment in every experiment is checked, a notification in red will appear after having added a compound to the experiment indicating that the assessment will need to be signed:



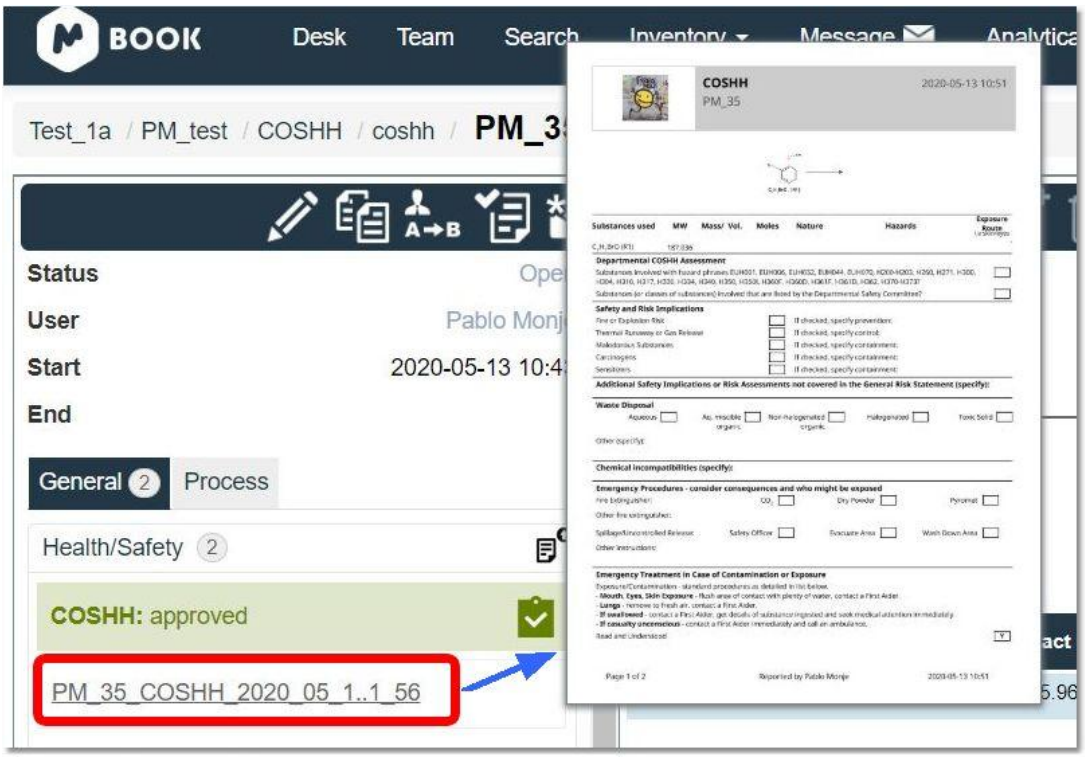
Fill the form with the relevant information, check the 'Read and Understood' box and click on the Save button.

If supervision is necessary, a message and an email will be sent to the supervisor requesting that the COSHH should be checked.

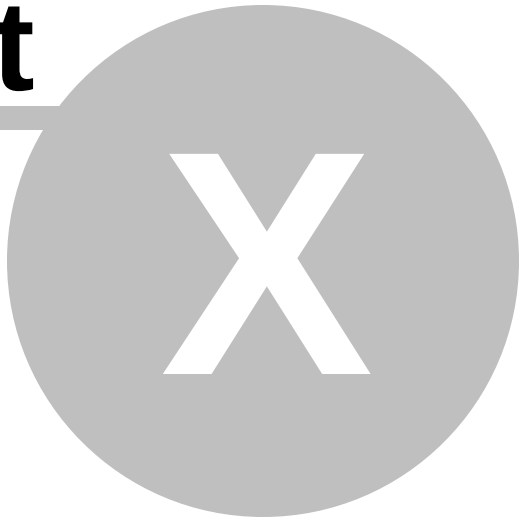


During this process, the experiment will remain blocked (the user, however, will be able to continue adding reactants, solvents, and products, but will not be able to edit the products in the stoichiometric table or to write the experimental section).

Once the supervisor has approved the COSSH assessment, the user will be able to continue with the experiment. The COSHH assessment can be downloaded in PDF format by clicking on the appropriate hyperlink:



Part



10 Further information

More information: https://mestrelab.com/learn-support?product_id=27197
FAQs: https://mestrelab.com/guide/mbook-faqs.html
Download this manual in pdf: https://mestrelab.com/pdf/manuals/Mbook-User-Manual.pdf

Thank you!

Thank you for reading this manual, and for purchasing this release version of Mbook. We will be very keen to read your feedback on the application, to hear about any bugs you may find and to also listen to any additional ideas or suggestions you may have.

Please remember that you can send all those, and any queries about the software, or requests for help, to:

support@mestrelab.com

Keep checking our web site (www.mestrelab.com) for additional information on our range of software packages, and for news on our company.