Mbook 3.1 Manual

Last Revision: 12-Sept-2022

Mbook

by MESTRELAB RESEARCH

This is the manual of Mbook

Mbook Manual

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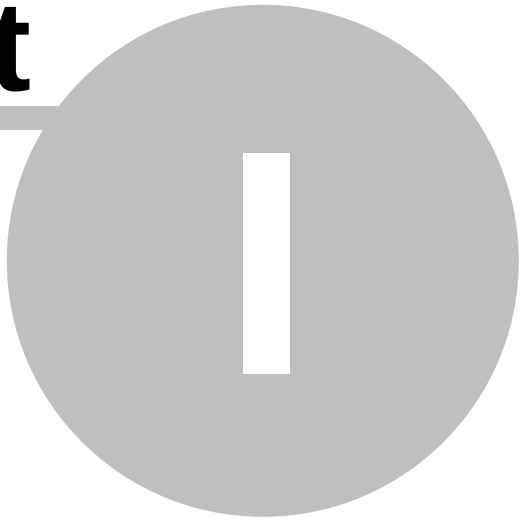


1 Introduction

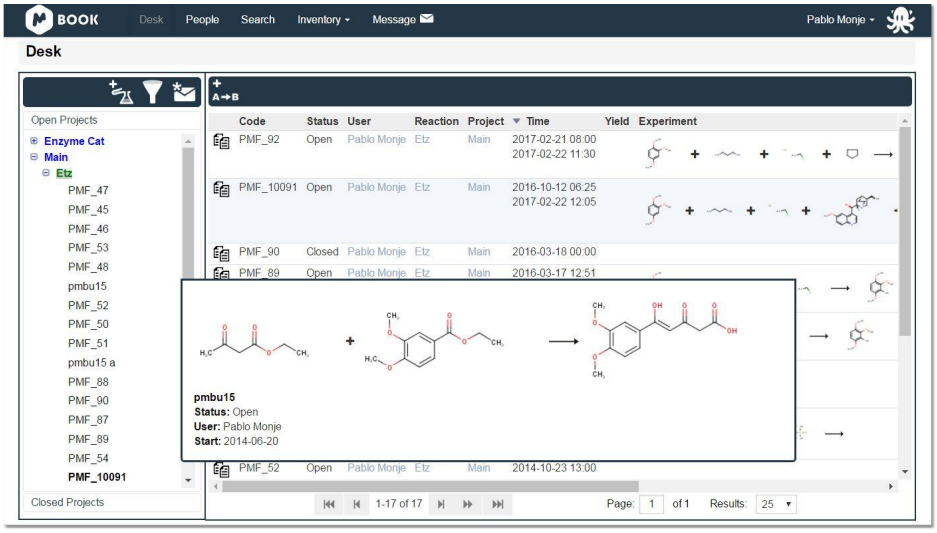
ABOUT MBOOK MANUAL

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 of the Group Manager, containing the list of Projects and a view of the experiments of interest. In the picture below, you can see the desk view with the list of projects (in blue), reactions (green) and experiments (black) with the applicable reaction scheme:



- **Inventory:** Set of compounds, stockrooms and suppliers.

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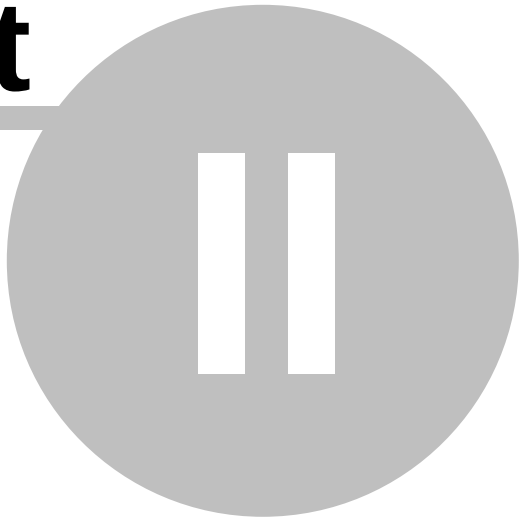
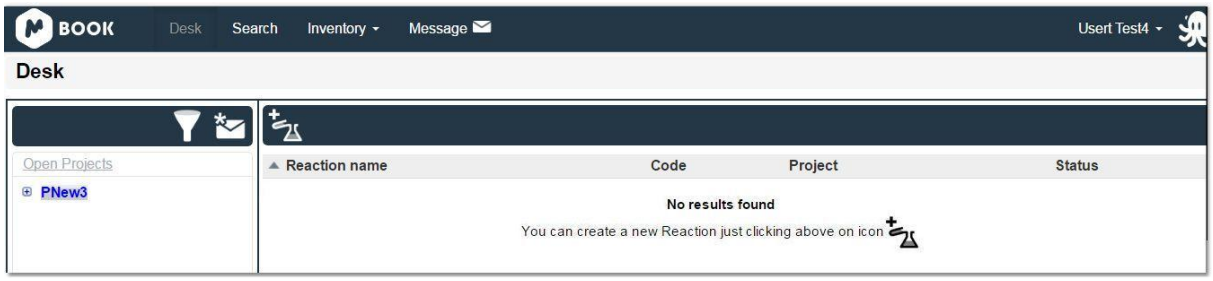


2 Starting with Mbook

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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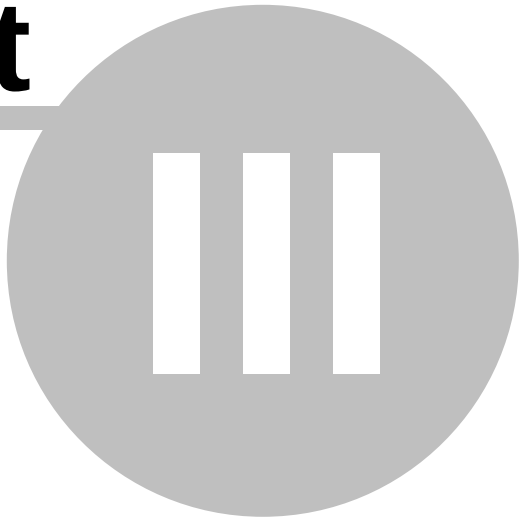


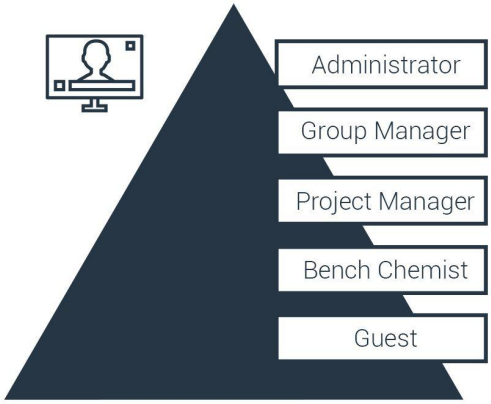
3 Users and Groups Configuration

Before you start creating users and groups, we strongly recommend you read the descriptions of the four types of users 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 provides several levels of access through user roles, limiting access depending on the privileges of the individual user (Administrator, Group Manager, Project Manager, Bench Chemist, or Guest).

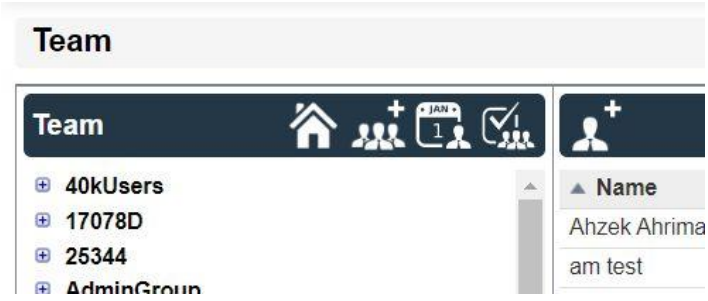


The permissions according to role are as follows:

BOOK	Group Manager	Project Manager	Bench Chemist	Administrator	Guest
Manage users	✓	✗	✗	✓	✗
Manage groups	✓	✗	✗	✓	✗
Assign structure, inventory & safety managers	✓	✗	✗	✗	✗
Assign witness power	✓	✗	✗	✗	✗
Manage projects	✓	✓	✗	✗	✗
Approve changes in structures	✓	✓	✗	✗	✗
Assign users to projects	✓	✓	✗	✗	✗
Approves experiments	✓	✓	✗	✗	✗
Manage reactions & experiments	✓	✓	✓	✗	✗
Witness experiments	✓	✓	✓	✗	✗
See projects, reactions & experiments	✓	*If part of the project*	*If part of the project*	✗	*If invited*

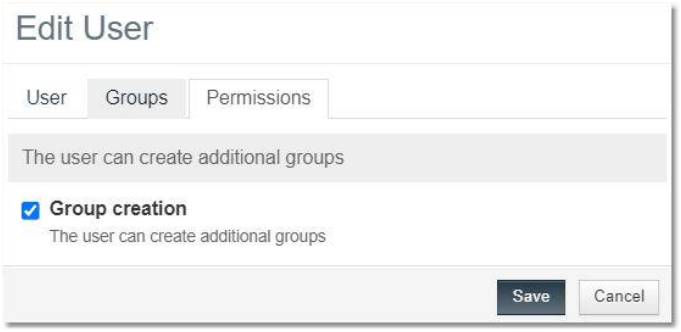
- **Administrator:**

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 has all the same permissions granted to Group Managers, except 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.

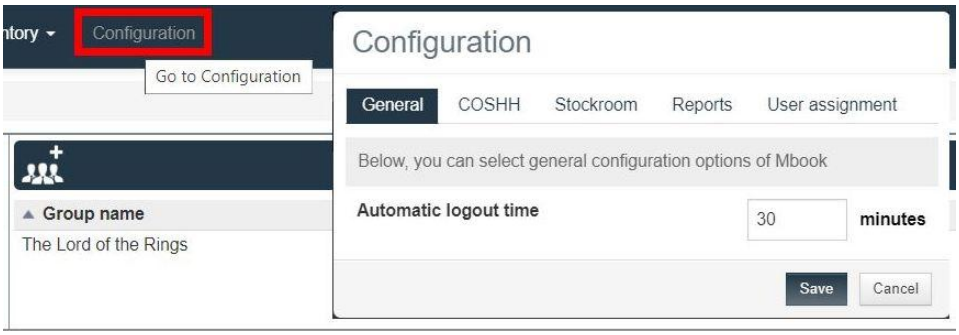


From the admin account you can also check the user activity or to activate/disable users.

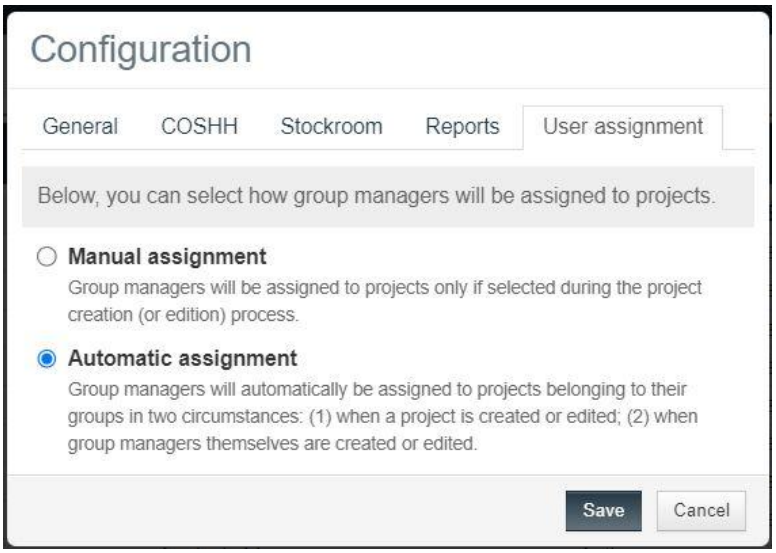
Admins can also change permissions to Group Managers to allow them or not to create groups:



From the configuration tab, the admin can control the automatic logout time (Minimun value: 15 minutes; maximum: 12 hours)



From here, the admin can also select some settings for the COSHH, Stockroom, reports and user assignments (for group managers and projects):



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), as well as Projects, reactions and 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 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 projects, reactions and experiments, but not users or groups; 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.

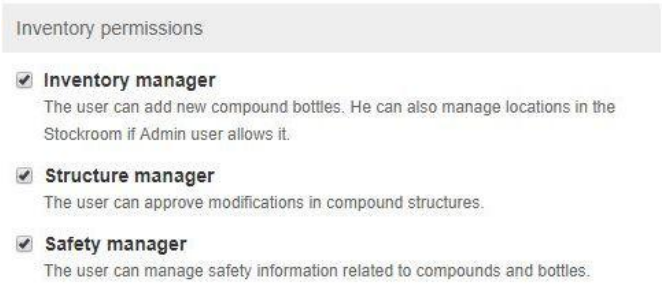
- **Bench Chemist:**

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. By default, Bench Chemists will only see their own experiments in the Desk Panel navigation tree, but this can be modified if required.

- **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 Safety, Inventory or Structure managers.

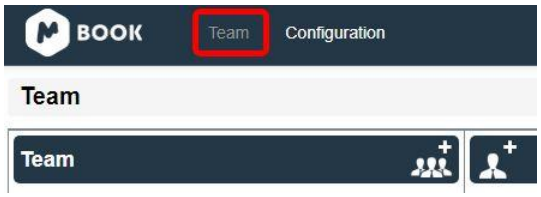


For further information about creating users and groups in Mbook, please follow this link.

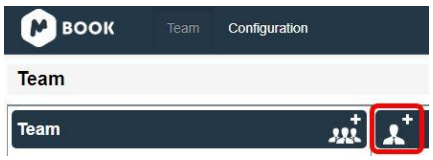
3.2 Create Users and Groups

ADMIN -How to create a user?

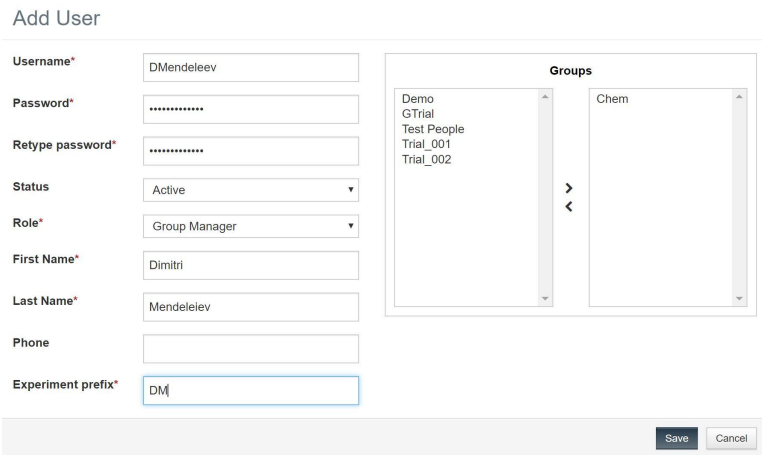
As mentioned, an Administrator will only be able to see the 'Team' tab to create and organize users and groups as an initial stage.



The Admin must create the first user by clicking on the 'Add User' button.



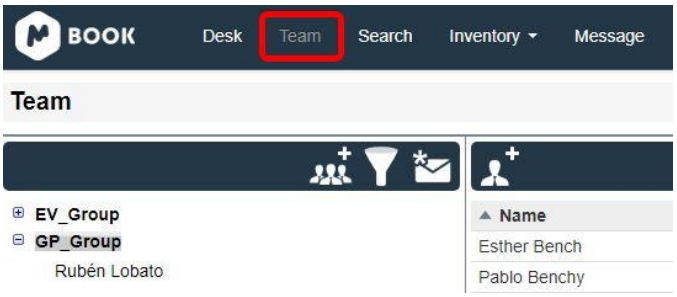
From here, the Administrator needs to enter a username (with a valid email address), password, role, etc... The Administrator can select a group (if there are any existing ones) to which the new user can be assigned:



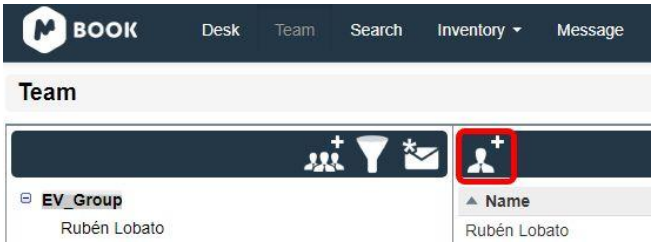
The Prefix field can be used to automatically generate experiment codes for experiments created by the user.

GROUP MANAGER - How to create a user?

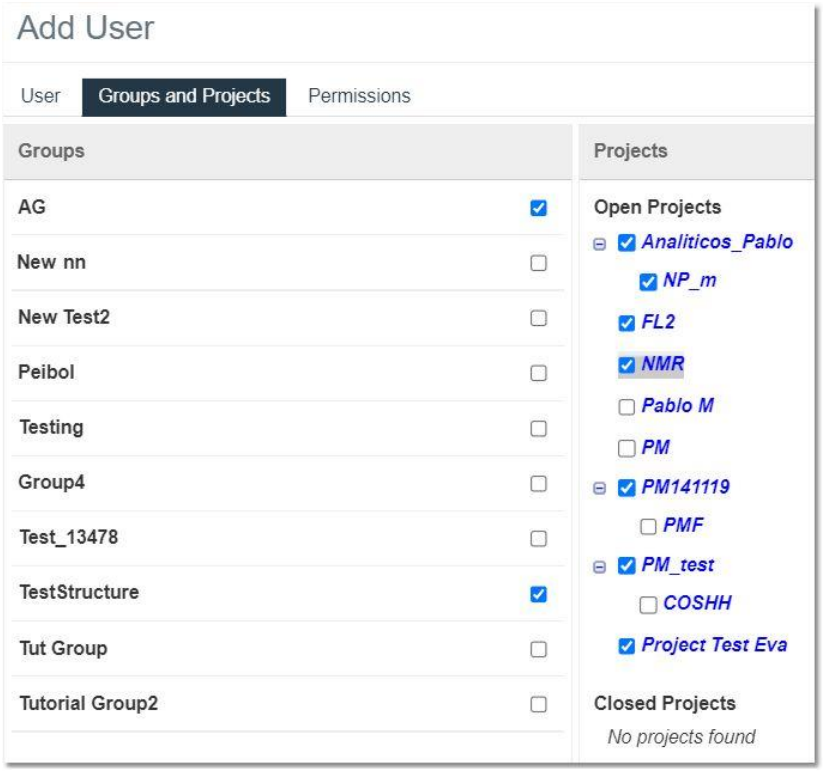
A Group Manager can also create users and groups (if the admin allows), among their other possible duties. As can be seen in the screenshot below, the Group Manager has more active tabs than an Administrator.



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

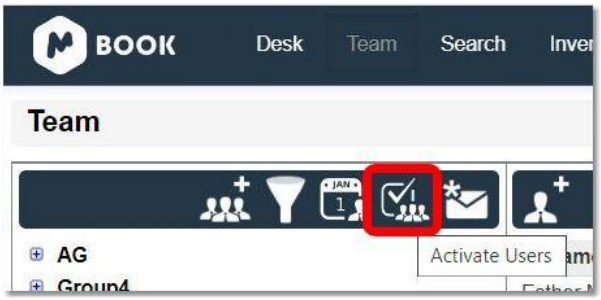


When the group manager is creating a new user, it is possible to assign him/her to any existing group and project by using the 'Groups and Projects tab':

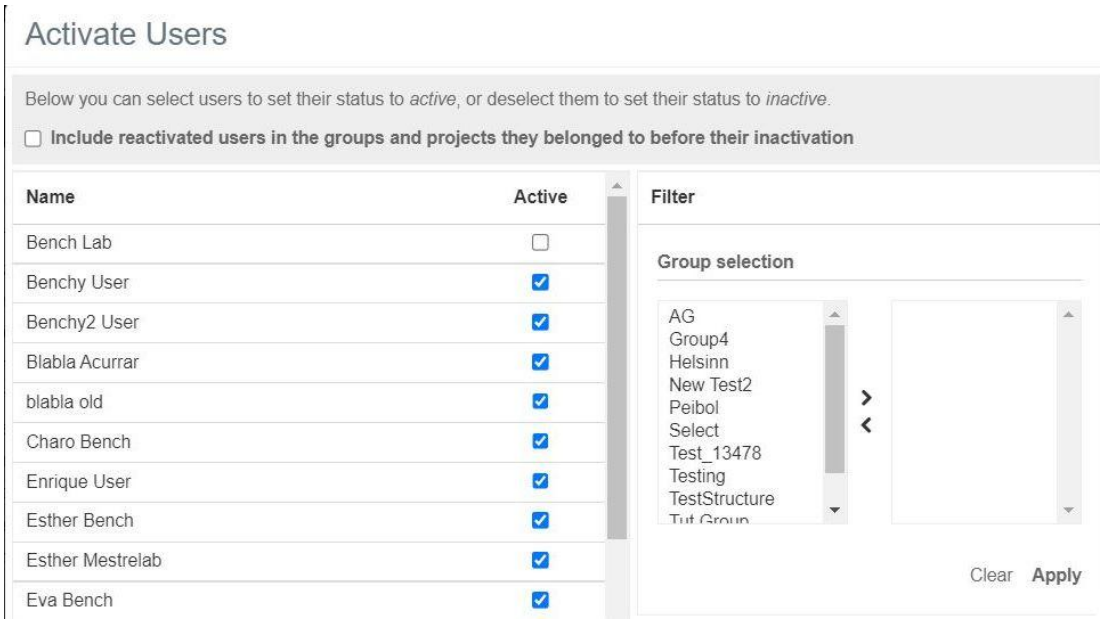


Please note that a Group Manager can also assign individual privileges to any user, for instance, as an Experiment Witness, an Inventory Manager, or a Structure Manager (which an Administrator cannot do).

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

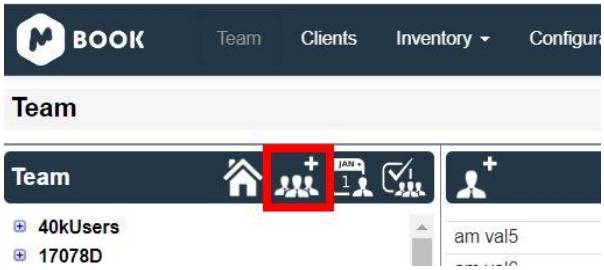


Note that when a user is inactivated in this way, he/she will be removed from all groups/projects at once. When the user is activated again, you will have the capability to include him/her back in the groups/projects he/she belonged to before the inactivation.

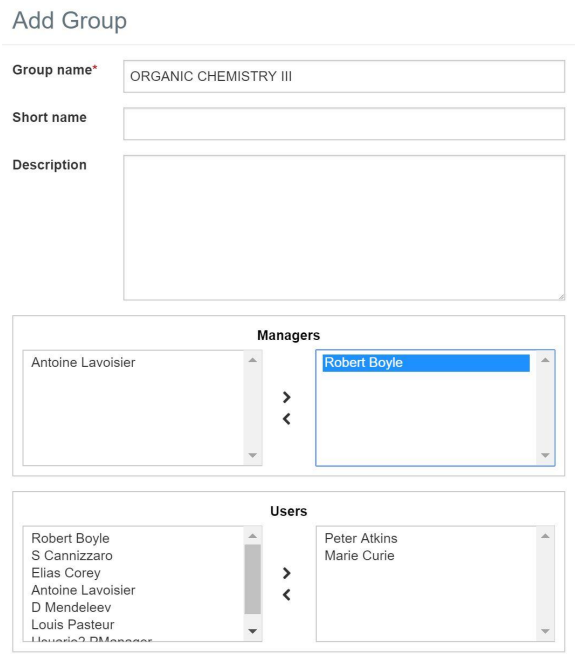


ADMIN - How to create a Group?

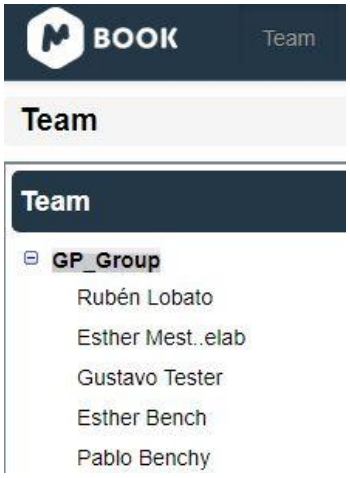
The Administrator can create a group just by clicking on the appropriate button:



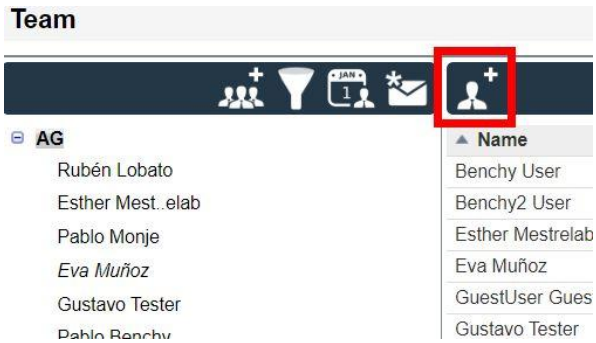
The Group can then be defined by filling in the form so invoked and can then add any existing managers and users as desired.



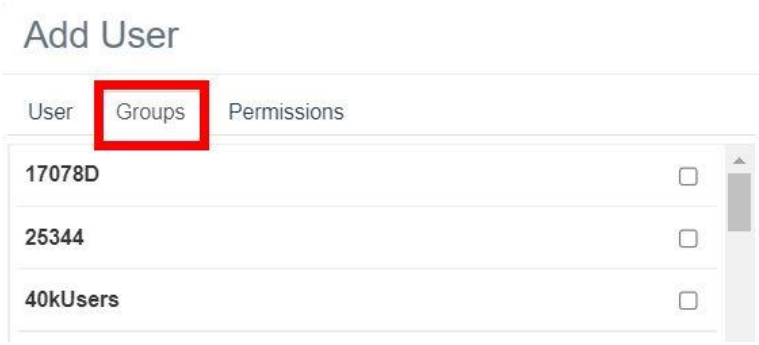
Once some groups have been created, you will find them listed on the left-hand side. You can click on any of them to list the users associated with a particular group.



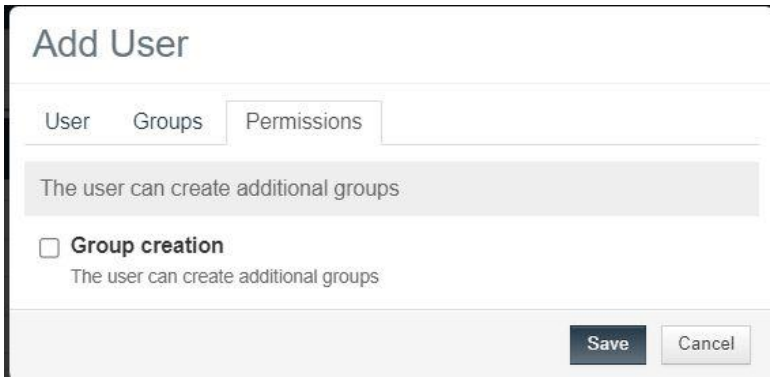
New users can be added to any existing group, just by highlighting the group (or any existing user in the group) and clicking on the 'Add User' button:



When you are creating a new user, you can assign him/her to any existing group by using the 'Groups tab':

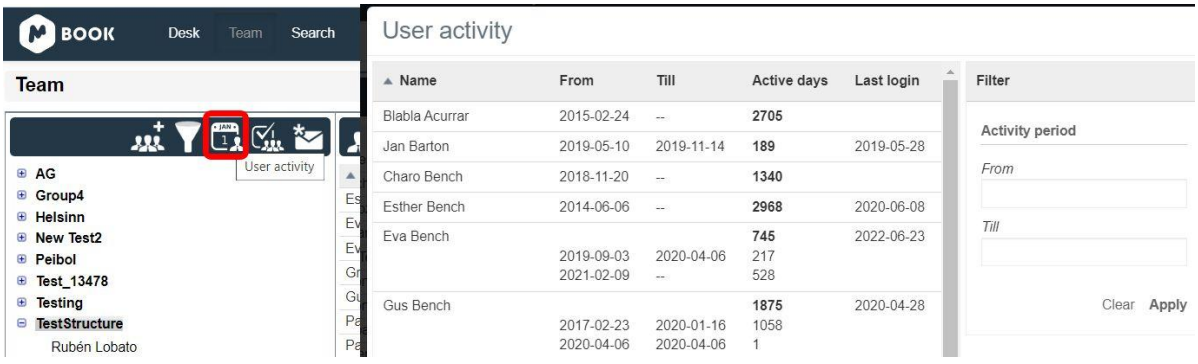


Use the permissions tab to allow the user to create groups.



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).

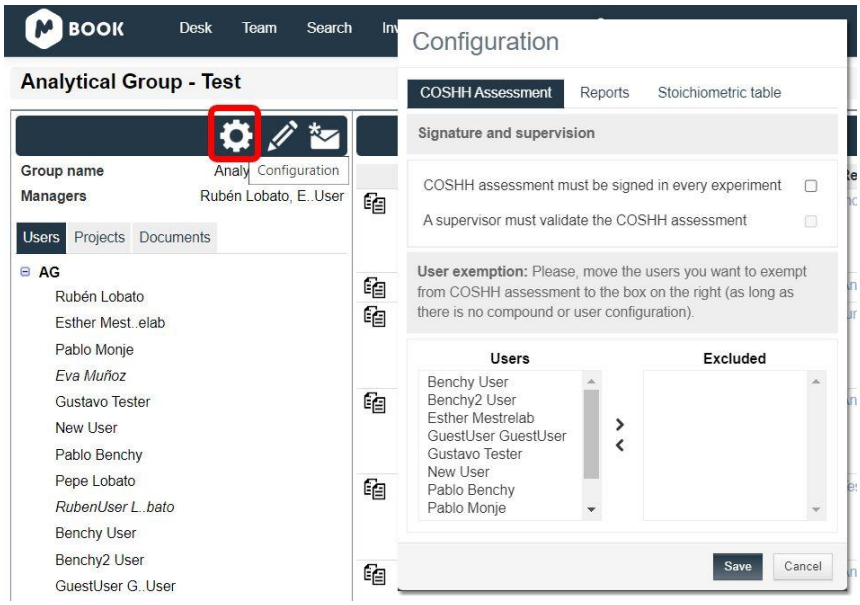
Click on the 'User Activity' button to check some relevant information about the users:



GROUP MANAGER - How to create a Group?

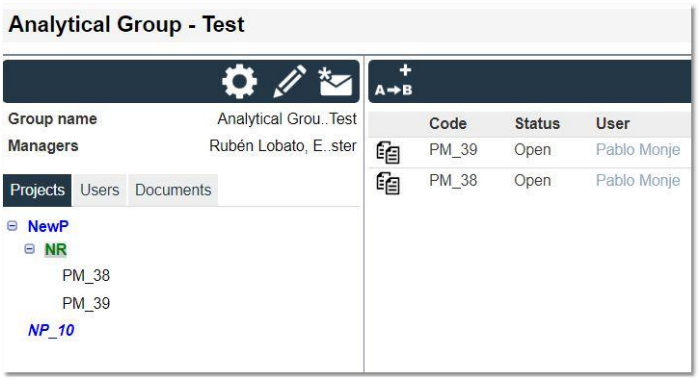
If the admin allows, the Group Manager can also create a group (as we described above for the Administrator role):

Double clicking on the group name will allow you to edit the group and configure some settings for the COSSH assessment, reports and stoichiometric table:

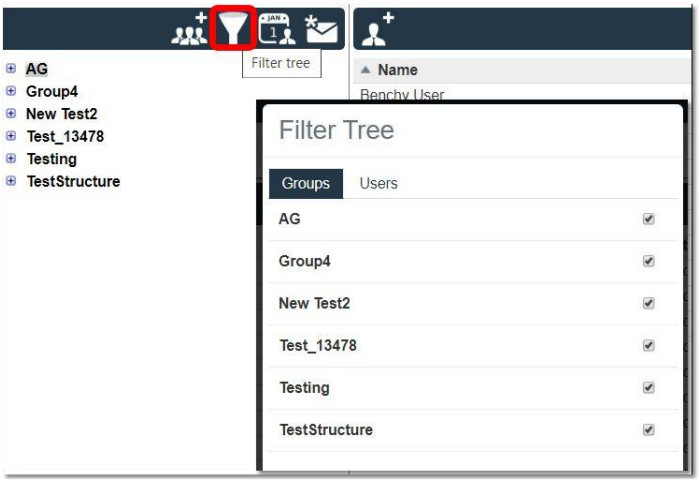


3.3 Managing groups

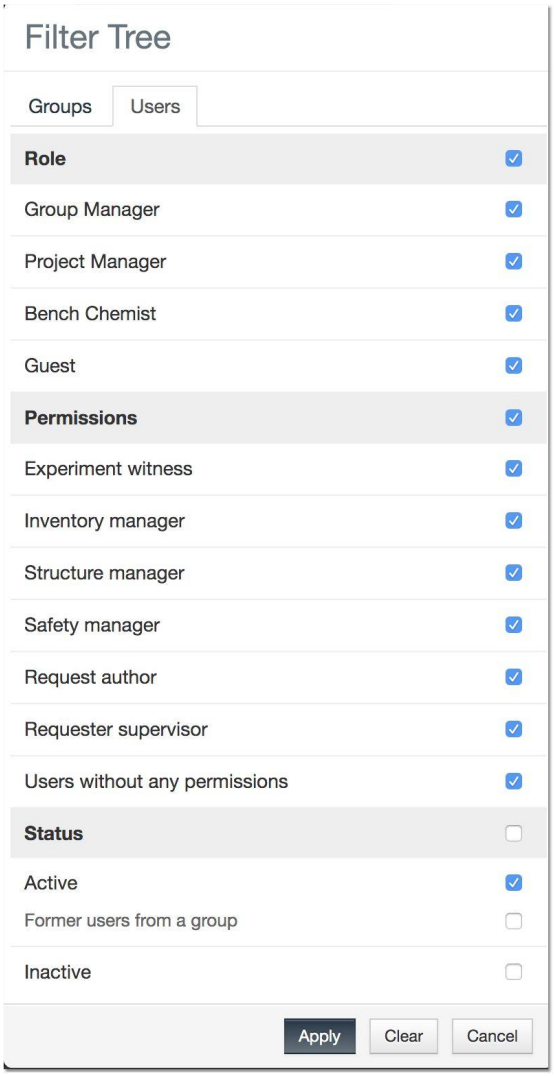
Double clicking on the group name will display the group's reactions and will allow you to send messages to all users or edit the current group. From here, you can also check the group documents:



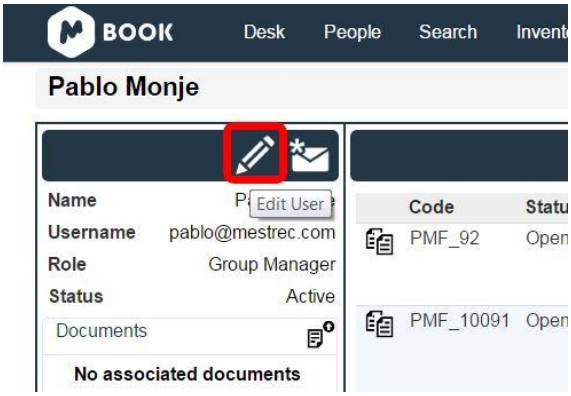
Going back to the ‘Team’ panel and clicking on the 'filter' button will allow you to filter the information by group and user, as shown in the panel:



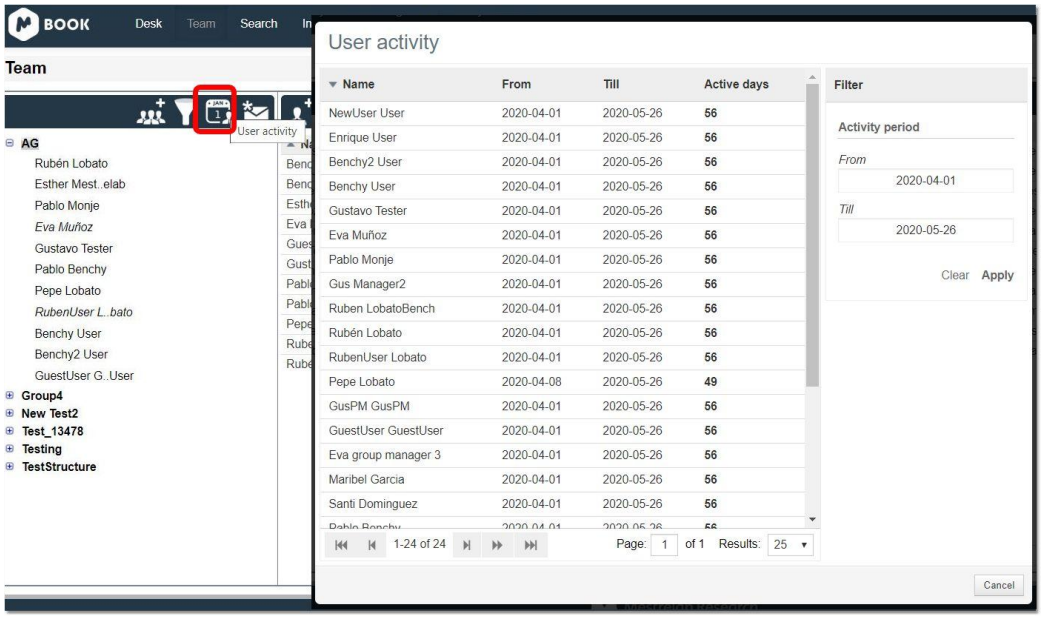
Selecting the users tab, will allow you to filter users by role, permissions, and status:



Left clicking on any existing user will display all the applicable reactions and experiments. Clicking on the 'Edit User' icon will allow you to edit a given user's details (password, status, role, etc.):



Clicking on the user activity button will display information about each user's active days:

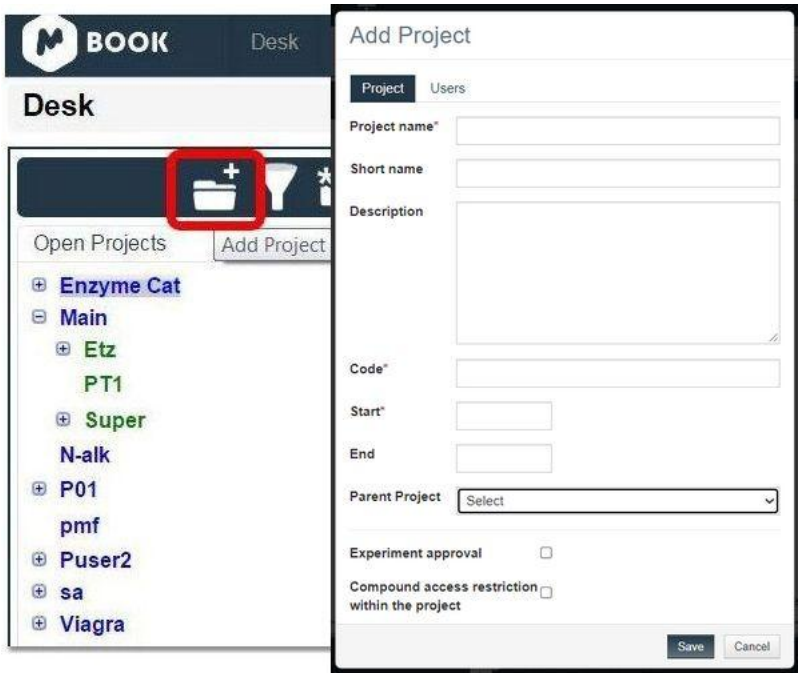


Part

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':

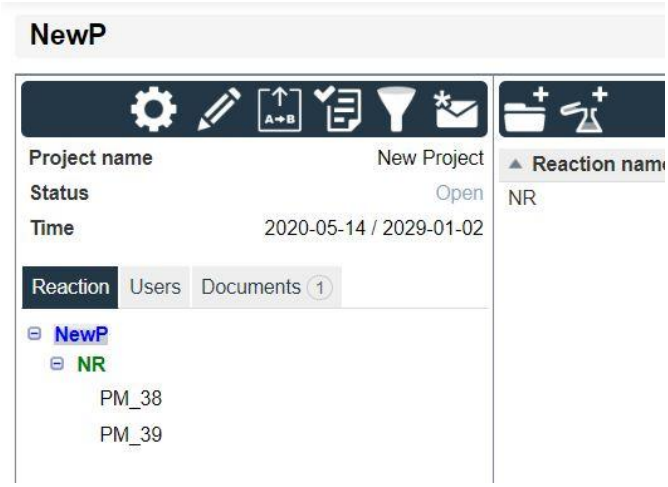


A user only has access to view and search the projects in which he/she is involved; these projects will be displayed in the Projects tree.

To add a new Project, the group manager will need to type a 'Project Name' and 'Project Code', 'Start Date' and the Groups involved in the new Project.

Once you have created the desired projects, these will become listed in the left panel.

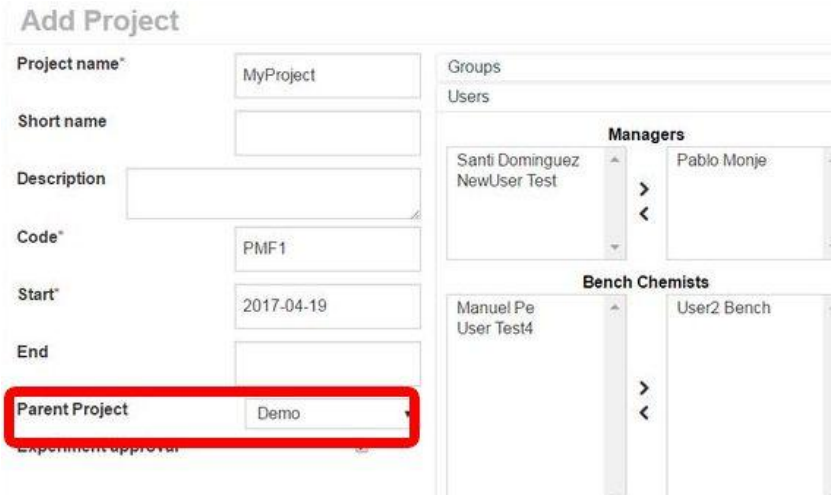
Double clicking on the Project Name will allow you to configure, edit, export, or report it:



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

You will also find certain tabs that allow to check the reactions (and experiments), users, and attached documents.

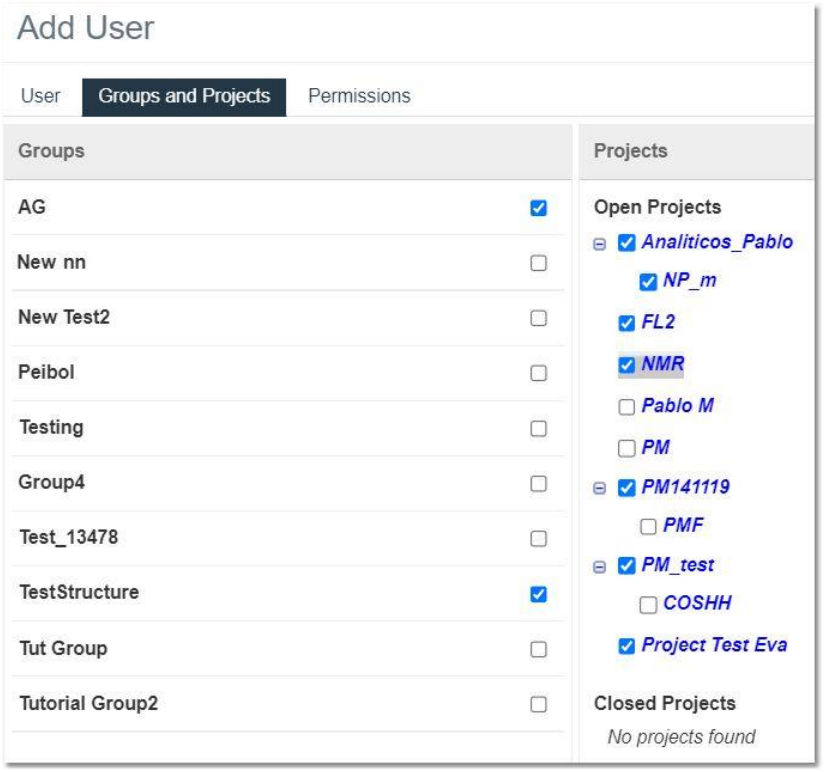
Subprojects can be created just by selecting the applicable 'Parent Project' in the 'Add Project' dialog box:



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.

When the group manager is creating a new user, it is possible to assign him/her to any existing group and project by using the 'Groups and Projects tab':

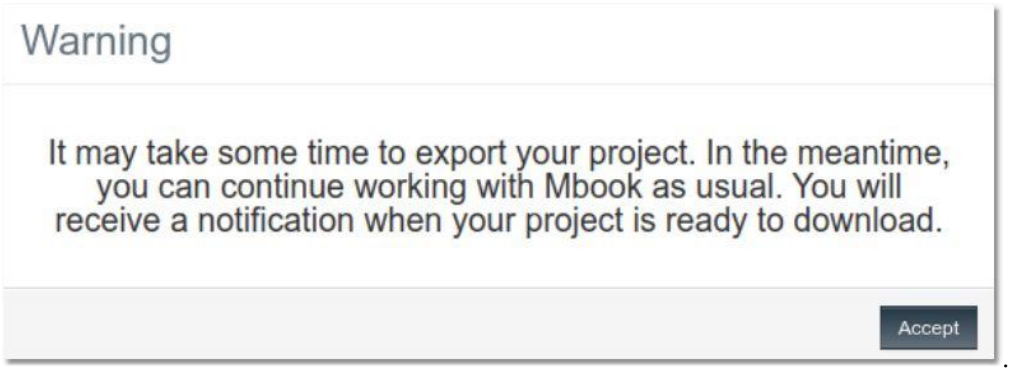


For further information about creating Projects in Mbook, please follow this link.

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).

After clicking the “Export Project” button, a new pop-up dialog will be displayed that will allow you to include documents from the project’s various entities (e.g., subprojects, reactions, and experiments). Once you have clicked on the 'Export button', you will be shown the dialog box below:



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.

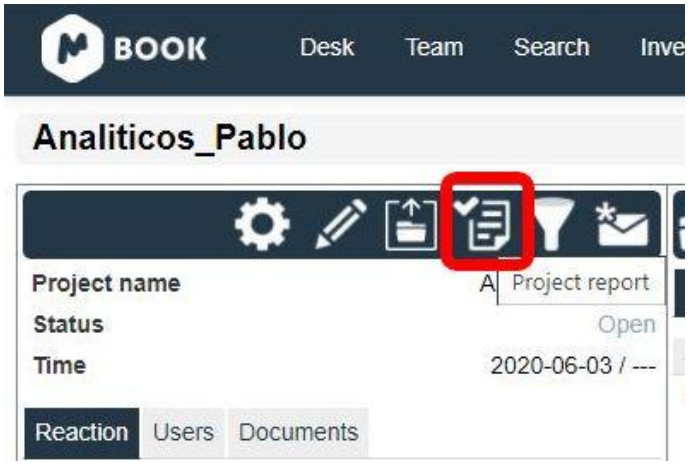
The generated ZIP file will contain:
-an XML file for the project
-a folder for each reaction
-an XML file for the reaction
-a folder named "experiments" containing a ZIP file for each of the experiments in this reaction
-this ZIP file (experiment) contains two files: an XML file with the experiment, 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.

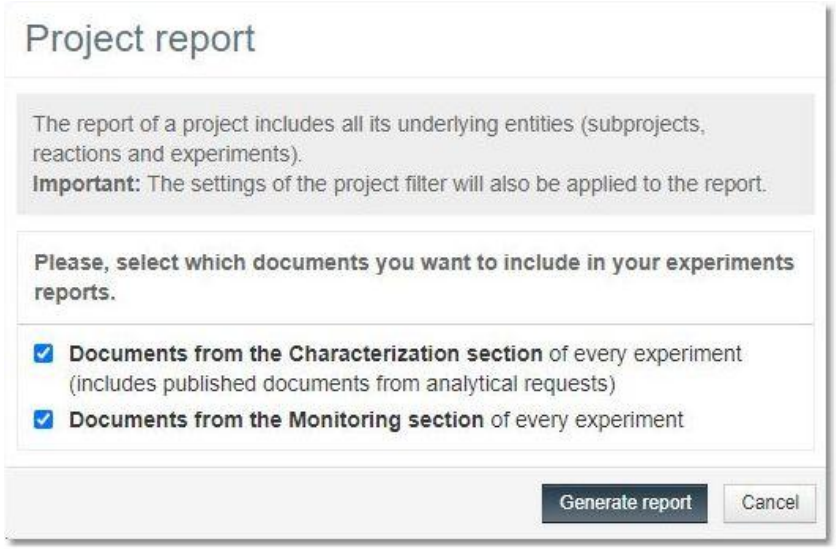
4.2 Report Projects

Group and Project Managers can generate PDF reports for an entire project (including subprojects, reactions, and experiments) just by clicking on the 'Project Report' button:

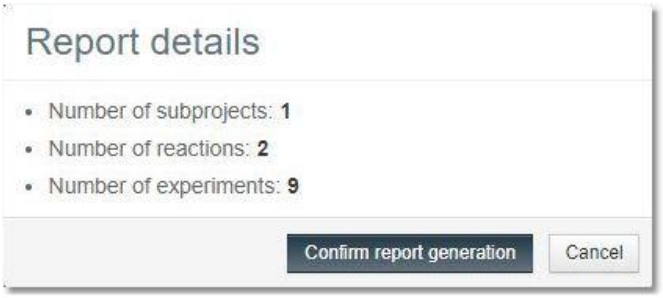


Clicking on the filter button will allow you to filter by “Users” and “Experiments”. The selection chosen will be used to generate the project report (in an otherwise identical manner to the reaction project and its filter).

After clicking the “Project report” button, 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.

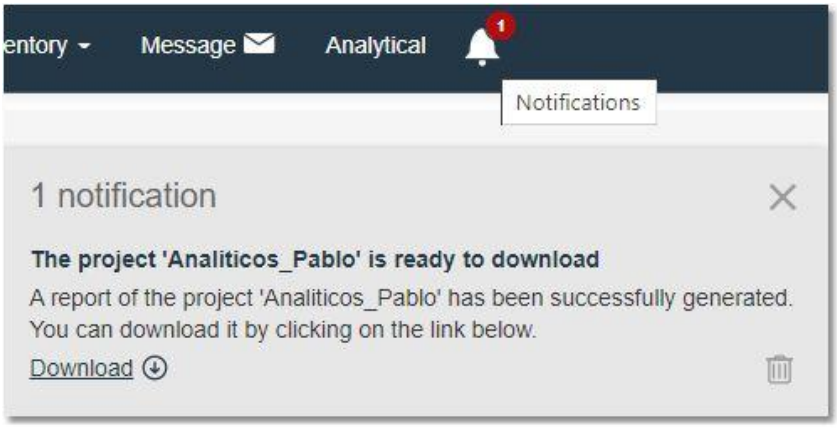


Clicking on the "Generate report" will display a summary window that includes the number of subprojects, reactions, and experiments:



Clicking on "Confirm report generation", will display a warning message informing you that this operation can take some time. You will receive a notification once the report is complete and can continue working as usual with Mbook in the meantime.

Once the project report has been created, a notification will be displayed on the window and you will be allowed to download or delete the report. The notification panel will then be cleared:.

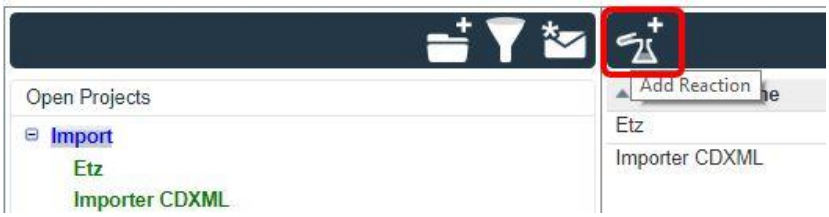


The project report is saved in the form of a zip archive (with the name of the project) containing a PDF file with a summary of the project and several folders (one per reaction).
Inside each reaction folder, you will find a reaction PDF report and the experiments folder, containing the individual PDF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

Part V

5 Creating Reactions and Experiments

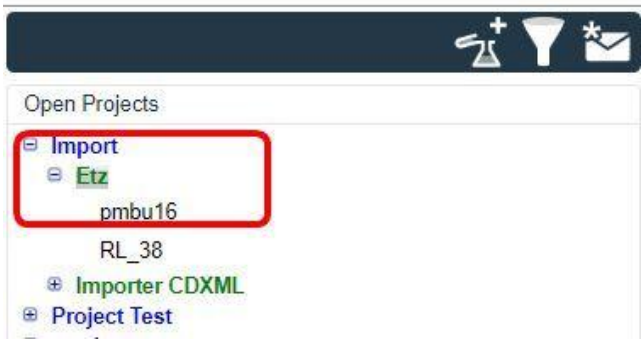
Highlighting any of the available projects in the left panel and clicking on the appropriate button will allow you to add reactions:



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

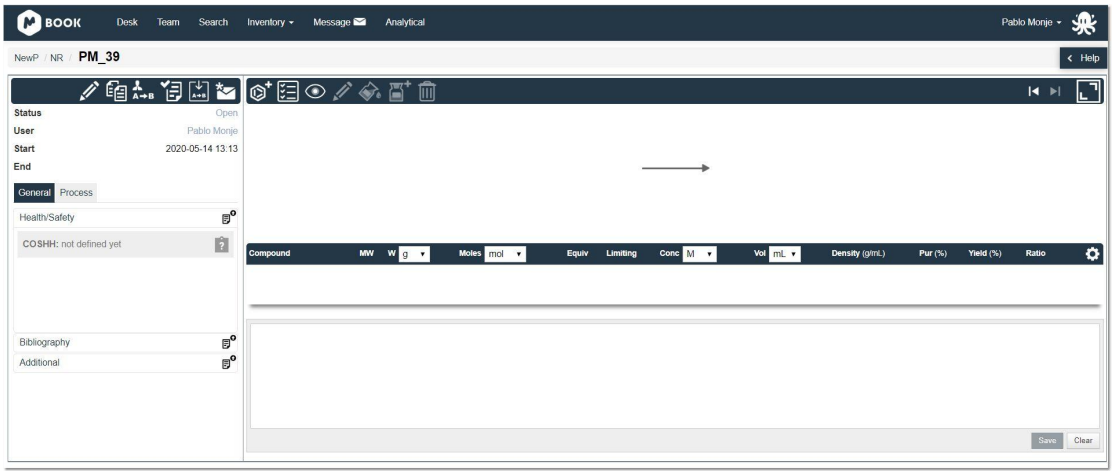
Once you have created the reaction, you will be able to add experiments just by highlighting the reaction and clicking on the appropriate button:

In the example below, we have created an experiment called 'pmbu16' in the 'Etz' reaction of the 'Import' project:



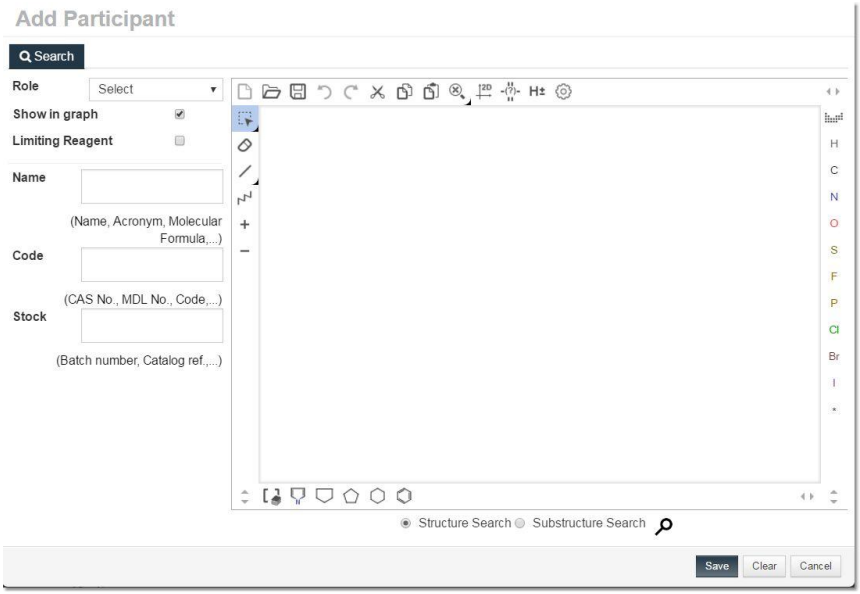
For further information about creating reactions and experiments in Mbook, please follow this link.

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



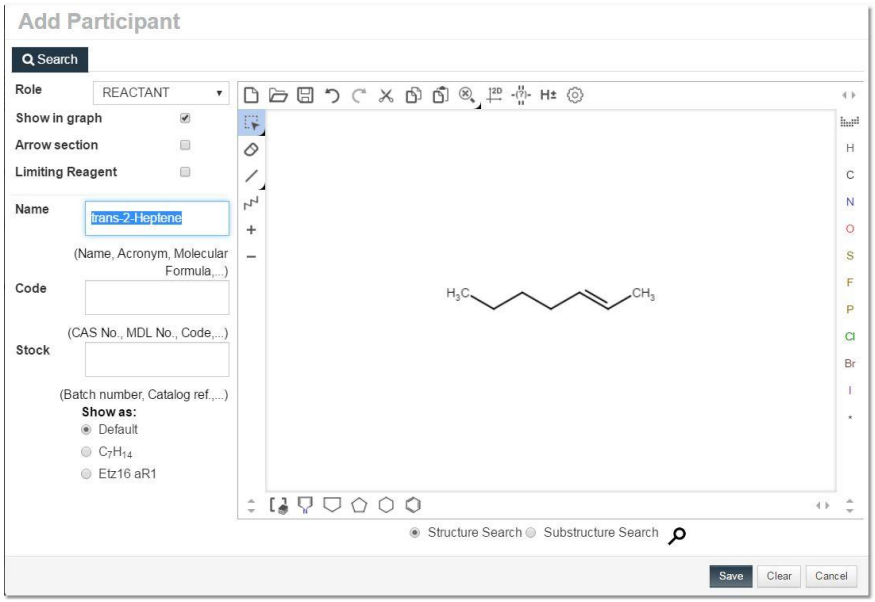
You will find a toolbar to Add  , Edit  , Show/Hide  , or Delete Participants  (reactants, solvents, and/or products) from the experiment, create  , or assign  sources, and to select the experimental conditions  (temperature, time, pressure, pH, etc.).

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

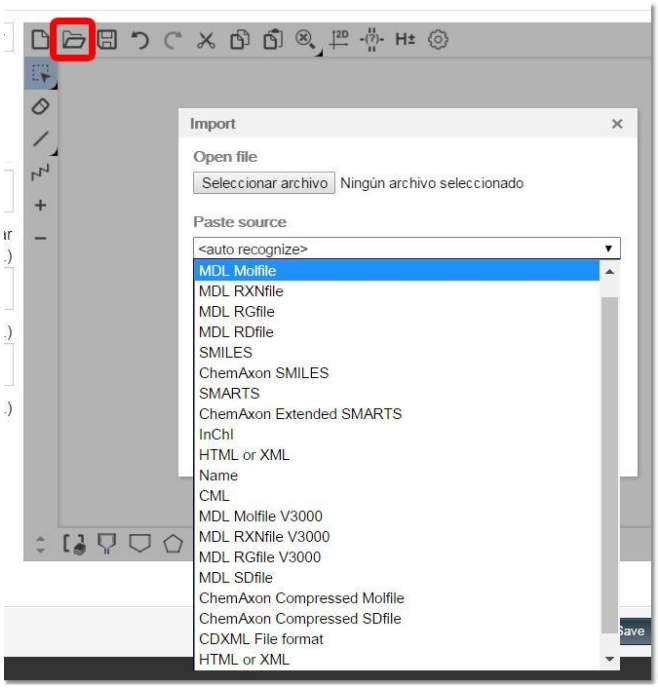


Clicking on the 'Role' scroll down menu will allow you to select the role of the new participant (reactant, solvent, or product). Check boxes will be available to include the new participant in the graphical reaction or in the arrow section and to select the 'Limiting Reagent'.

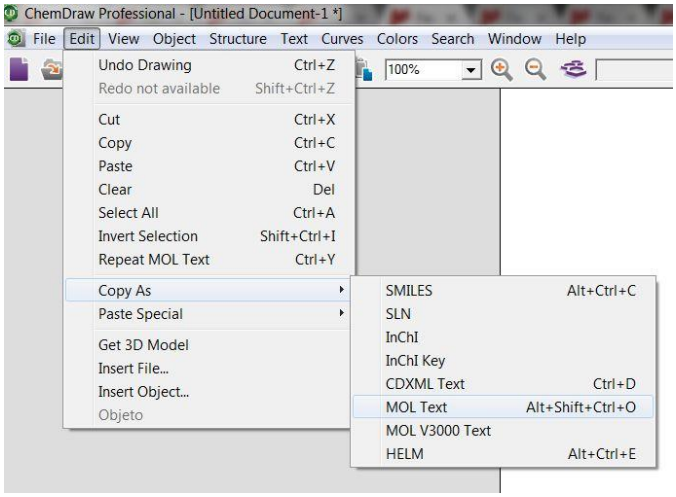
You can type the name of the desired compound (acronym, molecular formula, etc.) in order to search the database for that substance (this will be faster than drawing the molecule in the molecular sketcher, so we recommend you to attempt to find your reactants in the database in the first instance). Clicking on the Save button will add the participant to the experiment.



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):



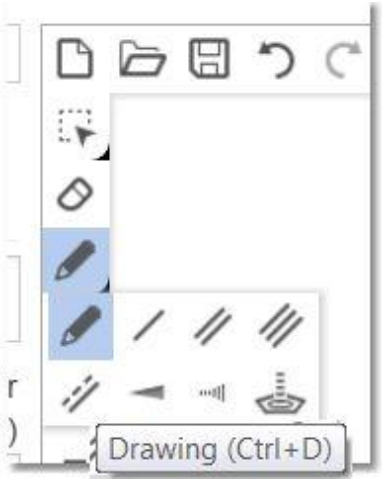
You can also copy and paste structures directly from ChemDraw to Mbook using the "Copy As: MOL Text" (shortcut Alt+Shift+Ctrl+O) option.



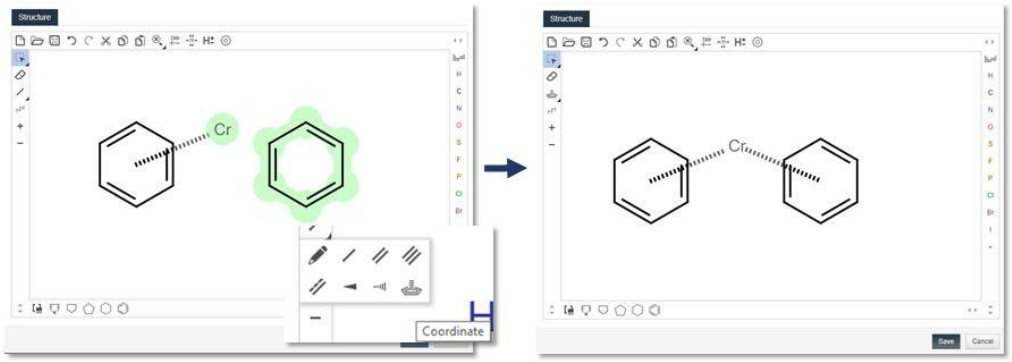
Of course, you can draw molecular structures using the sketcher itself (useful if your compound is not present in the database) or just drag and drop .mol files into the sketcher window.

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).

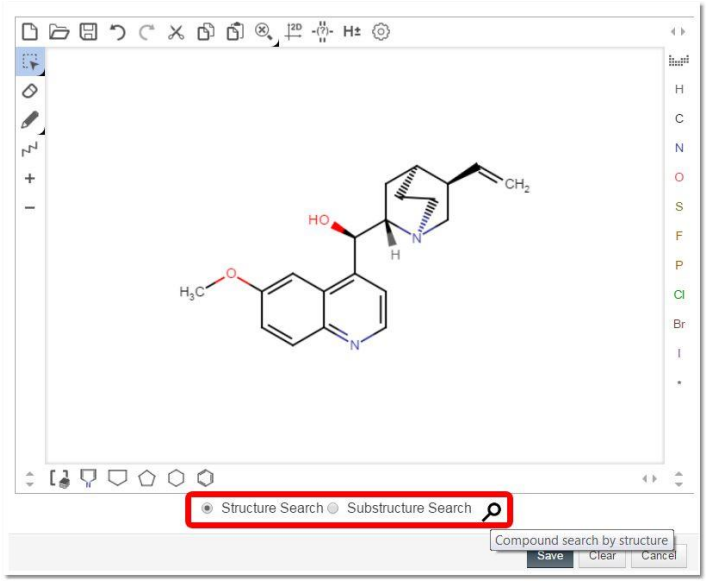


You can change the atom just by hovering the mouse over the atom and typing the applicable letter(s). You can also draw coordinate bonds for organometallic compounds. For further information in this regard, please follow this link.

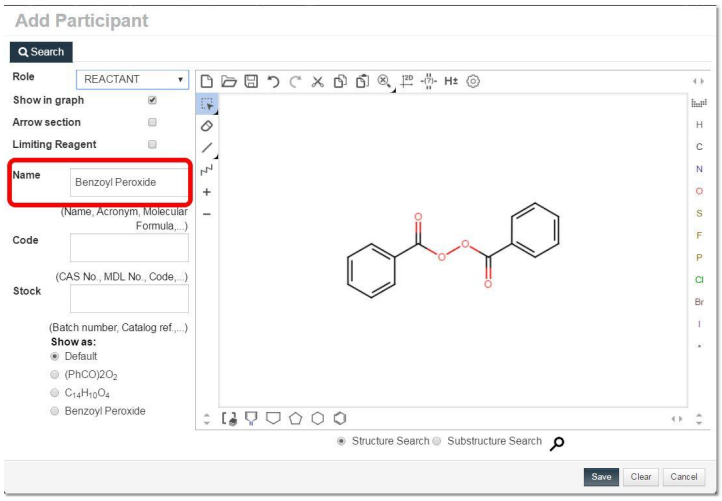


Mbook incorporates Marvin JS Sketcher. For further information about this program, please follow this link.

Once you have drawn the molecule, you can click on the 'Save' 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.

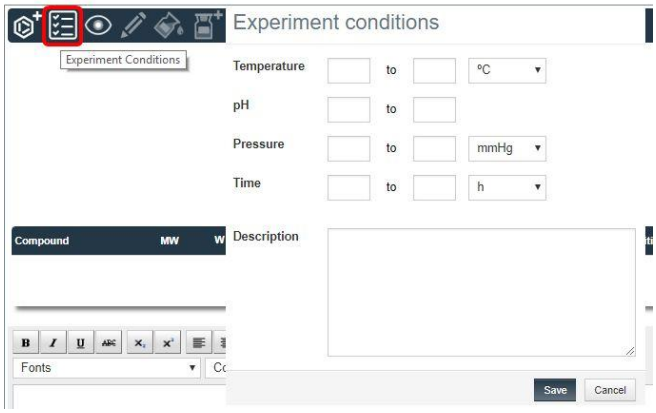


The next step is to add another reactant (benzoyl peroxide), just by typing its name in the edit box:



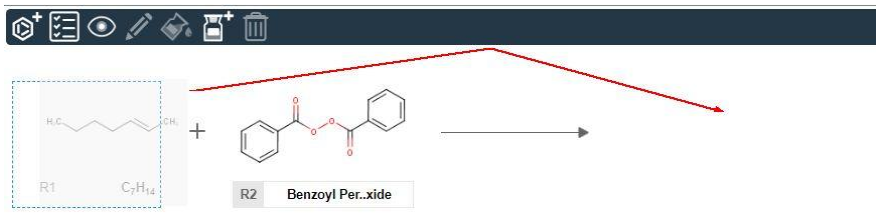
The solvent (CCl_4) will be added in the same way.

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

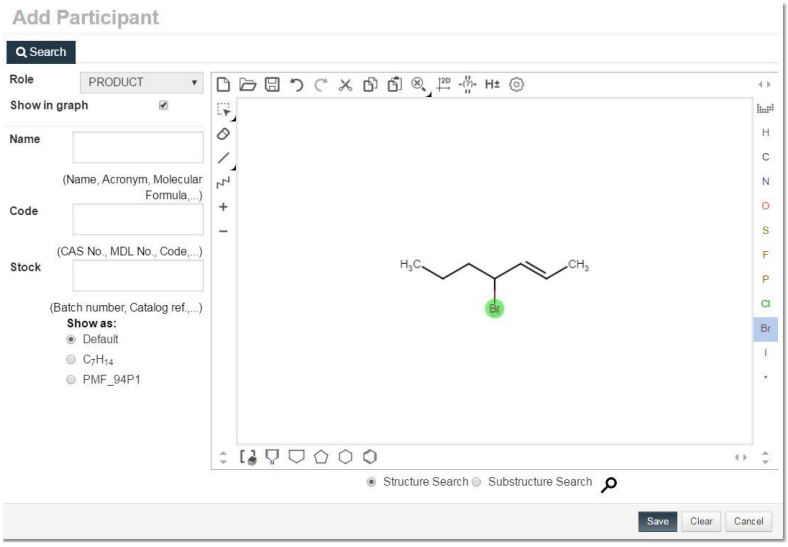


For further information about adding reaction participants and experimental conditions, please follow this link.

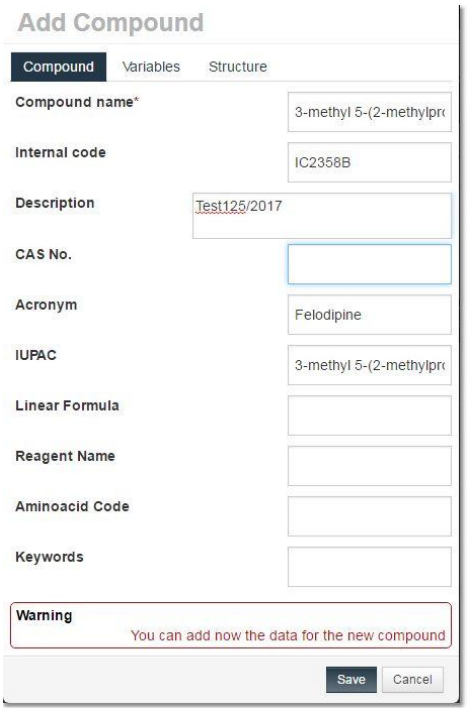
The next step is to add the product. If the structure of the compound is similar to any of the reagents, you can just click and drag the structure of the reactant to the 'Product' place:



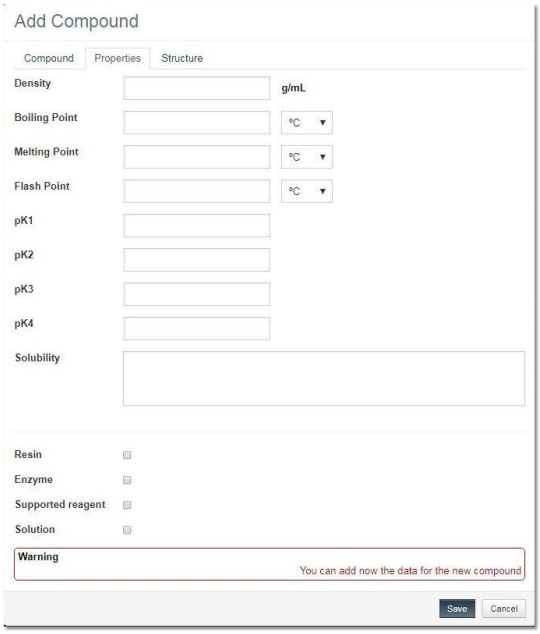
The sketcher will then be launched with the structure of your reagent (but as "Role=Product"), so you will only need to add the necessary changes (a bromine in this case) and click on the save button:



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

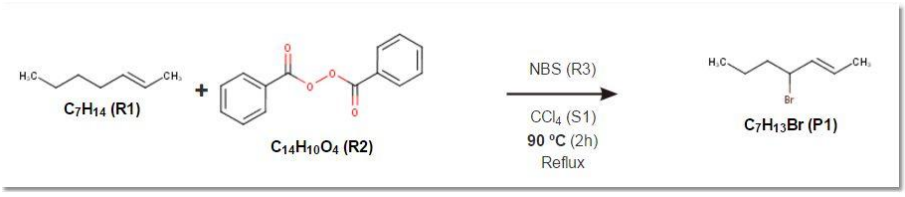


Clicking on the 'Properties' tab, will allow you to define different types of compounds (Resin, Enzyme, Solution and Supported reagent).



- 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.

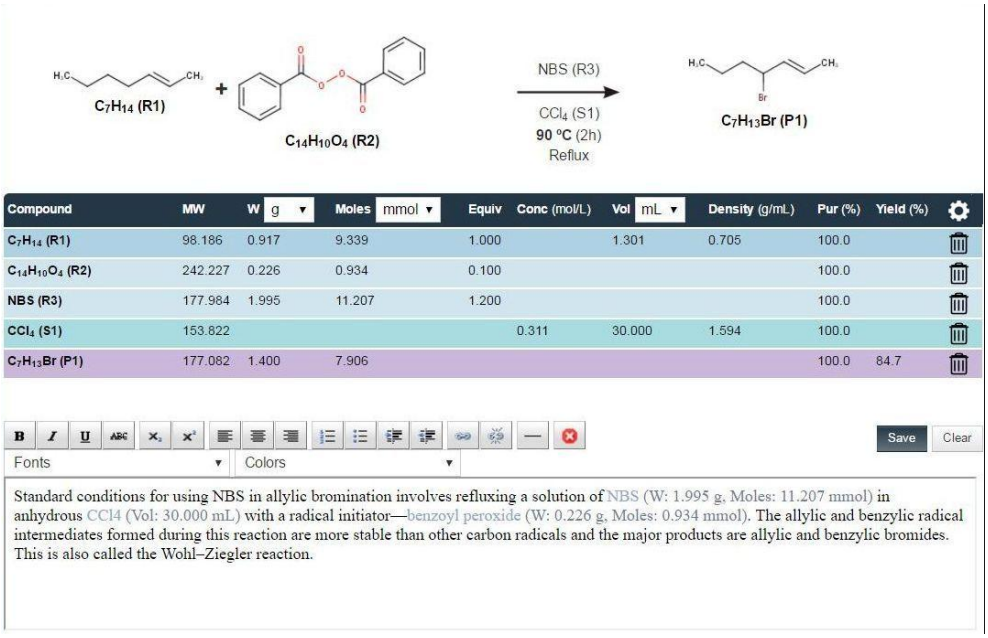
The resulting structure will be added to the Products:



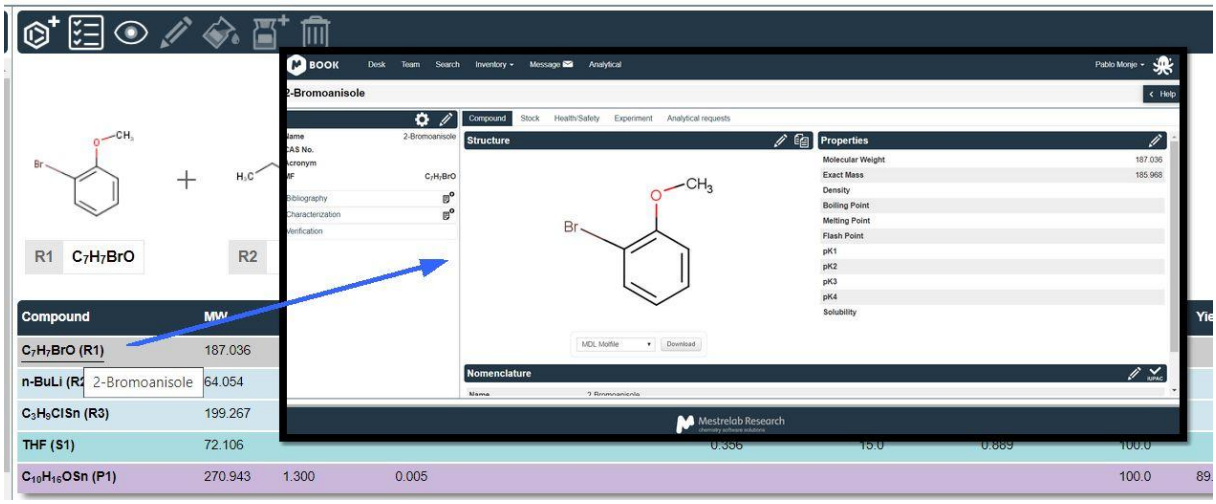
You can move the reactants from the arrow to the reaction section (and vice versa), just by dragging and dropping.

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.

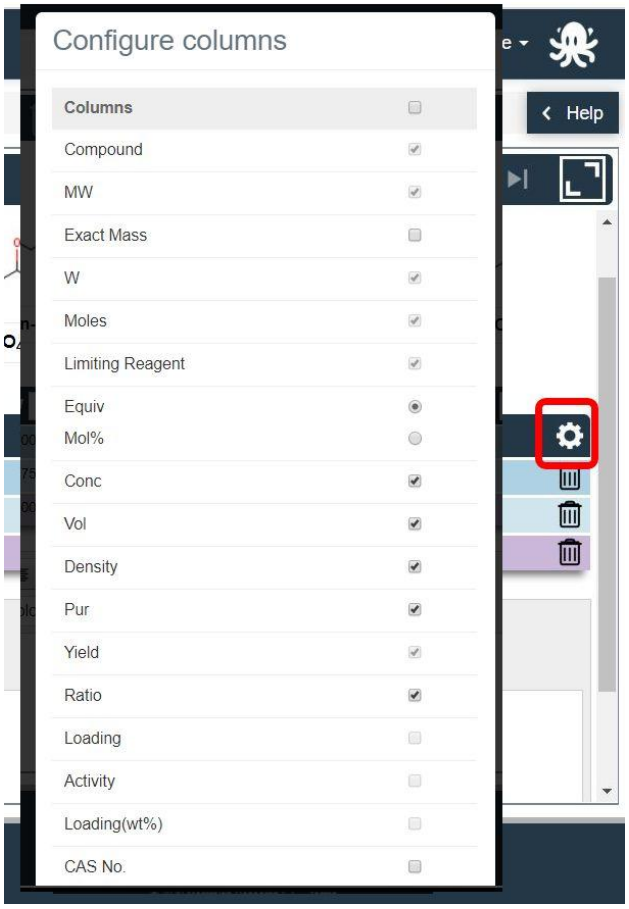
After inputting all the necessary information and formatting all the experimental procedures, click on the Save button:



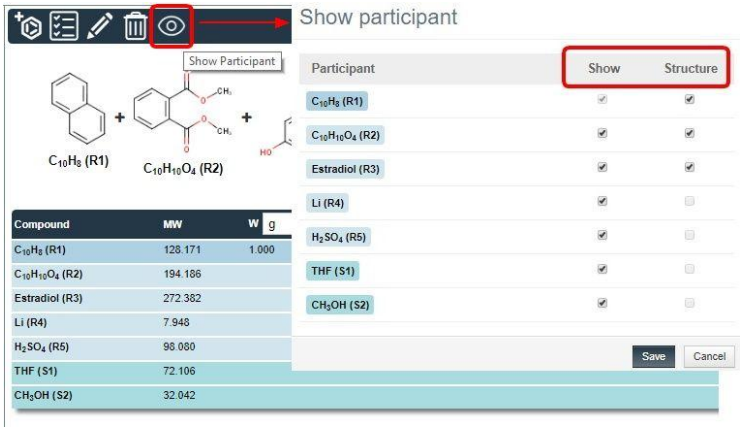
The compound names in the stoichiometric table include links to the inventory entries:



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

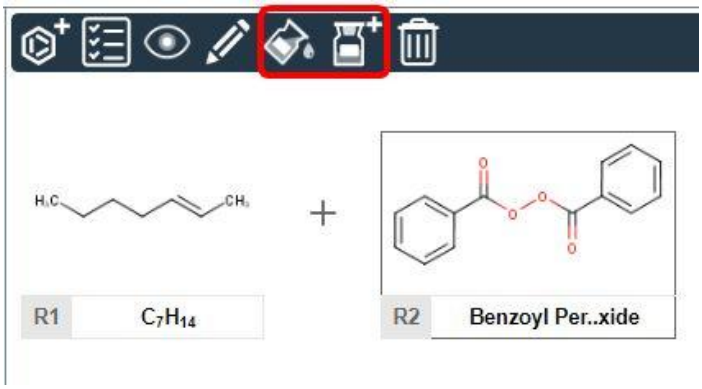


Clicking on the 'Show Participant' button  , will allow you to show/hide the molecular structure in the graph experiment, and to display the participant as a structure, name, or both:

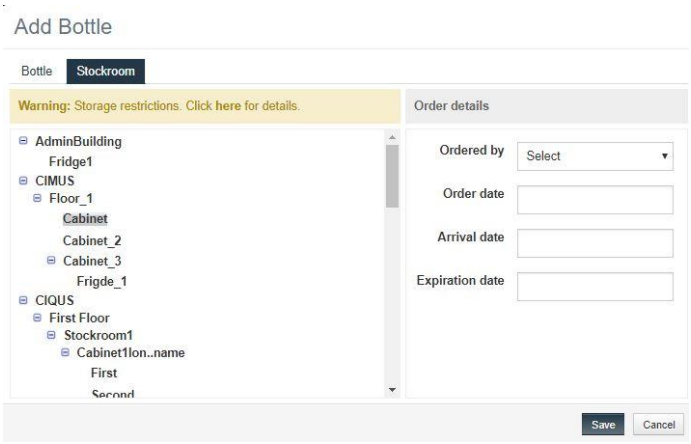


To edit or delete participants, highlight them and click on the applicable buttons  (from the toolbar or from the table).

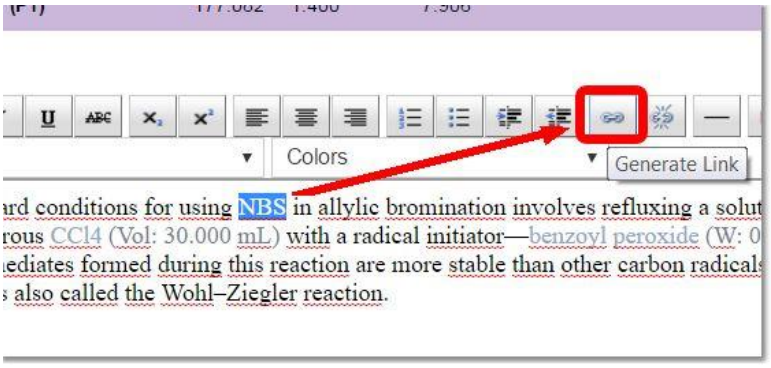
To create and assign sources, highlight the participant and click on the applicable buttons 
.



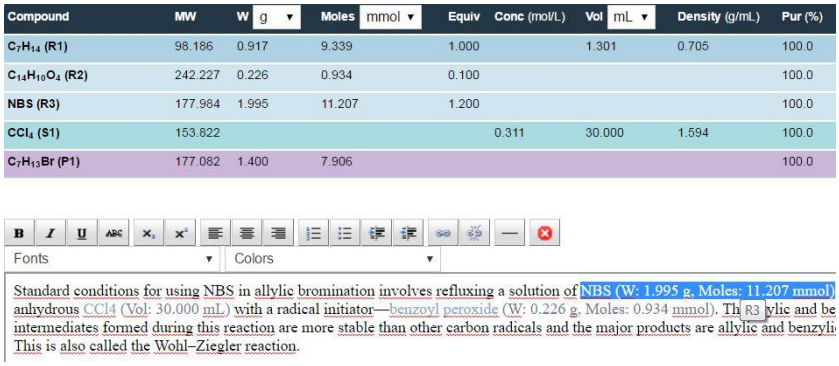
You can also add a location in the Stockroom for the bottle created:



You can create links in the experimental section to the participants just by highlighting the applicable text in the description and clicking on this 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 of the volume for solvents and for the amount, number of moles, and yield of the products:



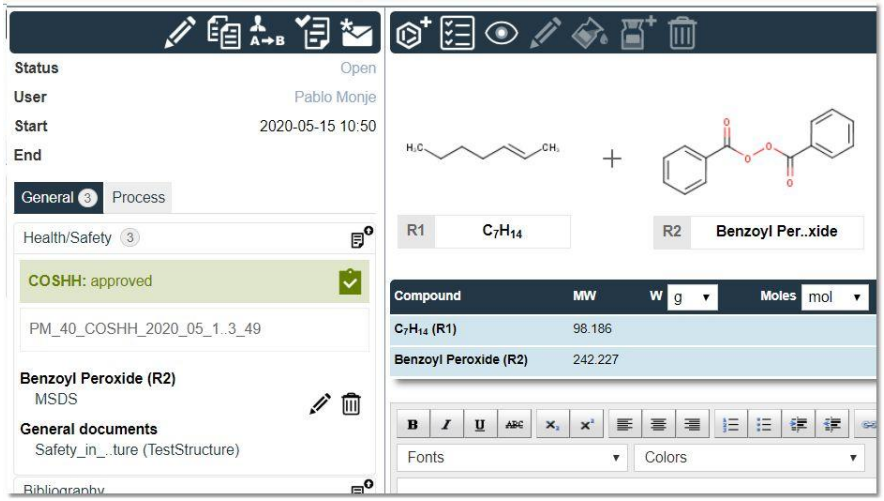
Compound	MW	W g	Moles mmol	Equiv	Conc (mol/L)	Vol mL	Density (g/mL)	Pur (%)
C_7H_{14} (R1)	98.186	0.917	9.339	1.000		1.301	0.705	100.0
$C_{14}H_{10}O_4$ (R2)	242.227	0.226	0.934	0.100				100.0
NBS (R3)	177.984	1.995	11.207	1.200				100.0
CCl_4 (S1)	153.822				0.311	30.000	1.594	100.0
$C_7H_{13}Br$ (P1)	177.082	1.400	7.906					100.0

Fonts Colors

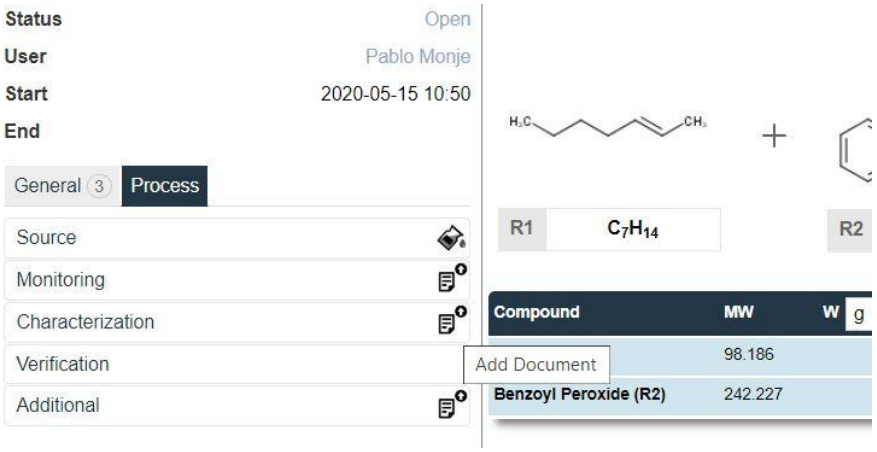
Standard conditions for using NBS in allylic bromination involves refluxing a solution of NBS (W: 1.995 g, Moles: 11.207 mmol) anhydrous CCl4 (Vol: 30.000 mL) with a radical initiator—benzoyl peroxide (W: 0.226 g, Moles: 0.934 mmol). Th R3 ylic and be intermediates formed during this reaction are more stable than other carbon radicals and the major products are allylic and benzyli This is also called the Wohl–Ziegler reaction.

To break a link, just highlight the word in the description and click on the appropriate button in the toolbar  .

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:



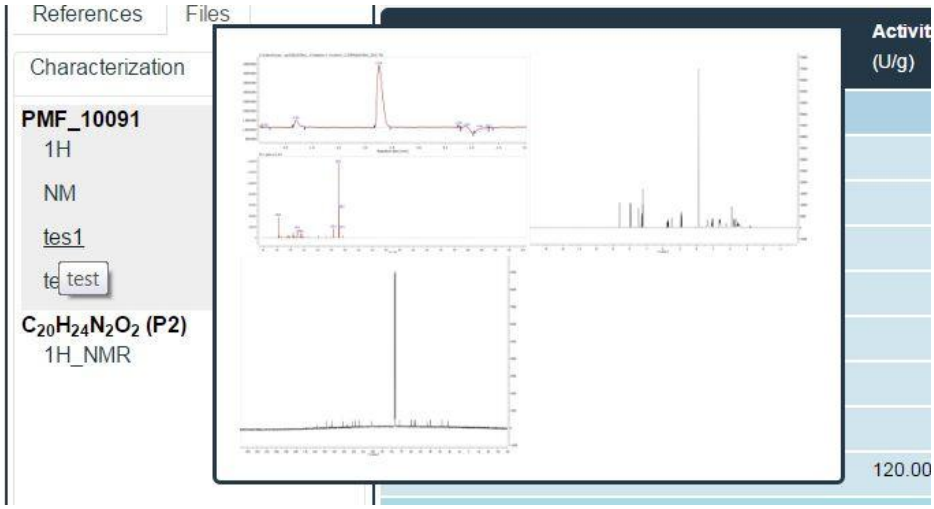
Selecting the 'Process' tab, will allow you to add other relevant documentation such as Mnova documents, the raw NMR/MS spectra in zip format, images, etc.:



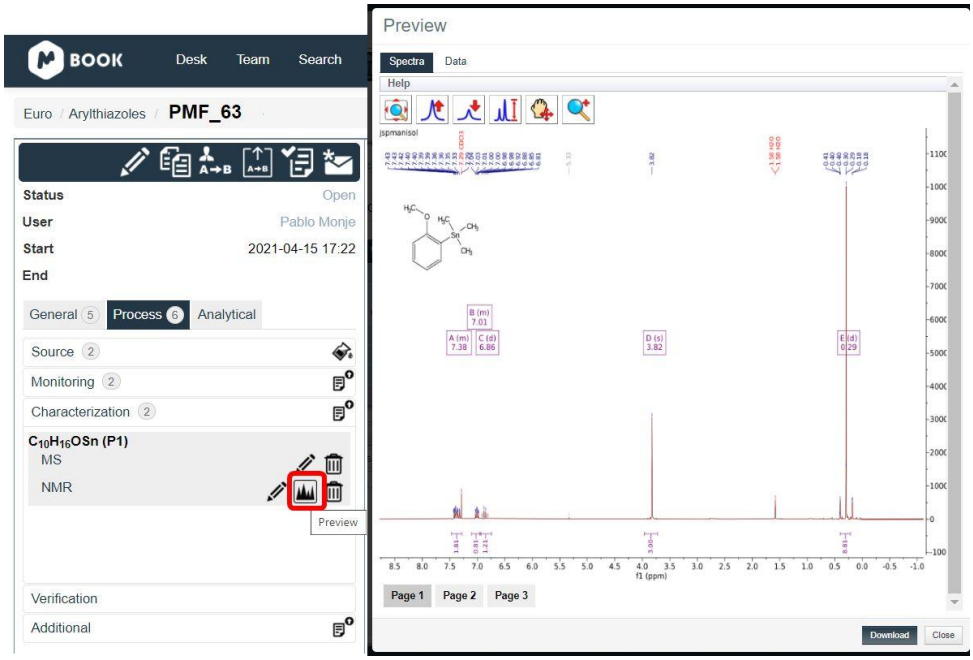
Once you have added the attachments, they will be listed in the appropriate panel.

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 hovering the mouse over the name of the document. If the Mnova document contains more than one page (or the zip file contains more than one raw dataset), you will get the preview in tile mode.

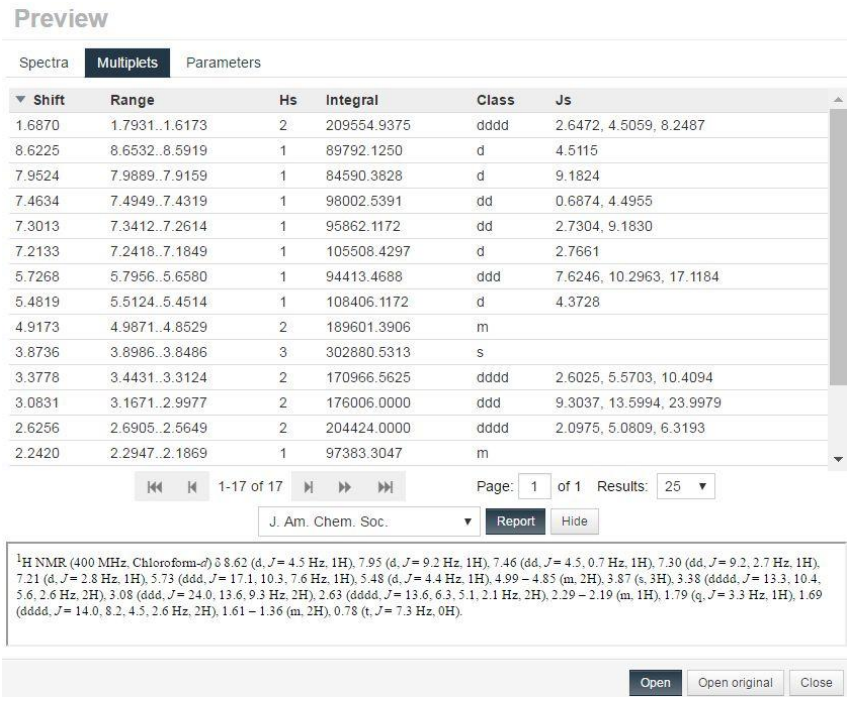


If you have loaded raw data in a zip file, the spectrum (or spectra) will be automatically processed. A large preview of the processed spectrum will be obtained by clicking on the Preview button.

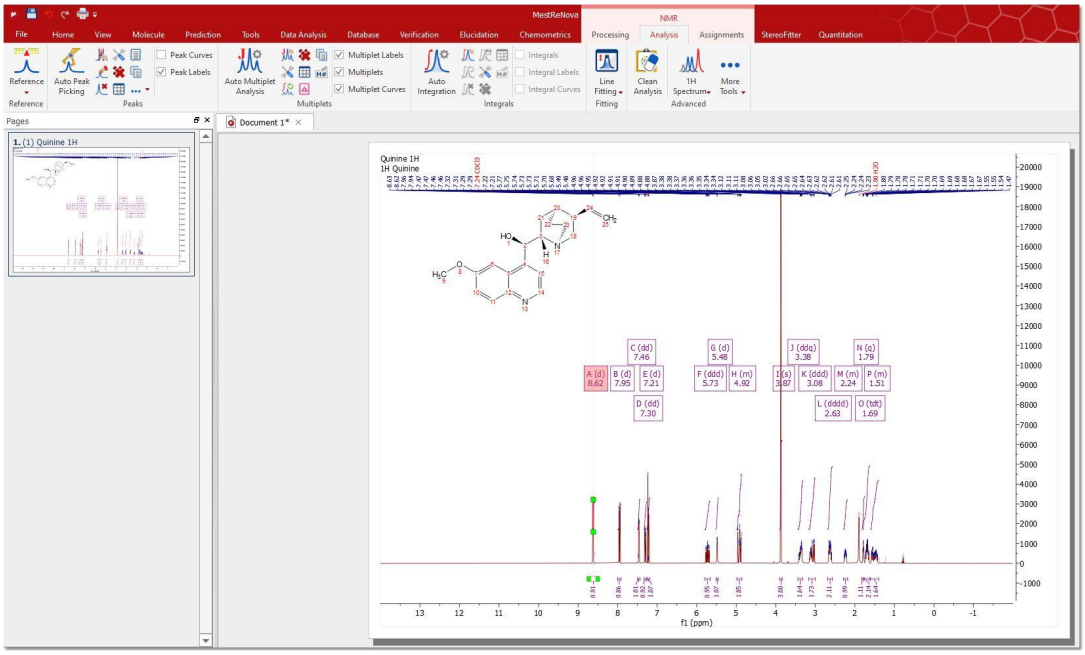


From the Preview, you can use the toolbar to 'pan', increase/decrease the peaks' intensity, or zoom into a region of interest:

You can also display the 'Multiplets Table' or generate a 'Mutiplet Report' in the journal format selected in the combobox (JACS, in the example below):

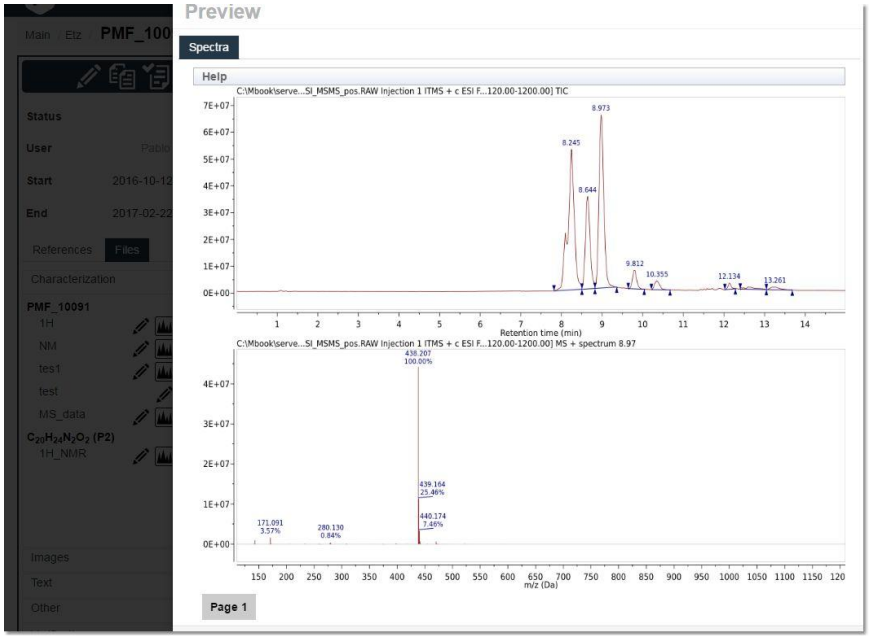


Clicking on the 'Open' button will load your Mnova document into Mnova (if you have valid licenses to do so), allowing you to reprocess the spectra or make any desired changes:



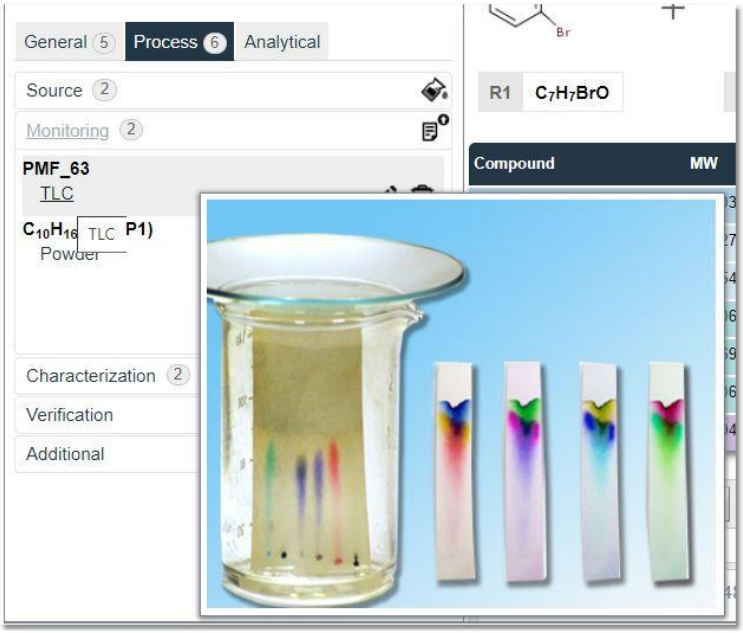
Both original raw files and Mnova documents are stored in the ELN. By default, when clicking on the link, the Mnova document will be opened; however, the original raw file can also be downloaded by clicking Edit and selecting the raw file from the same window.

Of course, you can also attach MS or ElViS spectra to your experiments:

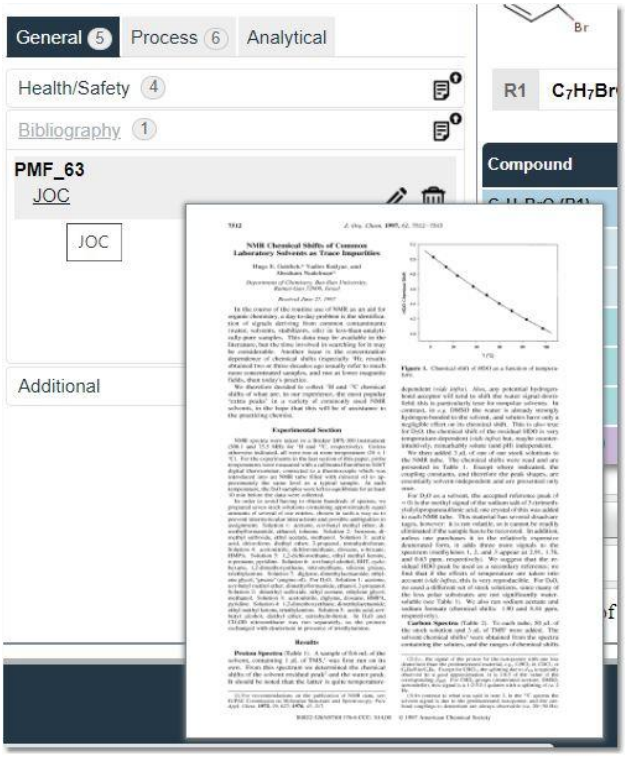


If you have a verification license, you can check whether your datasets match your structures. See this chapter for further information.

You can also add images (very useful, for example, when adding TLCs) to your experiments. Hovering the mouse over the 'image name' will generate a preview. These images can be included at the end of the report (with the description added).

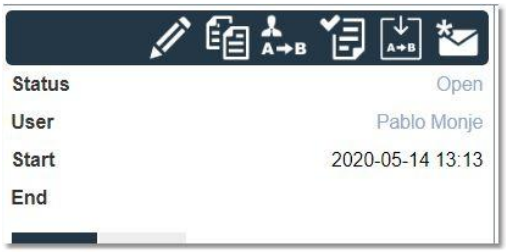


You can also add PDF files in the bibliography section. Hovering the mouse over the PDF link will display a preview of the first page of the document:

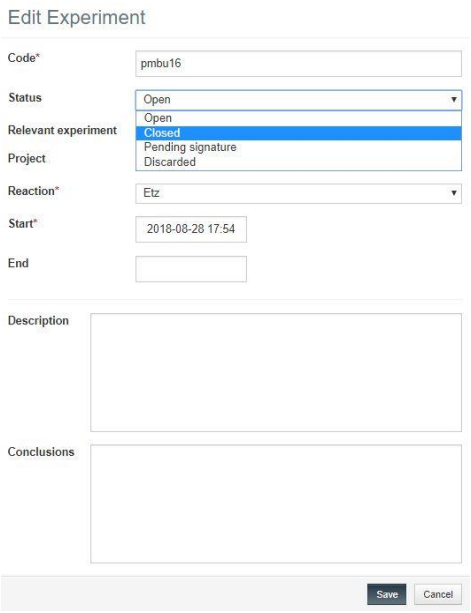


For further information about adding analytical documents to Mbook, please follow this link.

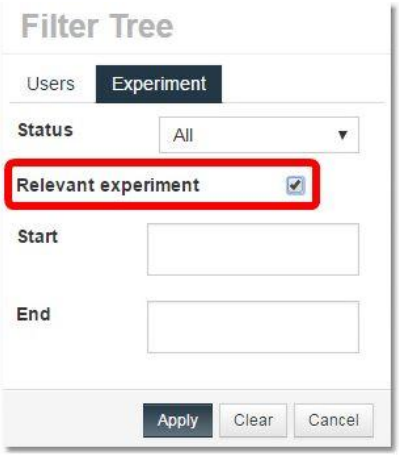
From the experiment panel, you can edit the description of the experiment, clone, assign the experiment to another user, generate a report as a PDF, import a reaction scheme from Chemdraw, and send a message with the report (to any member of the same group):



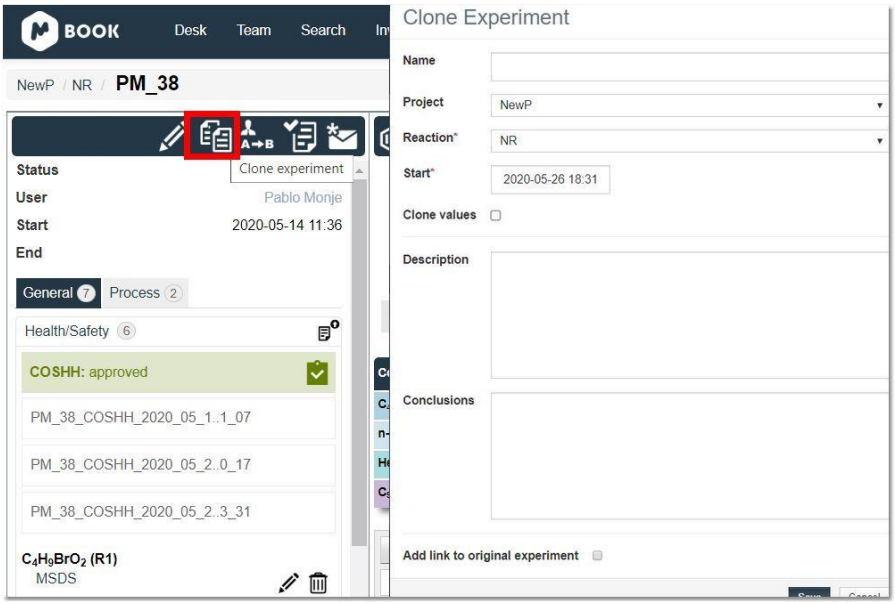
For reasons of integrity, it is not possible to delete experiments. However, clicking on the 'Edit Experiment' button will allow you change the status (from open to **closed** or **discarded**). From here, you can also rename the experiment code, modify the start and end dates, and type 'descriptions'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



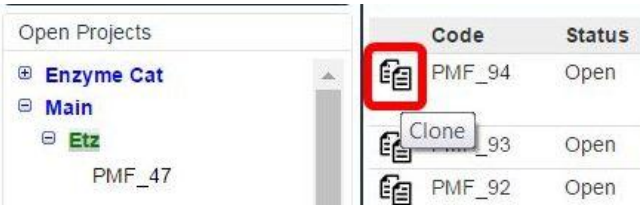
From the experiment tab, you can check the 'Relevant experiment' box. This type of experiment will be highlighted in blue in the desk, allowing the users to easily select the important experiments in a reaction (for cloning, reporting, etc.). You can also filter your searches using the relevant experiments:



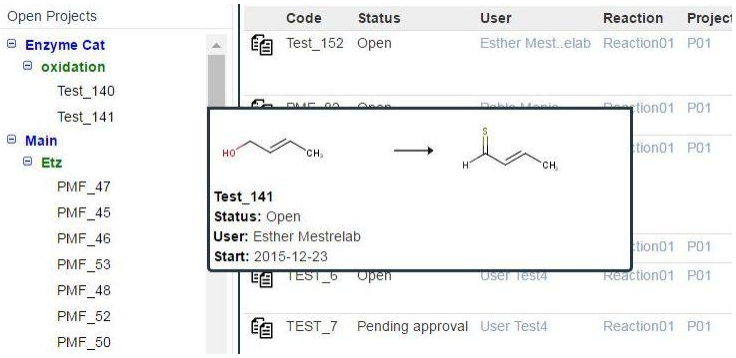
In the 'Experiment panel', you will also find a button that allows you to 'Clone' any experiment, a very useful feature for the creation of new experiments using existing ones as starting points (for instance, if you run the same experiment again under different conditions, or if you run a new experiment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



When the "Clone values" 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:

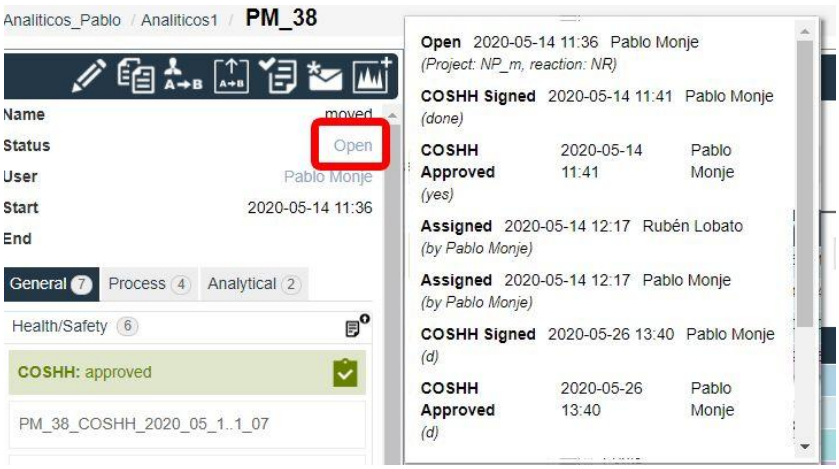


Once you have added your experiments, you will be able to navigate via the left panel using the expandable trees (hovering the mouse over any experiment will display a reaction preview):

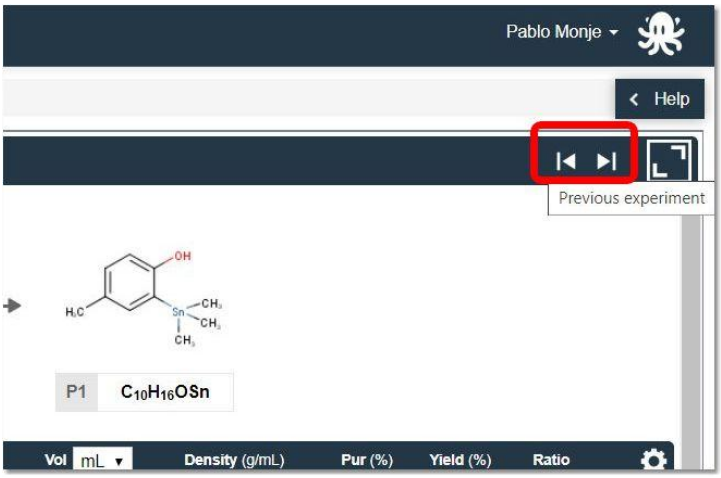


Clicking on any of the experiments on the left panel will show all the relevant information.

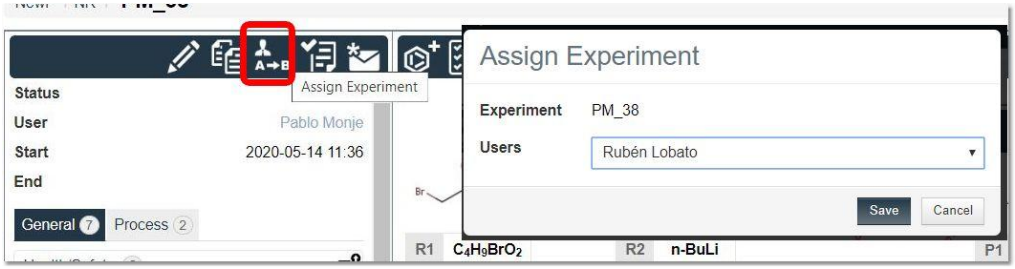
Clicking on the Status field will display the history:



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



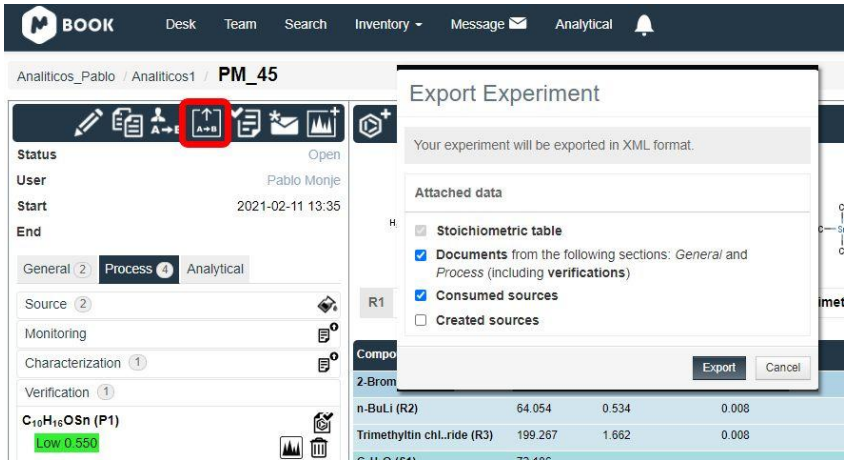
You can assign experiments to other group members by clicking on the applicable button:



See also:
Resources about creating Reactions and Experiments
Resources about drawing Structures with Coordinate Bonds.
Watch a miniclip about creating an experiment in Mbook by following this link

5.1 Export Experiments

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

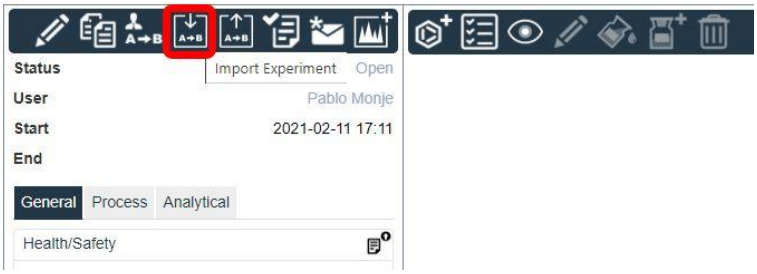


After clicking the "Export" button, a zip file with the name of the experiment code will be created. The zip file will contain several folders and files depending on the options checked in the export dialog:

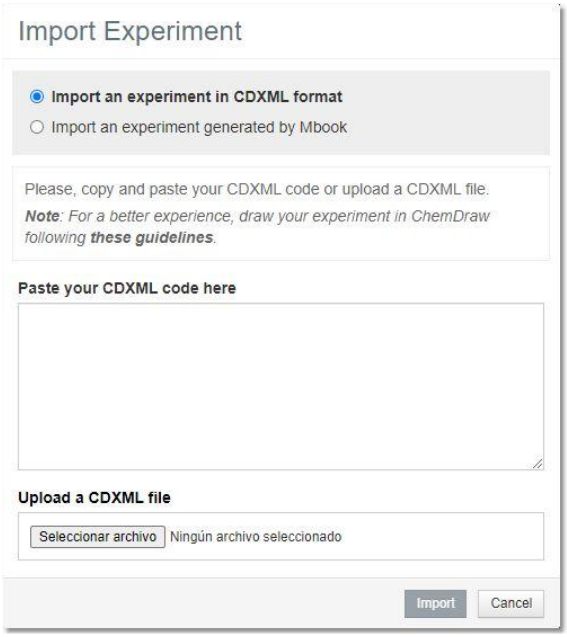
a) It will always contain an .sdf file containing the structures of all the participants (reactants, solvents, and products).
b) An .xml file will be always present with the description, history of the experiment (project, reaction, and owner) and consumed/created sources if the applicable options were checked.
c) If the option to include documents was checked, you will get one folder per General and process sections:
c.1) If you uploaded a raw spectrum file, the folder will contain the original file, the Mnova document automatically generated when uploading the file to Mbook.
c.2) If you uploaded an Mnova document, the folder will contain the original Mnova document.
c.3) If the user uploaded a PDF, image, or indeed a file any other format, the folder will only contain the original document attached to the experiment in its native format.

5.2 Import experiments

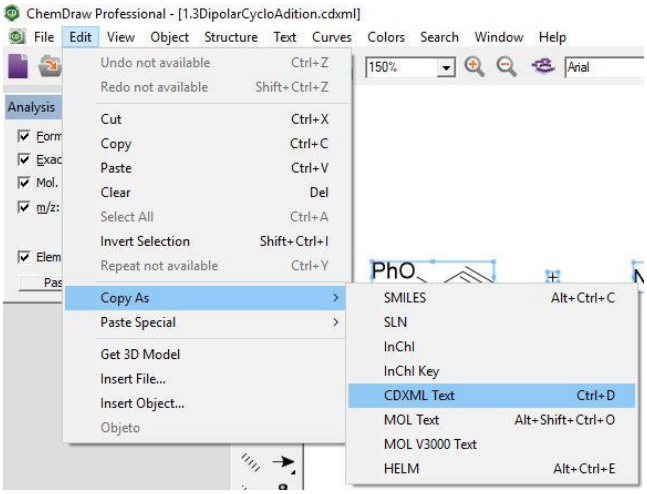
You can import experiments from Mbook (as zip archives) or from ChemDraw (in CDXML format) just by clicking on the applicable button (highlighted in red in the screenshot below):



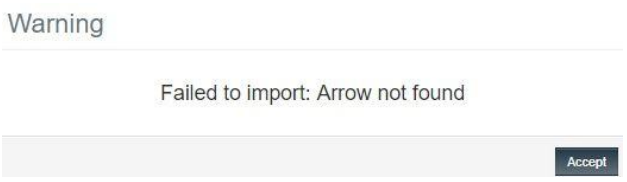
After clicking on this button, the user will be able to load the reaction scheme as a CDMXL file or to import a zip file containing an Mbook experiment:



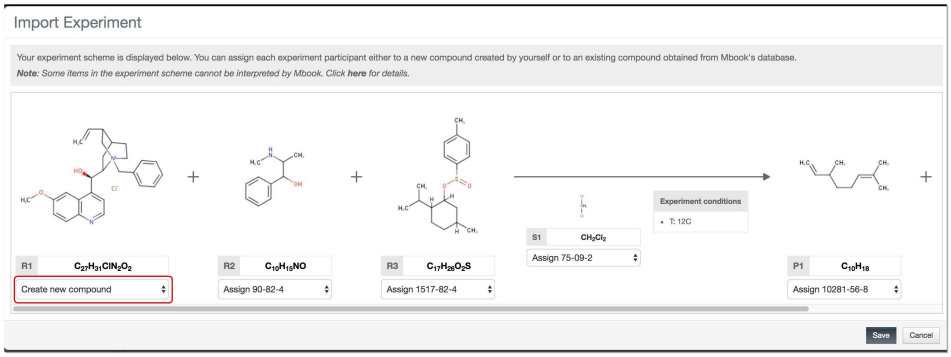
Another option would be to copy and paste the experiment from ChemDraw using the "Edit/Copy As: CDMXL Text" (Ctrl+D) command.



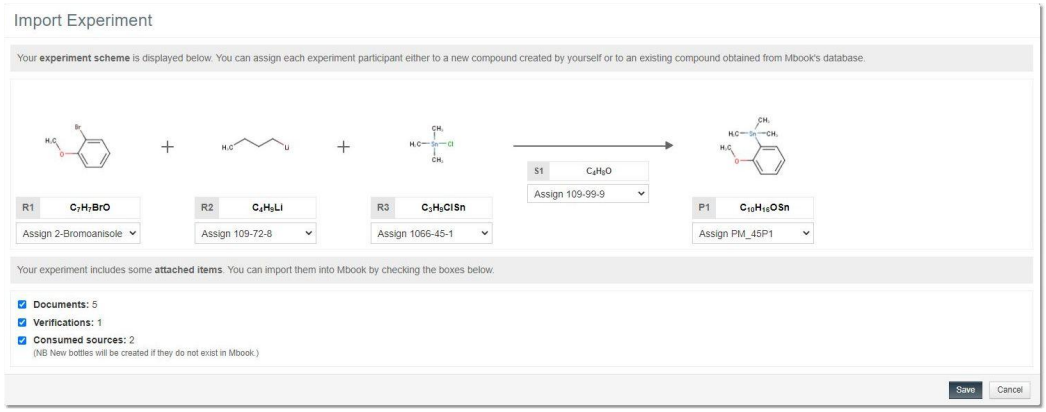
If the file is in another format or it does not have a reaction or a recognizable structure, a warning will be shown.



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 important 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.

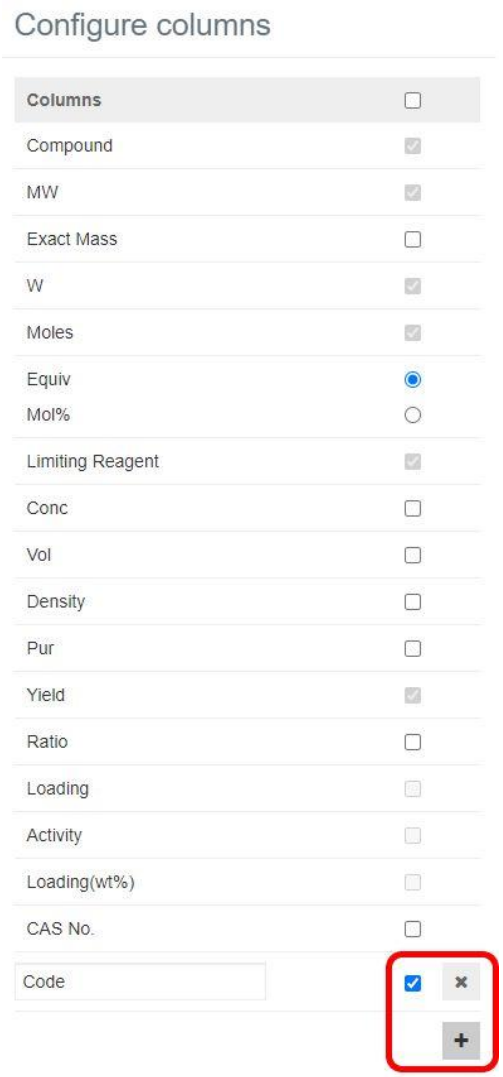
- If a Project Manager defines the column setup of the stoichiometric table for a project, this configuration will apply to every subproject and experiment.
- If no column configuration has been completed by the Group Manager or the Project Manager, chemists can define the column setup of the stoichiometric 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.

This will invoke the "Configure columns" pop-up window:



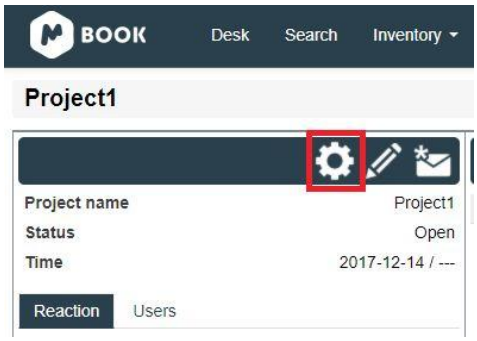
There are three types of available columns:

- 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, and Purity).
- 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).

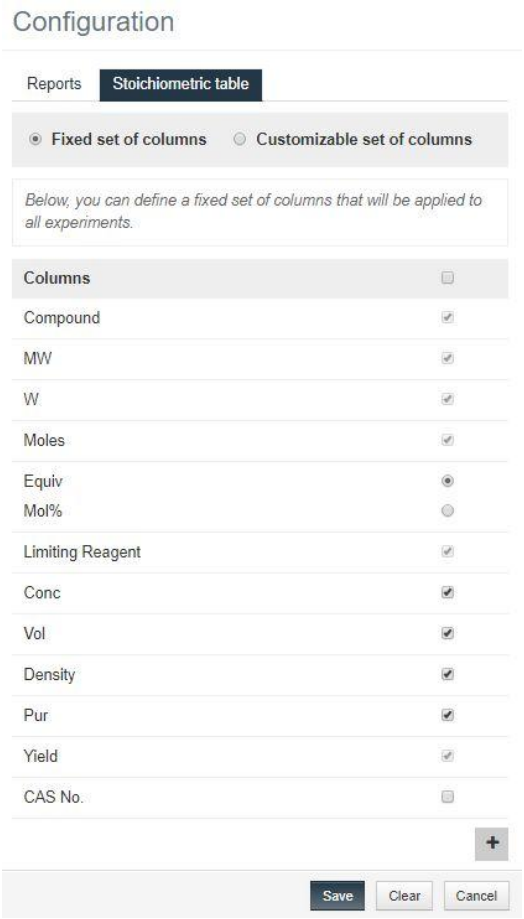
Users can also add their own custom columns to the stoichiometric table by clicking on the Plus icon (see picture above), specifying a name for each column header and ticking each column's checkbox. Custom columns can be removed at any time by clicking on the Delete (X) icon (see picture above). Finally, 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 Group Manager or the Project Manager

To open the column configuration section, the Group Manager and 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.



The following window will show up.



By clicking on the "Stoichiometric table" tab, the Group Manager and the Project Manager are able to define the column setup of the stoichiometric table for all the Group's or all the project's experiments, respectively. This column configuration section behaves the same way as the "Configure columns" window (see, above, "Column configuration by the experiment owner").

5.4 Searching

You can search for any existing experiment just by clicking on the 'Search' button and drawing the desired molecular structures of the participants:

You can also type any free text as keywords (experiment code, username, etc.) in the search field box. Use the filter button to restrict your results by project, user, or experiment.

5.5 Verification

This feature is included in the Enterprise package (it is not included in the Mbook Chemistry or Pro packages).

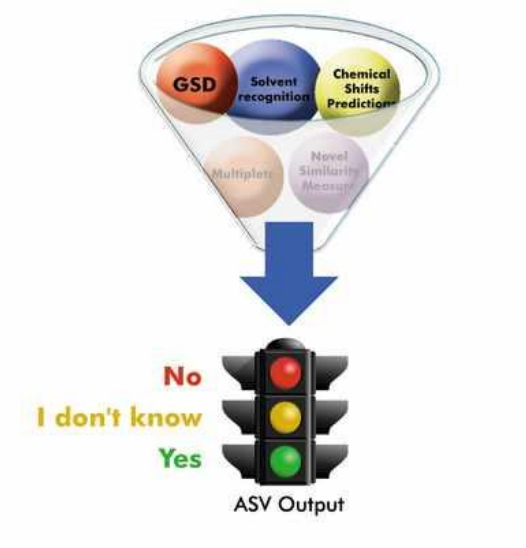
Mbook Verify is a new developing approach to structure verification via NMR and MS.

The pharmaceutical and biotechnology industries are currently facing very significant challenges that are resulting in major organizational and operational changes. The current trend is for pharmaceutical companies to outsource many of their Research and Development operations to third parties with specific specialties and areas of expertise in order to focus their own resources on areas where they are in a position to maximize value.

As a result, where many operations such as data mining, information sharing, and decisions about the chemical entities used to have to be carried out at an internal company level, these same functions now need to encompass the entirety of the supply chain and all partners involved in the company´s R&D efforts. In addition, it is desirable to standardize data formats and data handling to the greatest extent possible to keep tight control over quality, particularly when compounds are being transferred between organizations and to optimize the sharing of information to maximize productivity.

A further challenge that affects, among others, the analytical data domain, is the reduction in the resourcing of internal support teams. In the case of analytical data, this means that whilst progress in hardware capabilities and huge steps forward in automation allow us to generate vast amounts of analytical data with high throughputs, a bottleneck is being created by the ability of Analytical Departments to get eyes on data. In this situation, overseeing the data and proposed chemical structures proposed by partners outside the organization, and typically received in large numbers, is also becoming more difficult, and indeed in most cases has been abandoned as an achievable objective.

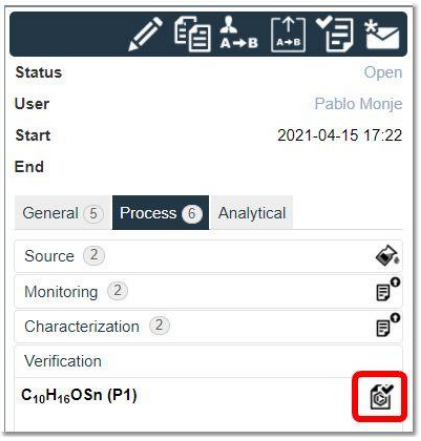
Mbook Verify evaluates a series of elements (GSD, solvent recognition, novel similarity measure, multiplets, and chemical shift predictions) and applies a scoring system to return a Yes/No/I don´t know answer. This makes it a very powerful screening system that is useful to chemists who need to validate decisions regarding the structure corresponding to their experiments, either in single or batch mode.



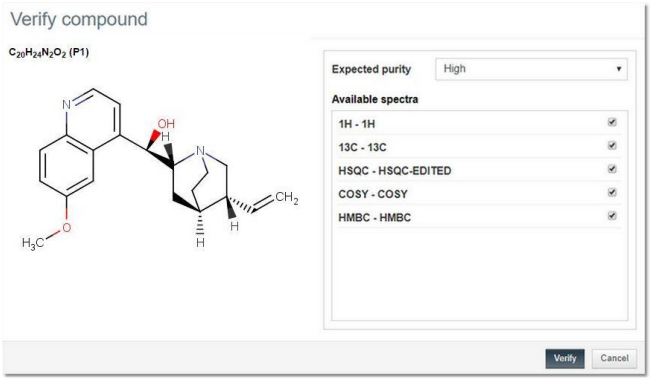
5.5.1 Running Verifications

To run a verification, you only need to have a ^{1}H, ^{13}C, HSQC, COSY, HMBC or MS associated with a molecular structure in your reaction scheme. You can upload the associated spectrum to the characterization section (under the 'Process' tab), raw datasets (in a zip file), or Mnova documents.

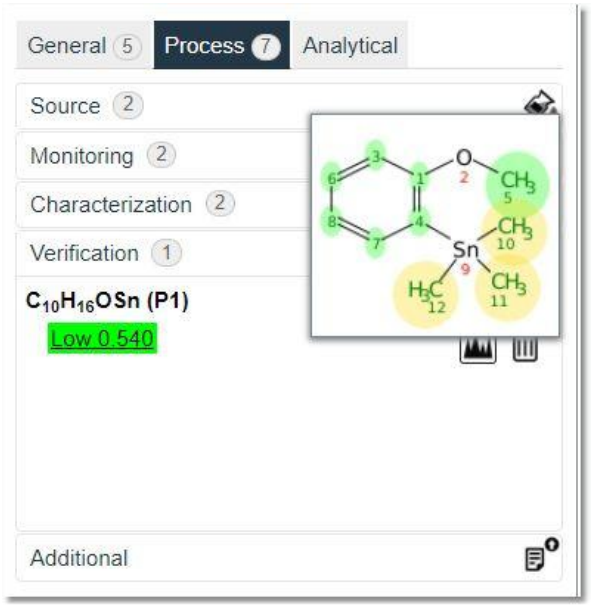
In the example below, we have uploaded ^{1}H, ^{13}C, HSQC, COSY and HMBC spectra associated with the Product (P1):



Clicking on the 'Verify' button (highlighted in red in the picture above) will display a dialog which will allow you to select the spectra involved in the verification (and the expected purity):



After having clicked on the 'Verify' button, you will get the result:



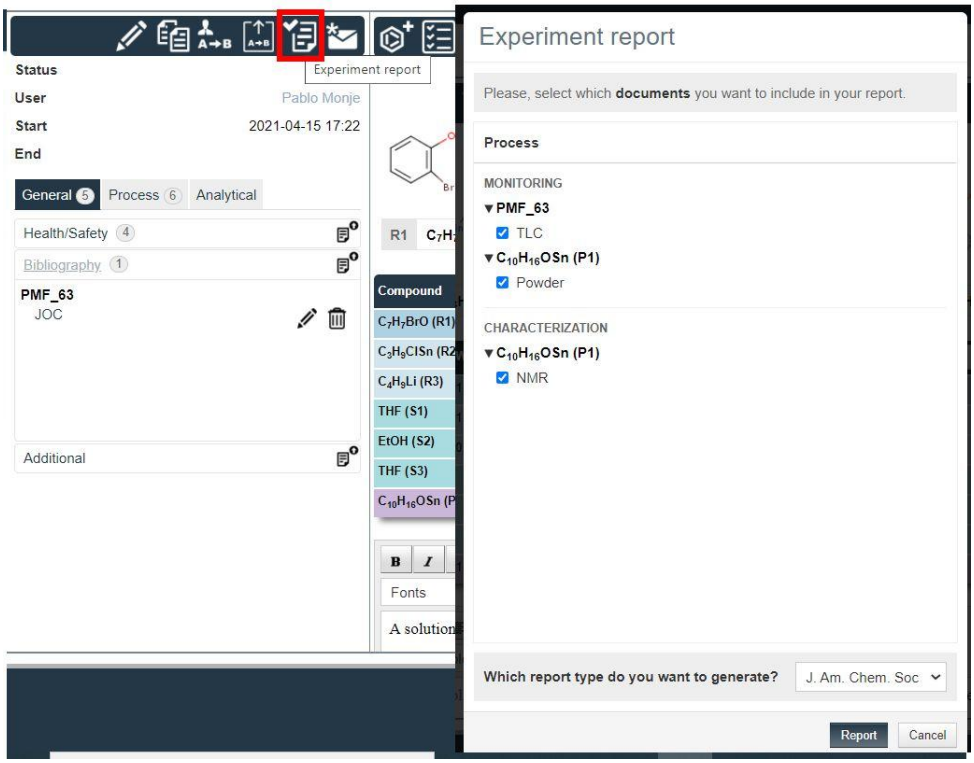
Clicking the 'Preview' button  will display a window with a molecule on the first page and the spectra on the remaining pages. Clicking on the 'Open PDF' button will display the results in a PDF file whilst clicking on the 'Open' button will load the document into Mnova.

See also:
Further information about Structure verification tools.

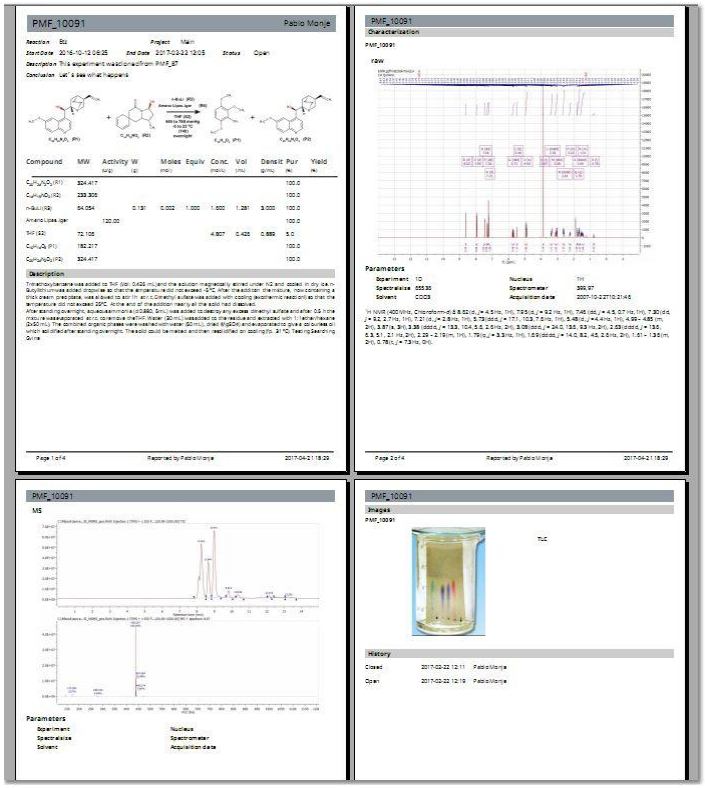
5.6 Generating Reports

You can generate experiments or reaction reports just by clicking on the applicable button 

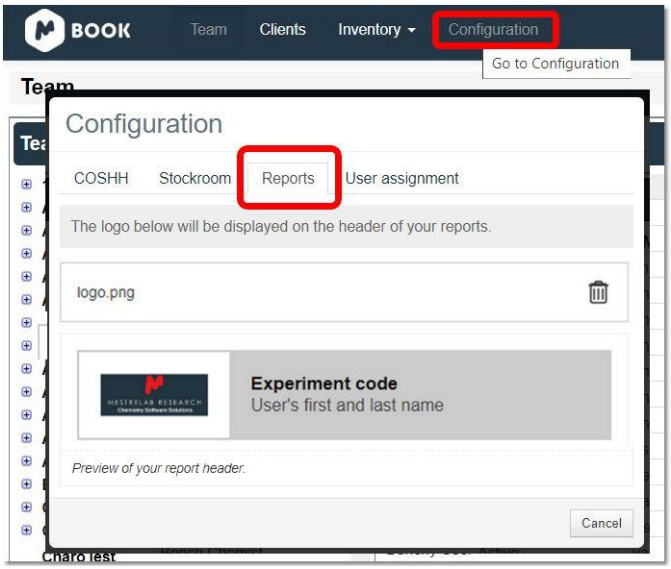
You can include the spectra used for the characterization and the images (with the description) in the report:



By clicking on the 'Report' 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:

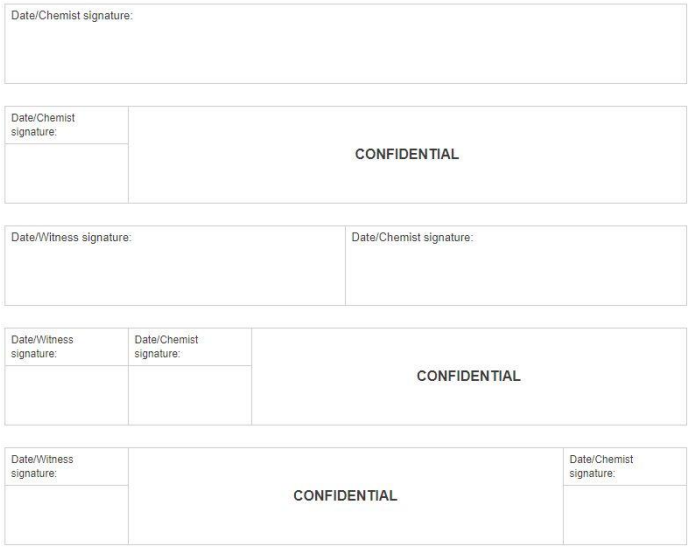


5.7 Report Footer

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

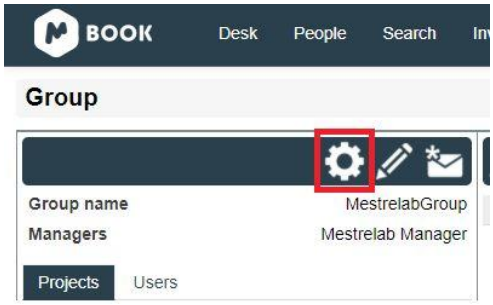
Report footers in Mbook contain one or two signature sections, as well as a text area where warning or informative messages are displayed. The picture below shows the five footer templates available in Mbook.



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.



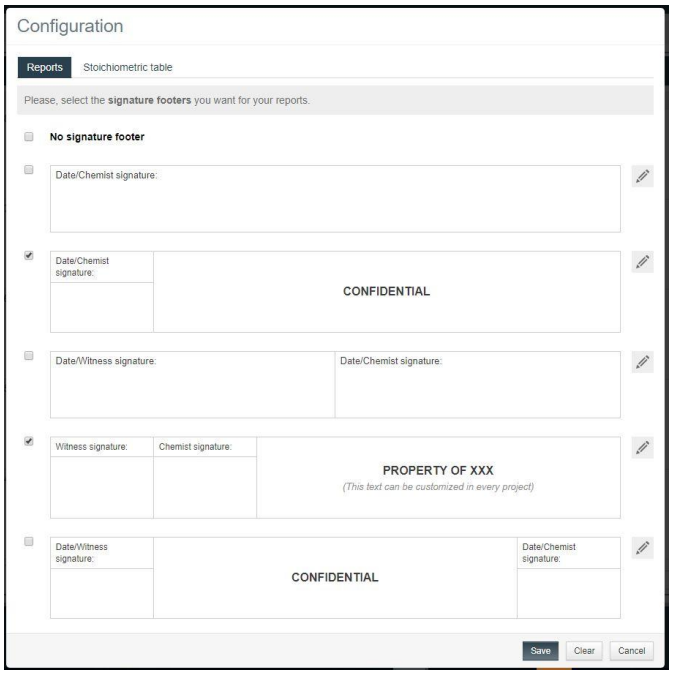
The report configuration window will pop up:

The Group Manager can select which footer templates are available to the Group's Project Managers by clicking on each template's checkbox (see picture below).

To customize a footer template, the Group Manager should click on the Edit (pencil) icon shown in the picture above, after which the footer template will become editable (see picture below). Once the footer template has been customized, the Group Manager should save the changes by clicking on the Tick button.

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.

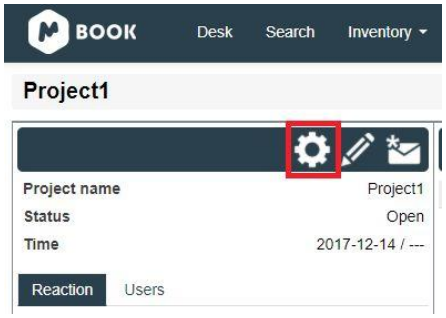
The image below shows an example where the Group Manager has customized and made two report footer templates available to the Group's Project Managers.



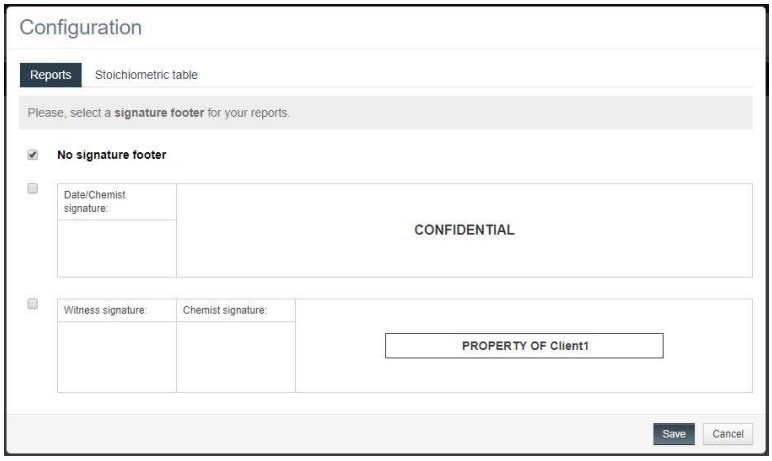
If no footer is needed for the Group's experiment reports, the Group Manager should check the "**No signature footer"** option.

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.



In the picture above, the text area in the last footer contains a message that was previously defined by the Group Manager as “Property of XXX” and has now been modified by the Project Manager with the text, “PROPERTY OF CLIENT1”.

Part VI

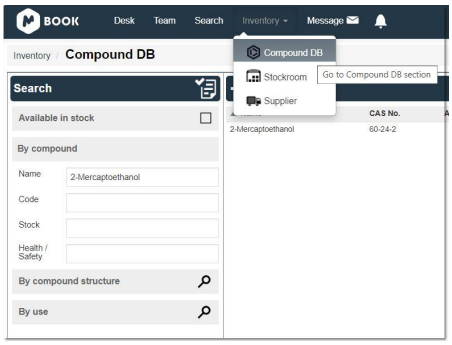
6 Main Toolbar

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.

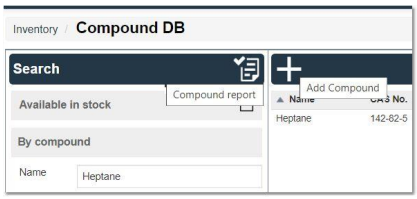
From the desk, you can search for experiments by molecular structure or by typing any free text just by selecting the 'Search' option:

Inventory

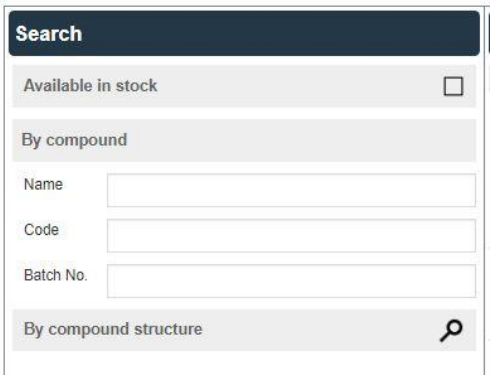
Selecting the 'Compound DB' from the Inventory scroll down menu will display the compound list:



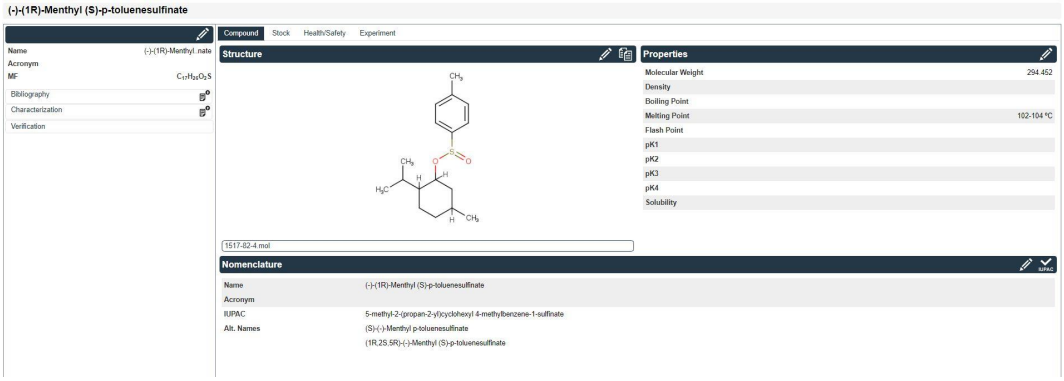
New compounds can be added to the database just by clicking on the appropriate button:



From the left panel, you will be able to search by name, code, batch number, or structure. When the "available in stock" option is checked, the search will only take into account those compounds currently listed as in the inventory:

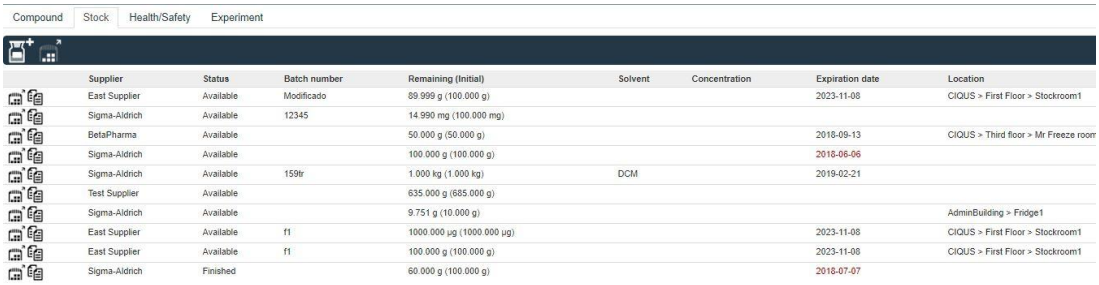


Left clicking on any existing record will display a dialog to add or edit the existing information (Name, Acronym, Molecular Formula, Melting and Boiling Points, Density, etc.):



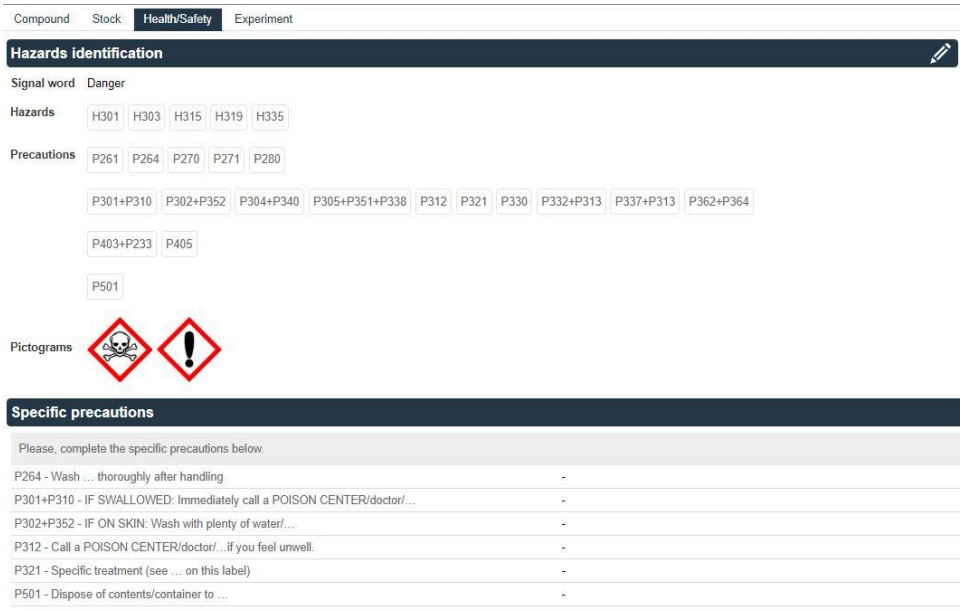
From here, you can get the MSDS document and download the .mol file of the applicable structure.

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

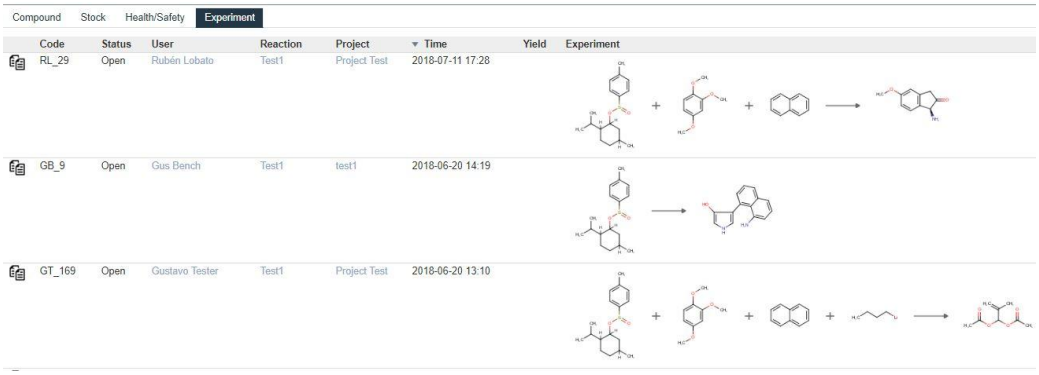


Supplier	Status	Batch number	Remaining (Initial)	Solvent	Concentration	Expiration date	Location
East Supplier	Available	Modificado	89.999 g (100.000 g)			2023-11-08	CIQUS > First Floor > Stockroom1
Sigma-Aldrich	Available	12345	14.990 mg (100.000 mg)				
BetaPharma	Available		50.000 g (50.000 g)			2018-09-13	CIQUS > Third floor > Mr Freeze room
Sigma-Aldrich	Available		100.000 g (100.000 g)			2018-06-06	
Sigma-Aldrich	Available	159tr	1.000 kg (1.000 kg)	DCM		2019-02-21	
Test Supplier	Available		635.000 g (685.000 g)				
Sigma-Aldrich	Available		9.751 g (10.000 g)				AdminBuilding > Fridge1
East Supplier	Available	f1	1000.000 µg (1000.000 µg)			2023-11-08	CIQUS > First Floor > Stockroom1
East Supplier	Available	f1	100.000 g (100.000 g)			2023-11-08	CIQUS > First Floor > Stockroom1
Sigma-Aldrich	Finished		60.000 g (100.000 g)			2018-07-07	

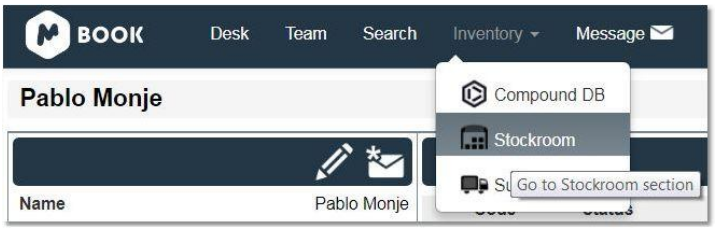
The 'Health/Safety' panel will allow you to check and modify the hazards and precautions assigned to the compound:



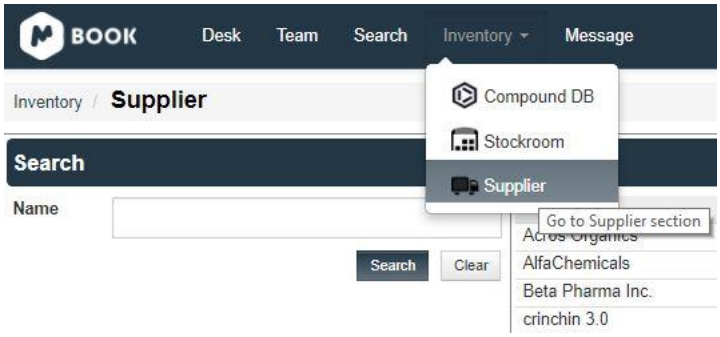
Clicking on the 'Experiment' button will display the list of experiments where the compound has previously been used:



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

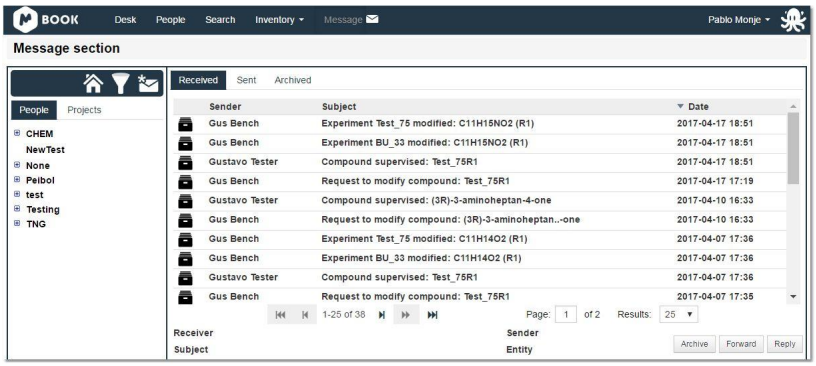


The Supplier option in the toolbar will allow you to search/edit/add suppliers to your database:



Message

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



The Message panel shows a complete list of experiments open and the list of messages related to a given user by default. Clicking on the 'Home' button  will restore this original view after navigating the trees.

Part

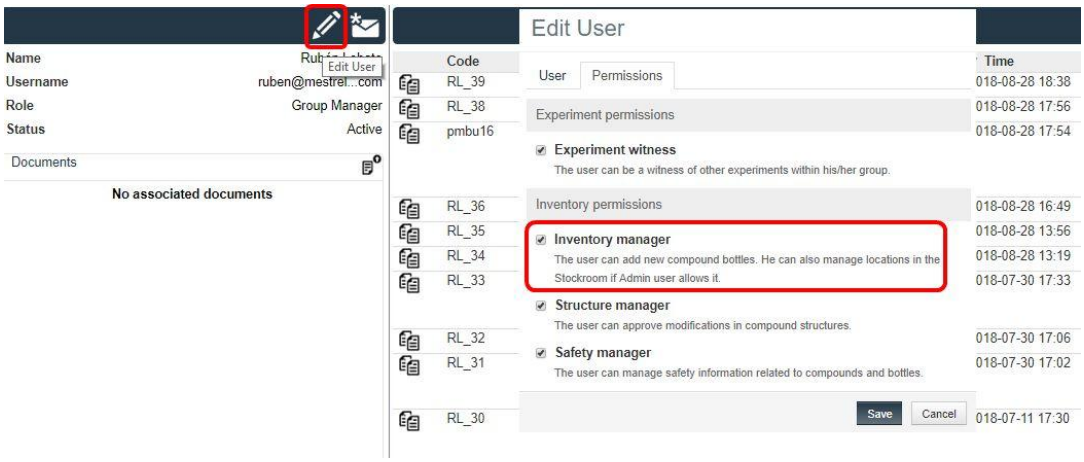
7 Inventory

This feature is included in the Mbook PRO, Mbook Analytical and Enterprise packages (it is not included in the Mbook Chemistry package)

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. This tool has been automatically updated on your Cloud version; for in-house installations, you will have to update to Mbook 1.1.

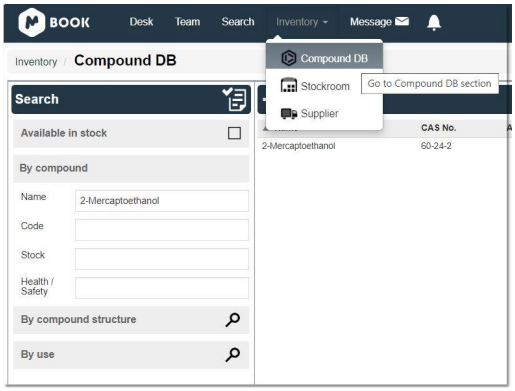
Preliminary step: Become an inventory manager!

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 at the top right corner of the screen and select "edit user". Here you can enable or disable the inventory manager privileges for any of the other users.

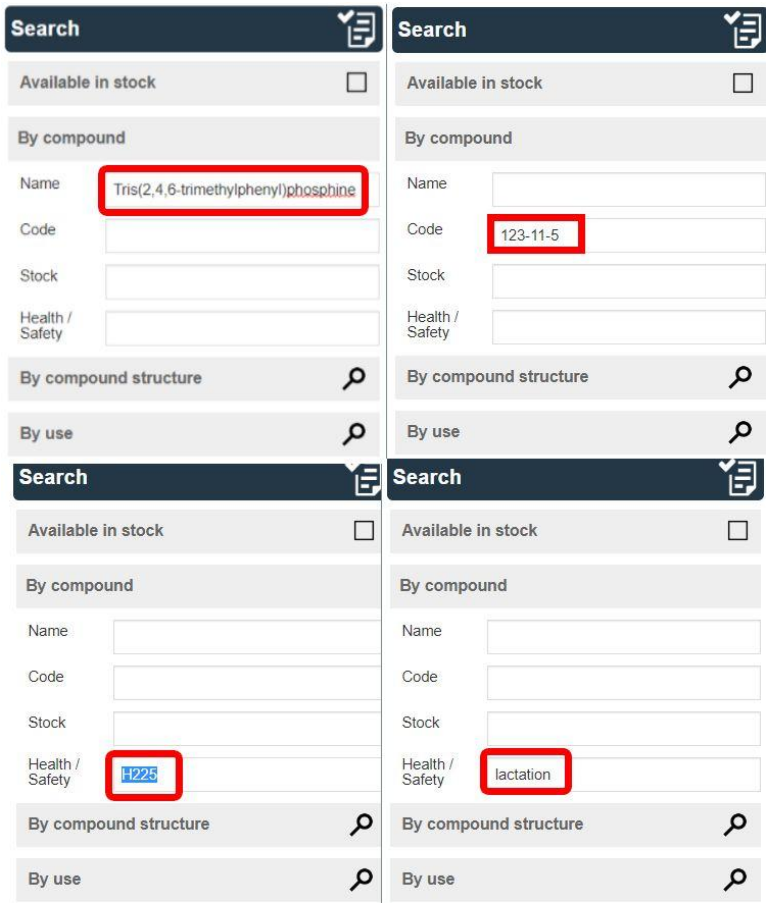


The inventory menu

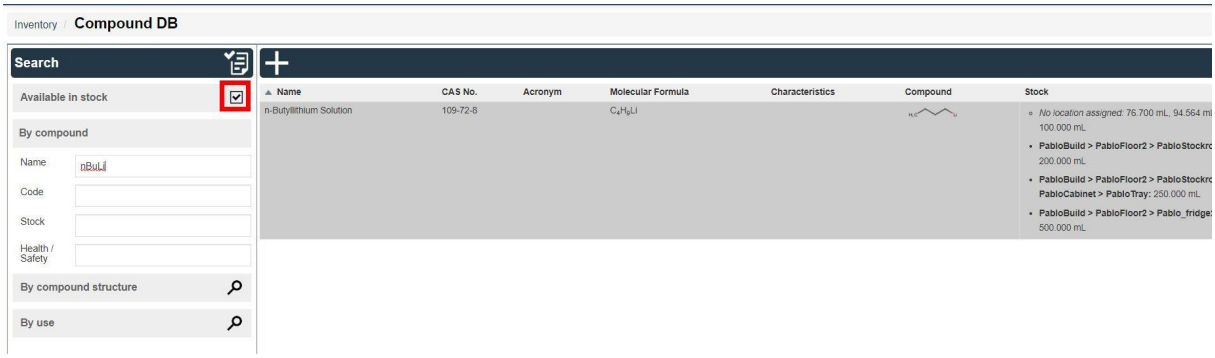
The inventory tool can be found on the top bar menu and is linked to the compound database entries. You can enter or edit new suppliers as well as searching for any compound in your Mbook database.



You can search by name, 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.

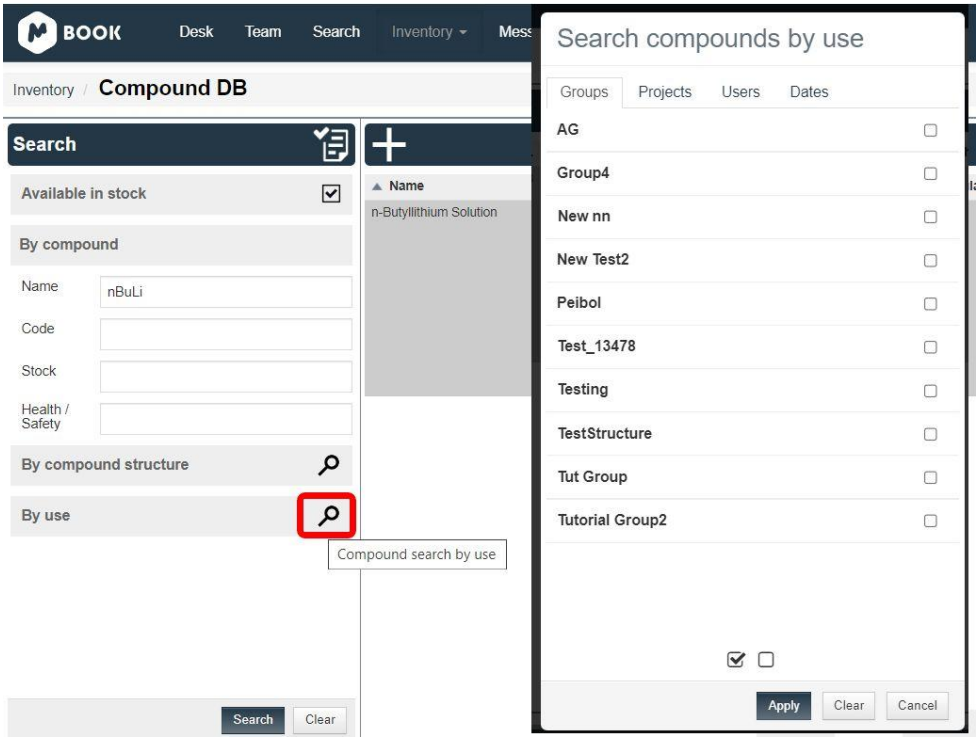


You can search by compounds available in stock, just by checking the applicable box:

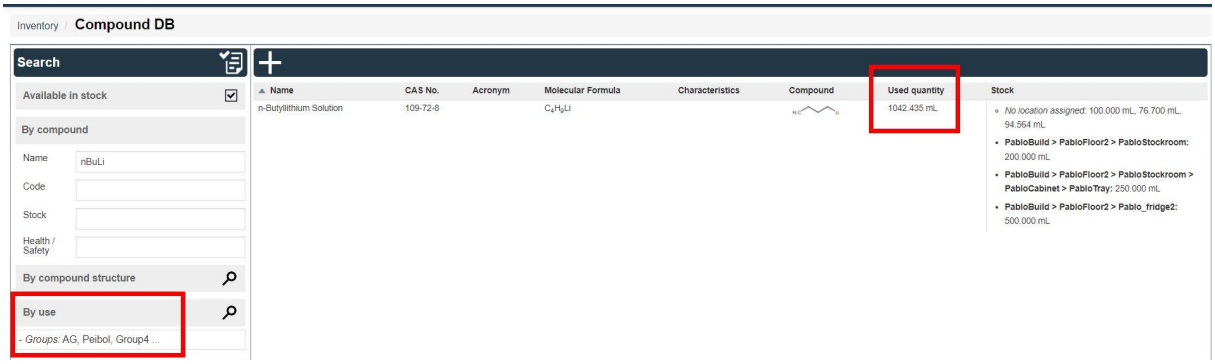


Use the option to search by compound Structure to load or draw a molecule and search for it.

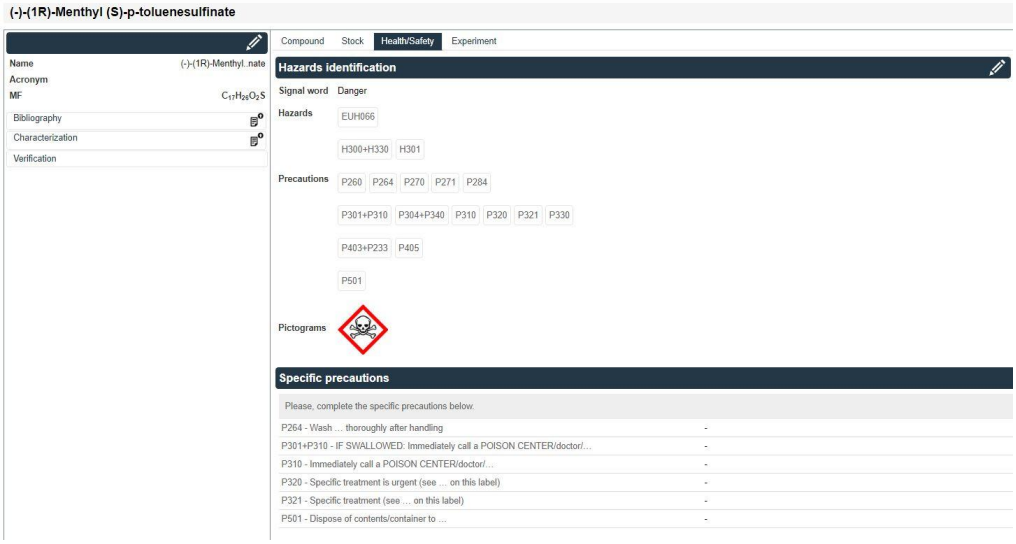
The search mode “By Use” allows you to search by compounds used by a group, project and/or user:



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



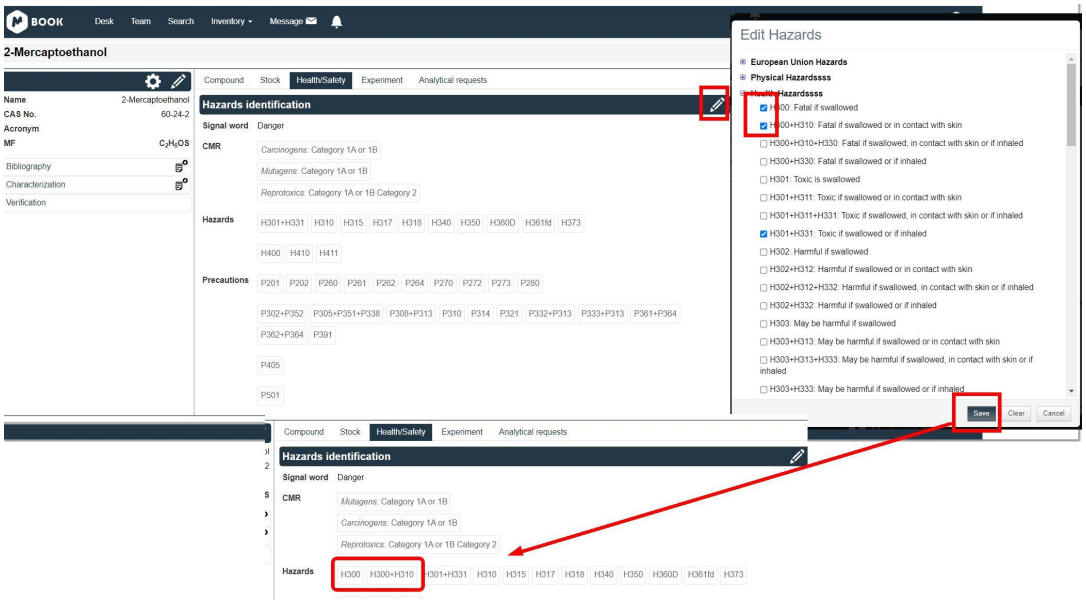
You can categorize compounds using the CMR (carcinogenic, mutagenic or reprotoxic) categories. The CMR categories are related with the H phrases according to the table below:

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.

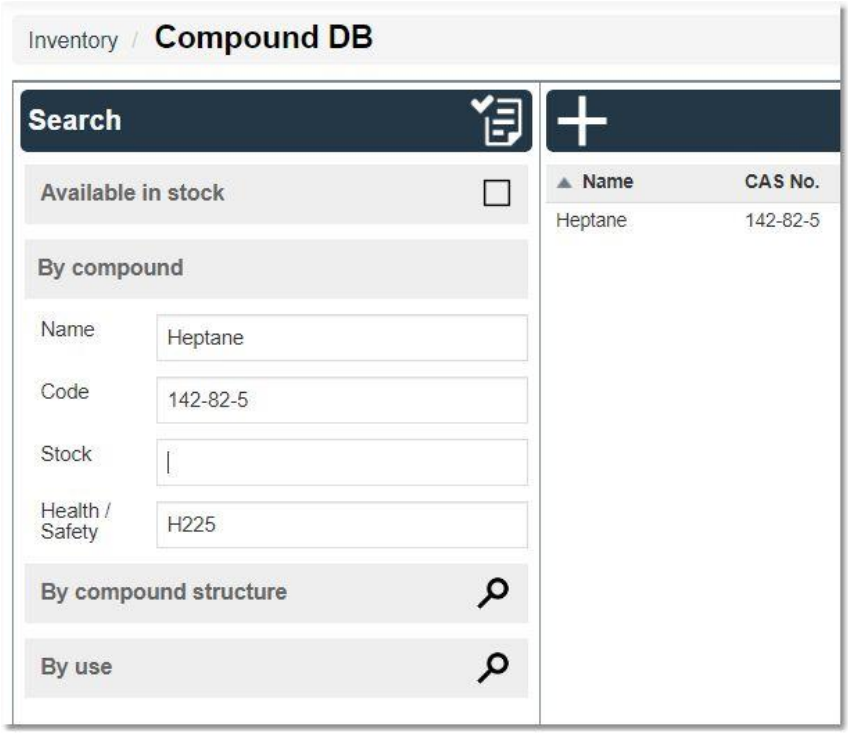
Source: Regulation (EC) No 1272/2008[2]

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



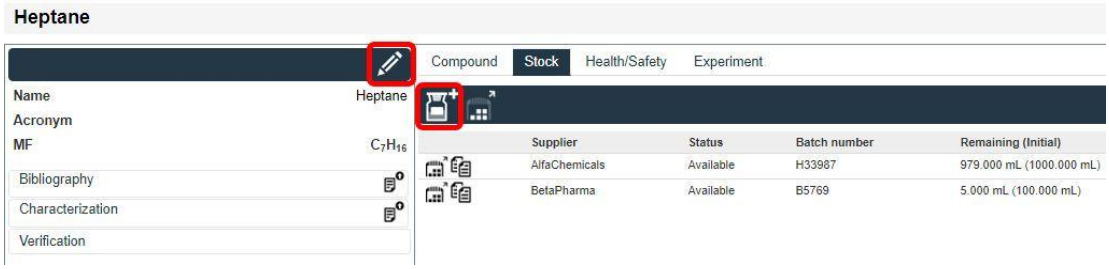
A practical example

Let´s go to the main menu and select Inventory/Compound DB and search "heptane" as an example:

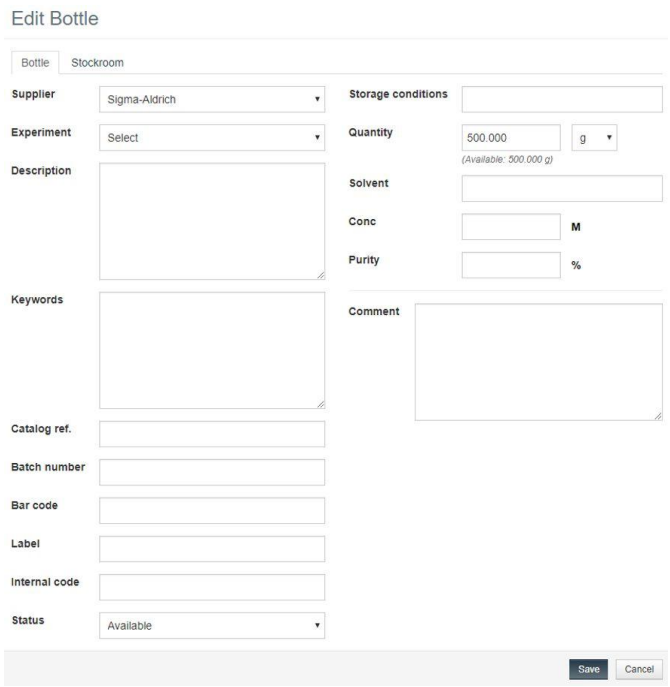


(You can also search by code, stock or Health/Safety: by the H phrases or CMR categories, or even by searching by keywords as Lactancy, Lactation, Carcinogens, Mutagens, Reprotoxics is available using this field.)

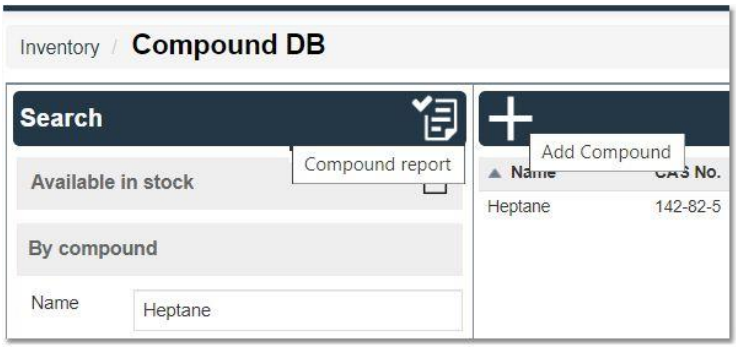
Click on “Heptane” in the list and go to the “Stock” tab for this compound. Here you can see we have two different entries for two different suppliers. This window also displays details such as status, batch number, and remaining number for each of the bottles.



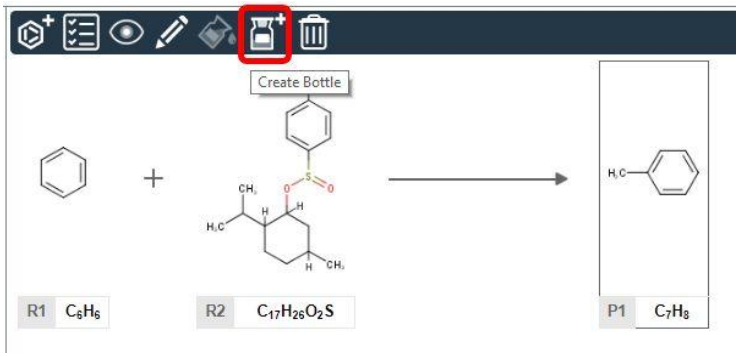
As an inventory manager you can add a new entry or edit the information relating to any of these bottles, such as the description, quantity, purity, order date, who ordered it, etc., and then just save any changes made.



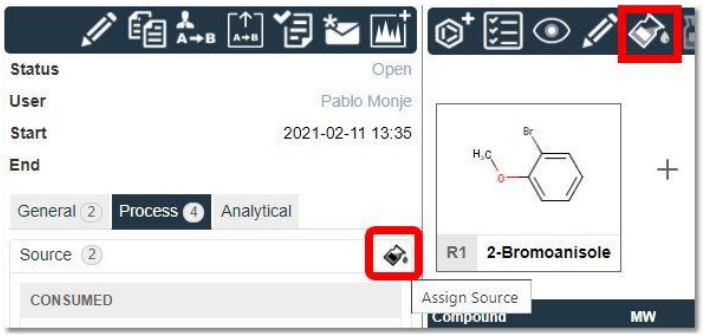
Clicking on the 'Compound Report' button will export to PDF the compound list. You can add new compounds to the inventory just by clicking on the appropriate button (from the compound DB):



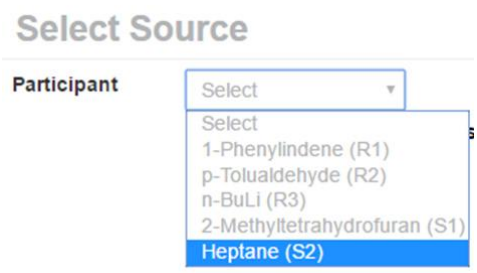
You can also add bottles to the inventory from the reaction scheme just by highlighting the appropriate product and clicking on the 'Create bottle' button:



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 heptane (or your preferred reaction participant) by clicking on the "Assign Source" icon.

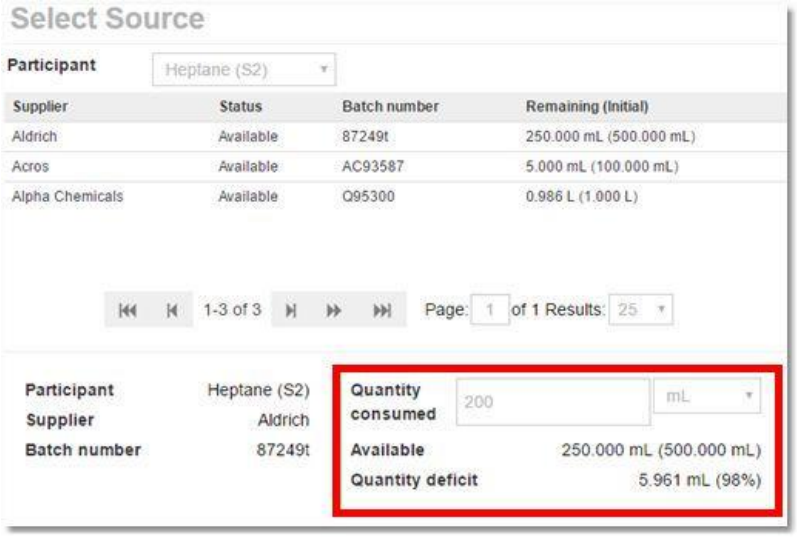


You can now set the amount you have used of each chemical for any of the source entries.



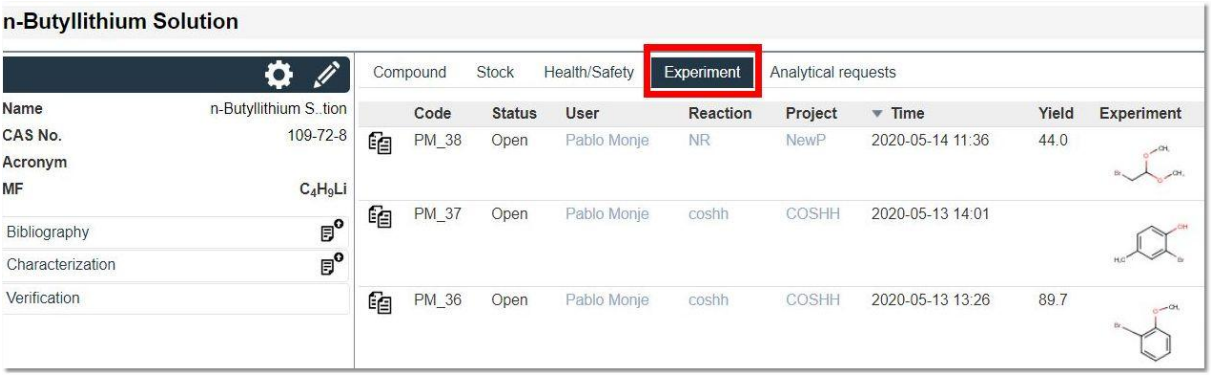
Besides the available number of each of the source bottles, it also displays the "quantity deficit". This shows you the amount of participant required for the reaction as per the stoichiometric table.

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.

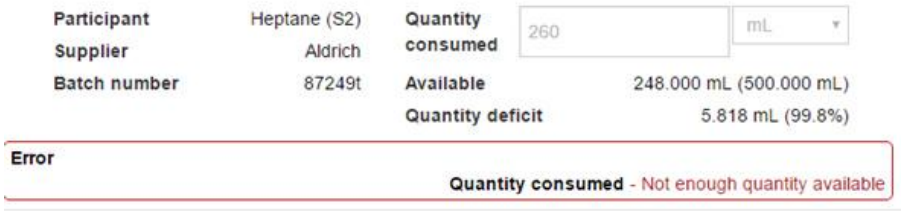
When selecting a compound from the Inventory/Compound DB, the experiment tab displays the list of experiments where this compound has been used:



Warning messages

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

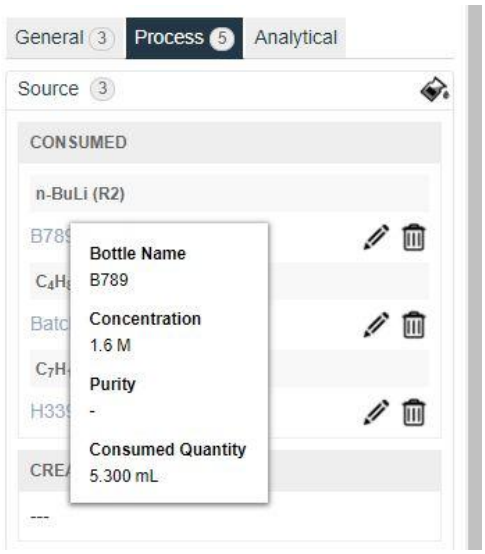
- If the value of the quantity consumed is greater than the number of bottles you have available, you will see the following error message:



- 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:



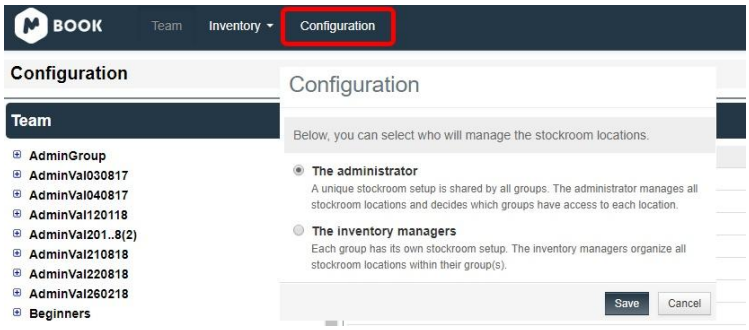
See also:

Resources about Inventory tool.
Resources about drawing Structures with Coordinate Bonds.

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.



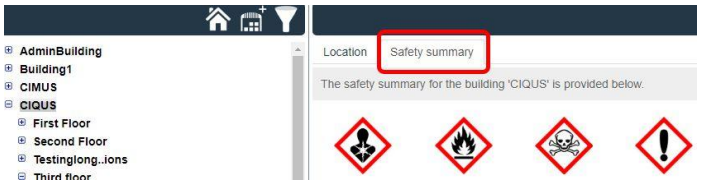
'The Administrator' option is the default configuration.

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 and the safety summary for each of 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.



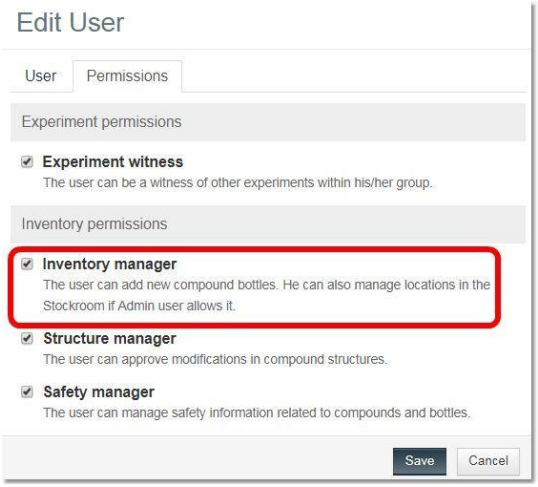
Inventory managers can assign bottles to the existing locations created by the administrator but cannot create new locations.

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.

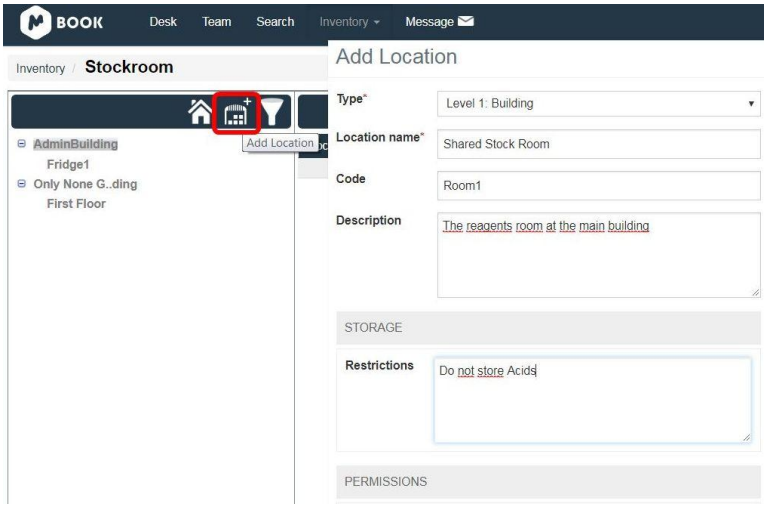
The group managers will be able to give 'inventory manager' permissions to any existing user:



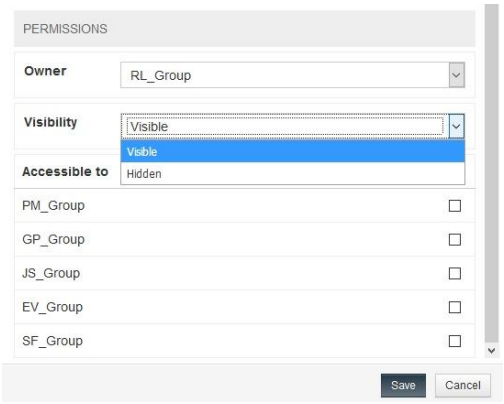
The stockroom menu

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

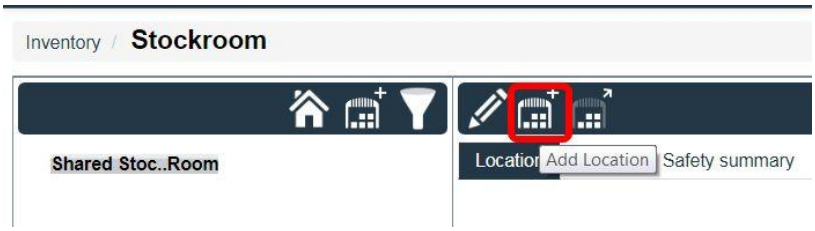
The first step is to 'Add a location':



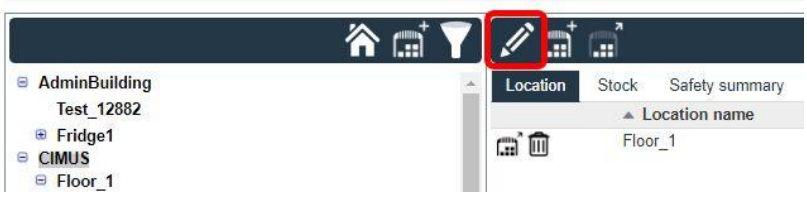
From here, you can enter the type (Level 1 in this example), location name, description, storage conditions (see above), and manage permissions (Group owner, visibility, and allowed groups) for the new location:



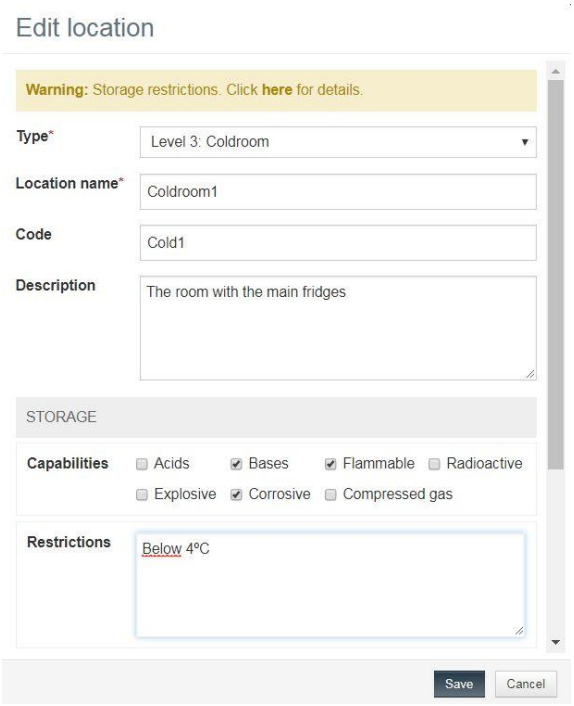
Once you have created the location in the first level, you can continue adding further levels by clicking on the 'add location' button:



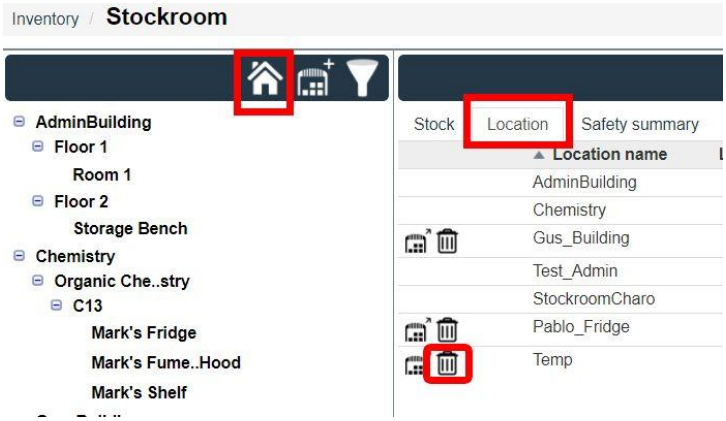
You can also edit a location by clicking on the appropriate button:



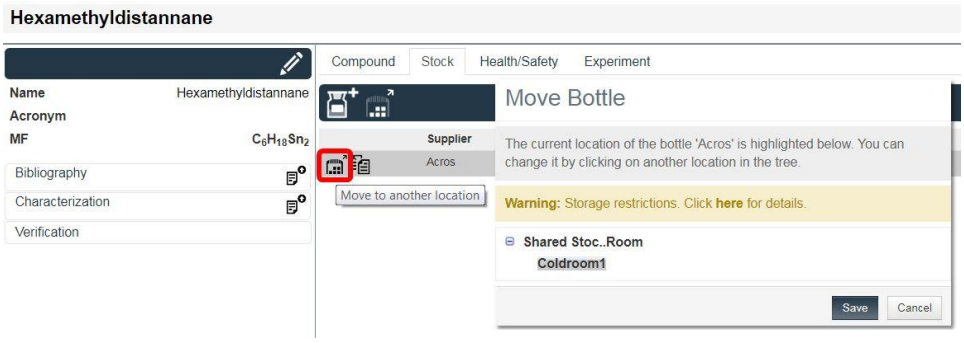
In this case, we will create a location in level 3 (coldroom). You can define further restrictions and permissions for this level:



You can delete any empty locations by selecting 'Home/Location' and clicking on the 'Delete' button:



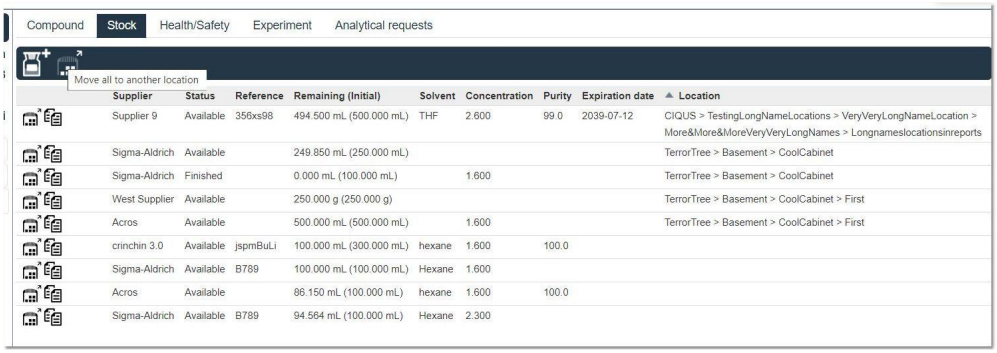
The next step would be to add an existing inventory entry to one of those locations:



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

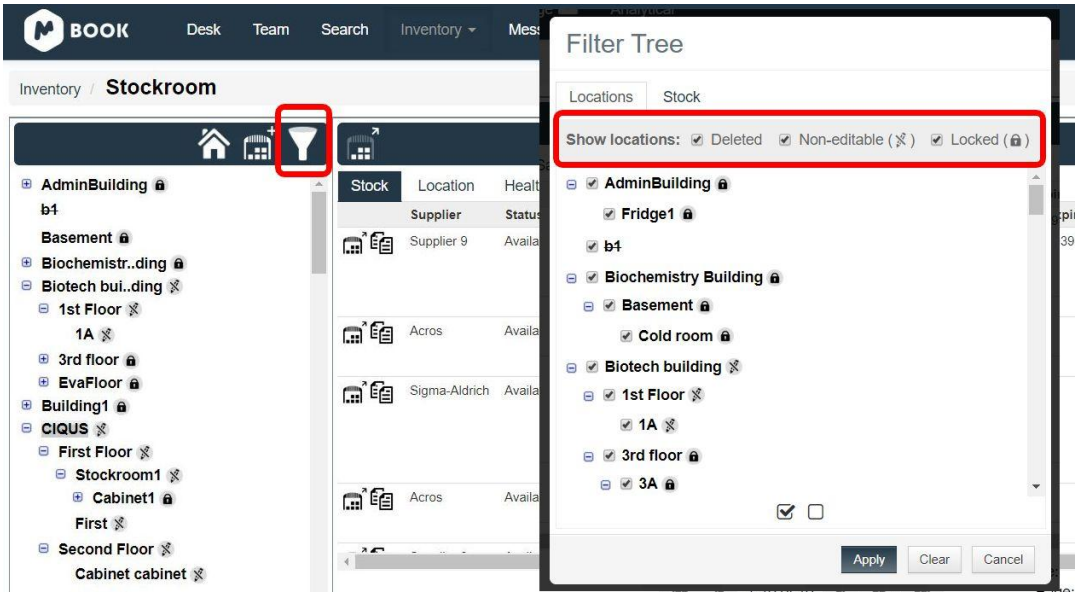
After having clicked on the 'Save' button, the location will be updated:

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 .

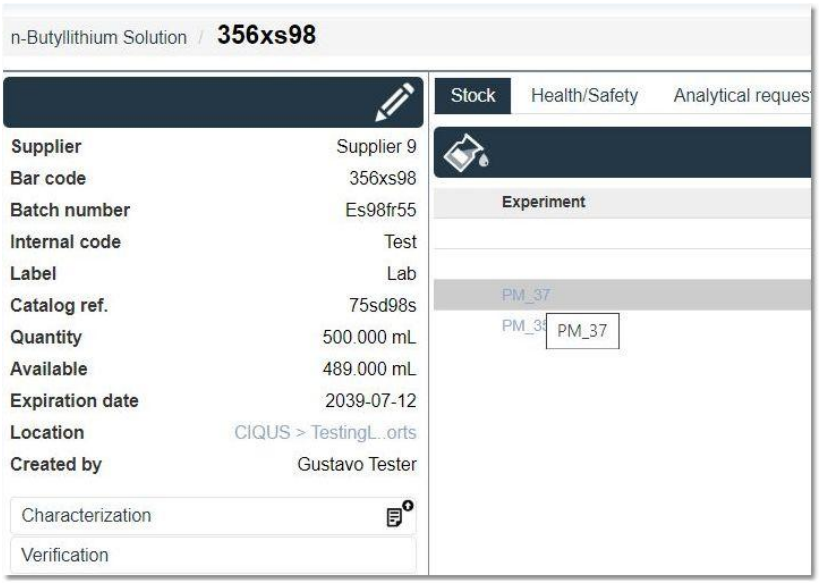


You can create bottles for products from the experiment panel:

Use the filter to display 'deleted', 'non editable', and/or 'locked' locations:



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:



See also:

Resources about the Inventory tool.

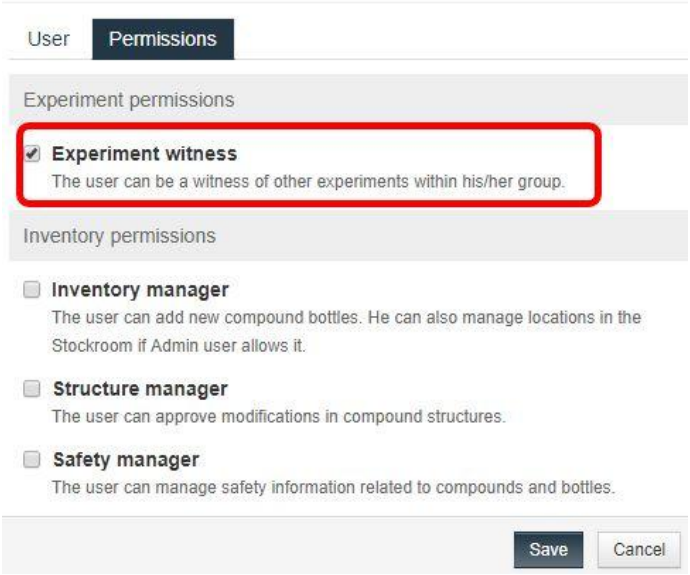
Watch a miniclip about this functionality by following this link

Part VIII

8 Experiment Witnessing, Approval and Structure Managers

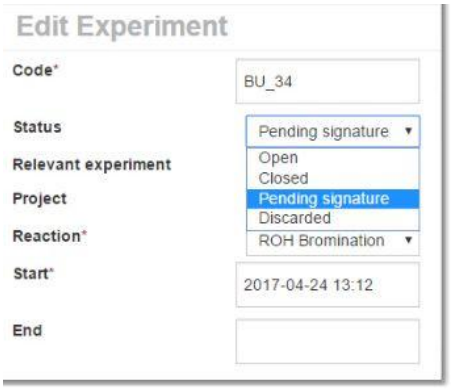
Experiment Witness

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:



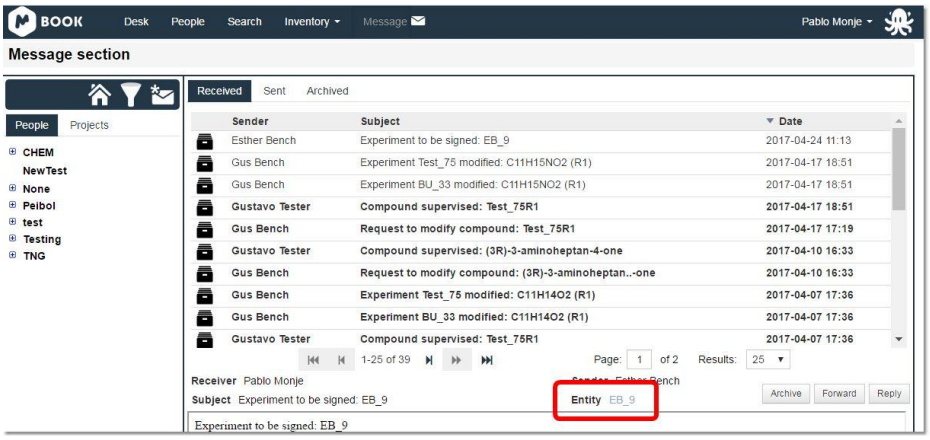
The group manager can allow any given user to be a witness to other user's experiments if those experiments are accessible by that particular user.

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).

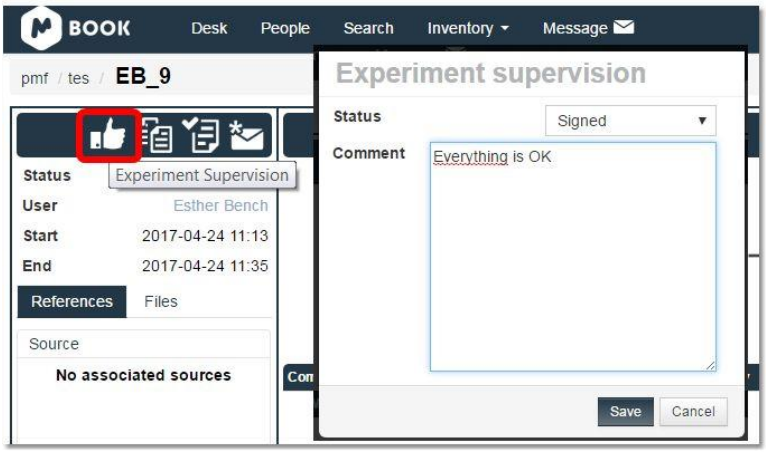
The witness will receive a notification in his/her inbox (displaying an envelope in the toolbar):



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):



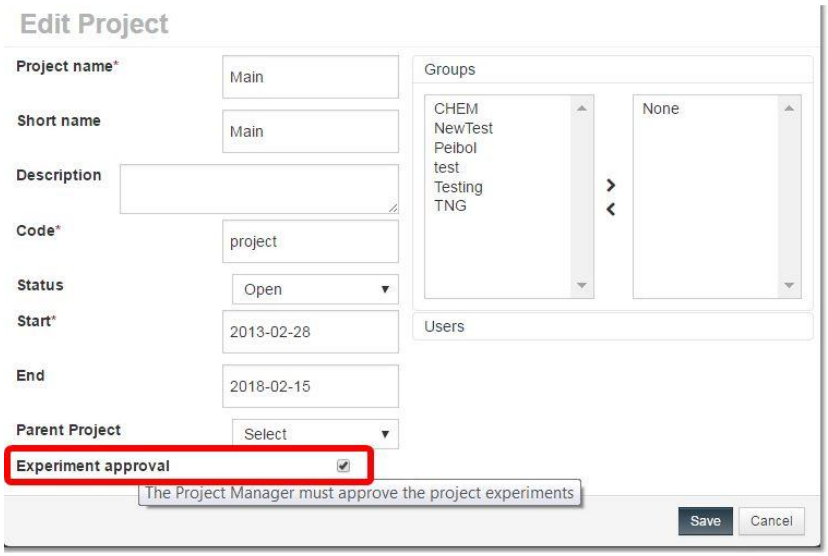
After clicking the Save button, the supervision icon will disappear and the status of the experiment will turn to 'signed'. Once the experiment has been signed, it can no longer be edited by the owner (unless the owner of the experiment is the project manager).

Experiment Approval

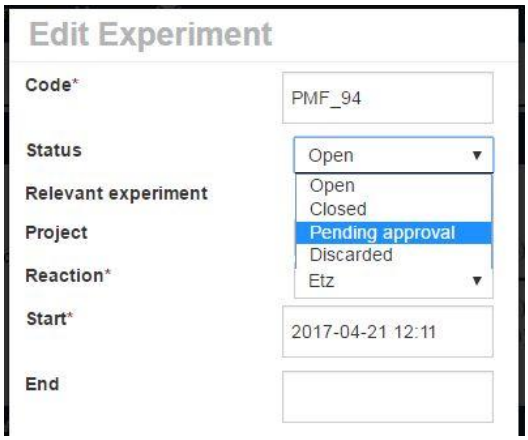
In certain companies/groups, experiments, once finished, must be **approved** by authorized users.

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:

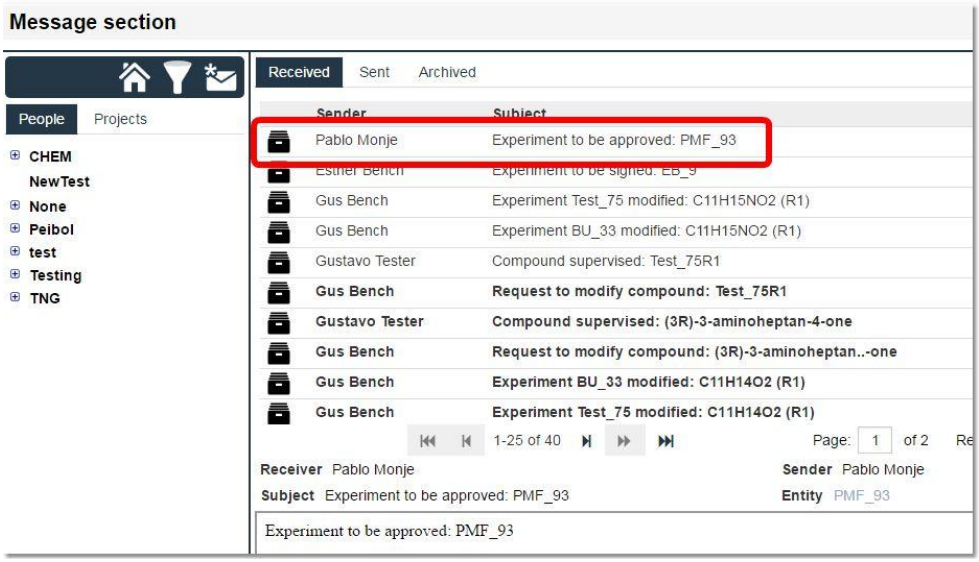


When the status of an experiment is switched to "Pending approval", a message is sent to the group manager(s) of the project to inform them that there is an experiment that needs to be approved:

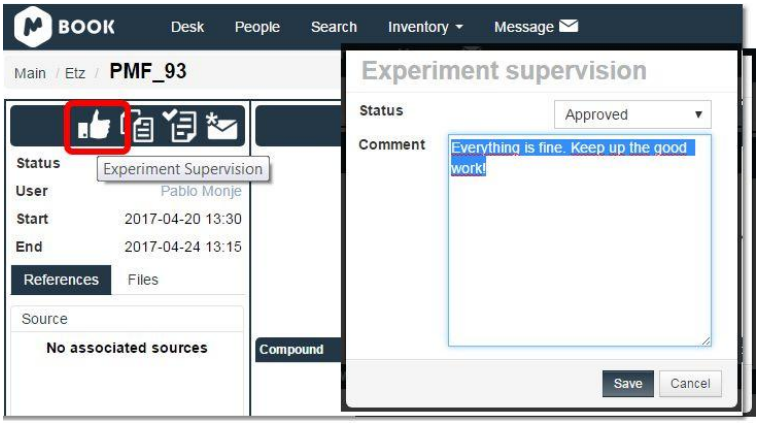


NOTE: If both witness and approval process are active, once an experiment is signed, the approval process will be launched automatically (the experiment owner does not need to trigger this action manually).

The privileged user can load the experiment using the 'Entity' link:



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



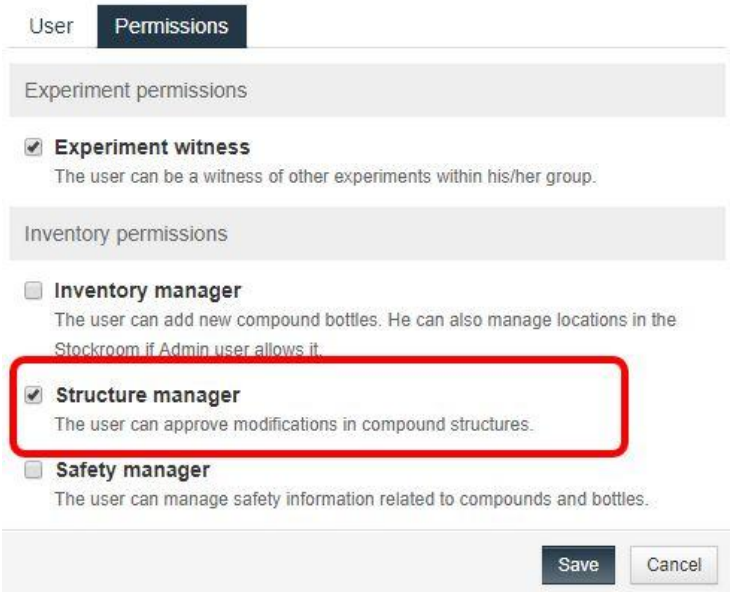
After approval, the experiment state will change to "Approved", and the experiment owner will receive a notification of such. After the experiment is approved, it cannot be edited by the owner:

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

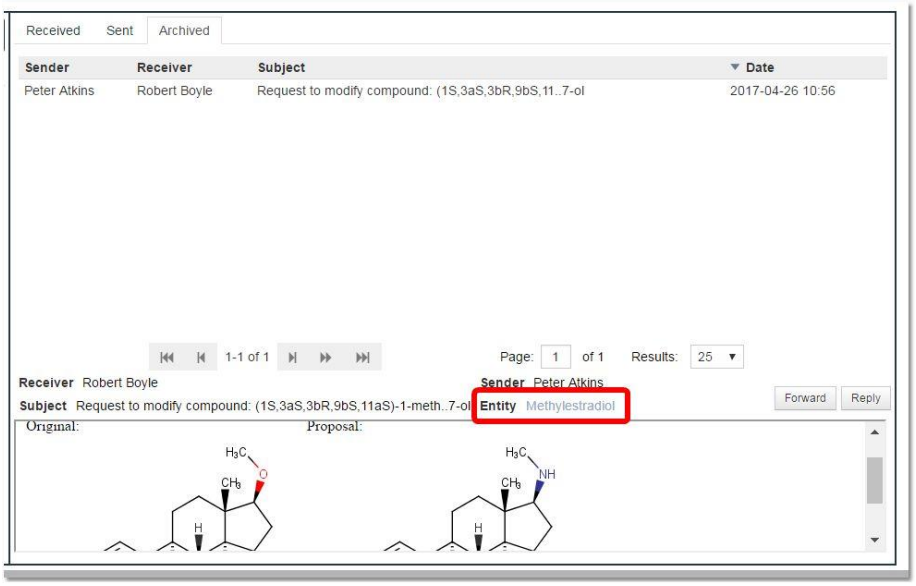
By default, Group and Project Managers will have "Structure manager" permissions.



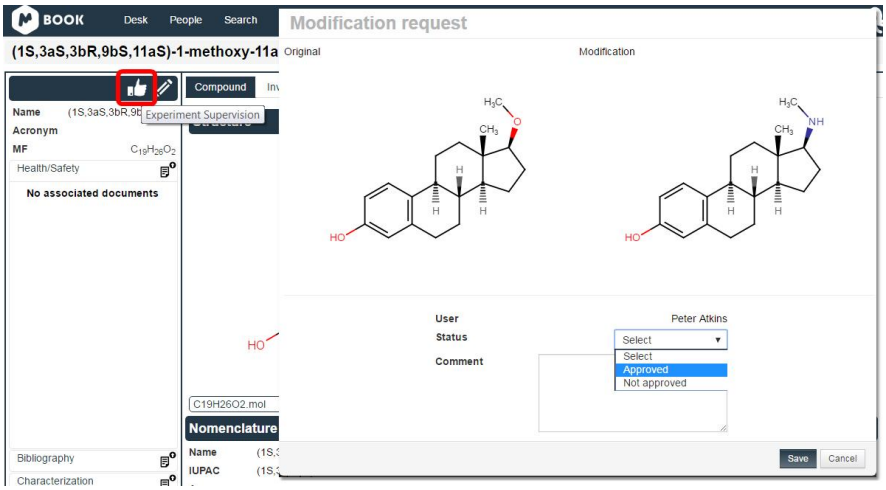
Any user can modify a compound that they have created (compounds created by other users, however, cannot be changed) that are only used in their experiments. A message informing about that change will be displayed to them:

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:

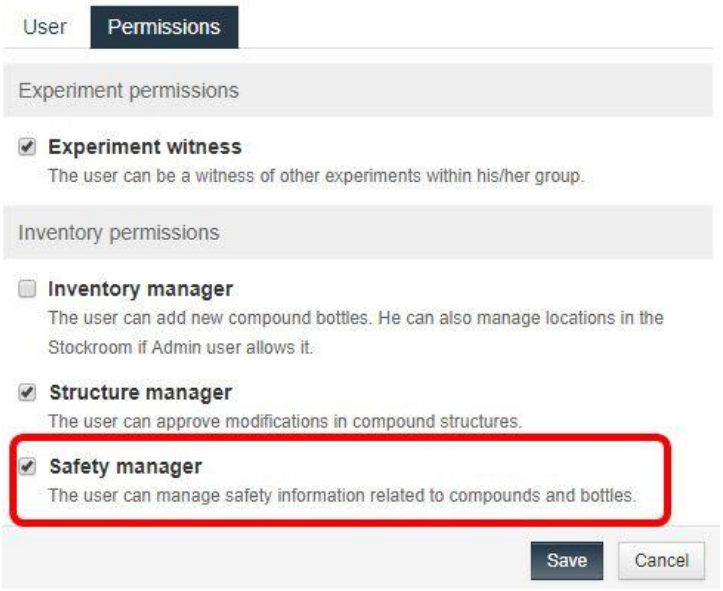


If the modifications are approved, the changes will be applied immediately and a message will be sent to the users associated with the experiments and to the applicable project managers (informing them about the approval).

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

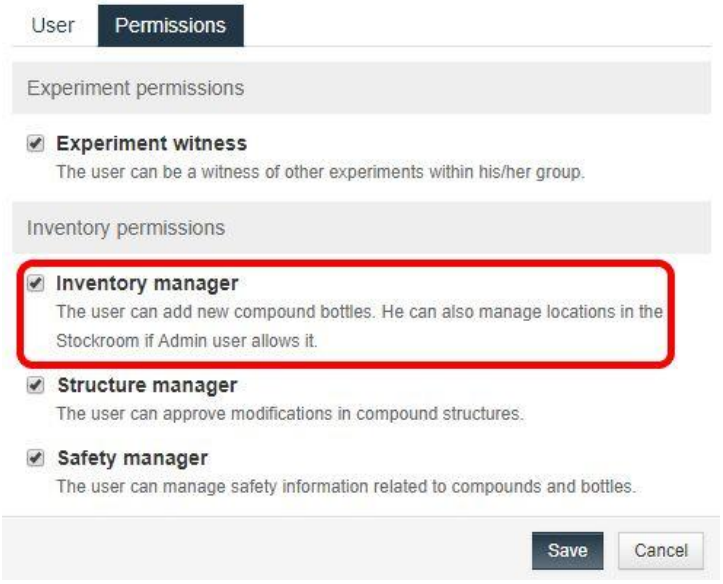
Safety Managers

This user can manage safety information related to compounds and bottles. The group manager can assign these permissions to any existing user (except guests):



Inventory Managers

This user can manage locations in the stockroom (If the administrator allows it) and add or edit compounds bottles in the Stockroom section:



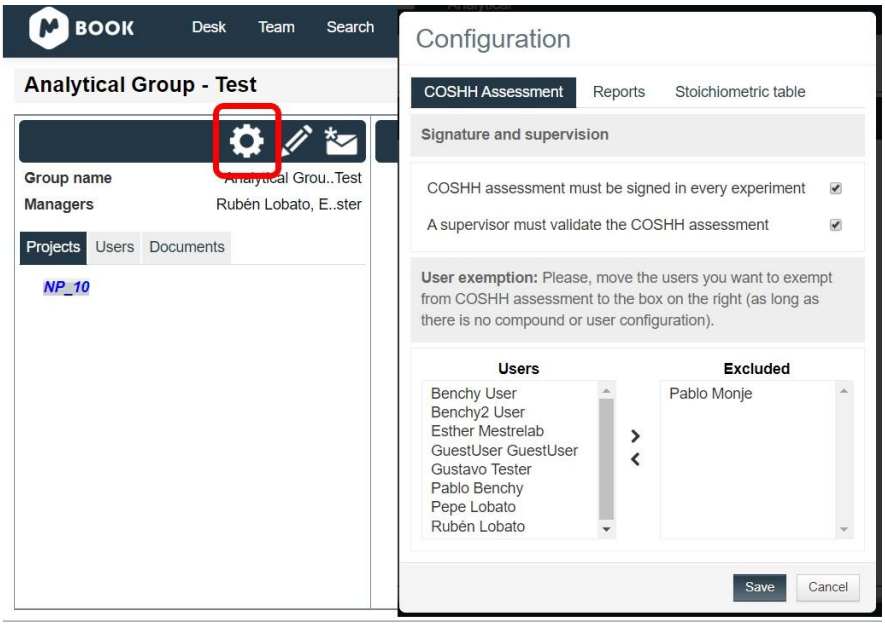
Part

9 COSHH

This feature is included in the Mbook PRO and Enterprise packages (it is not included in the Mbook Chemistry package)

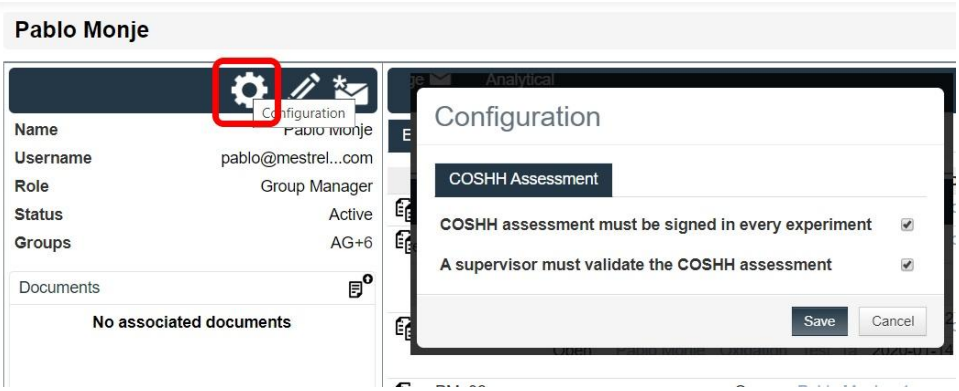
You can include COSHH assessments for groups, projects, users, and compounds.

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:

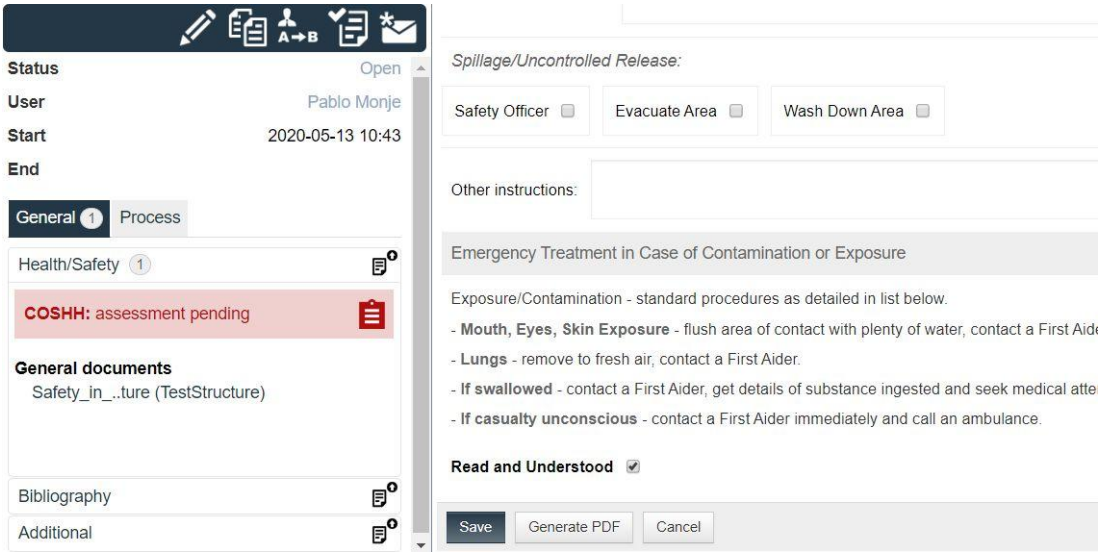


Note: parent COSHH project configurations take precedence over child project configurations.

For user and compound configurations, the setup is somewhat similar:

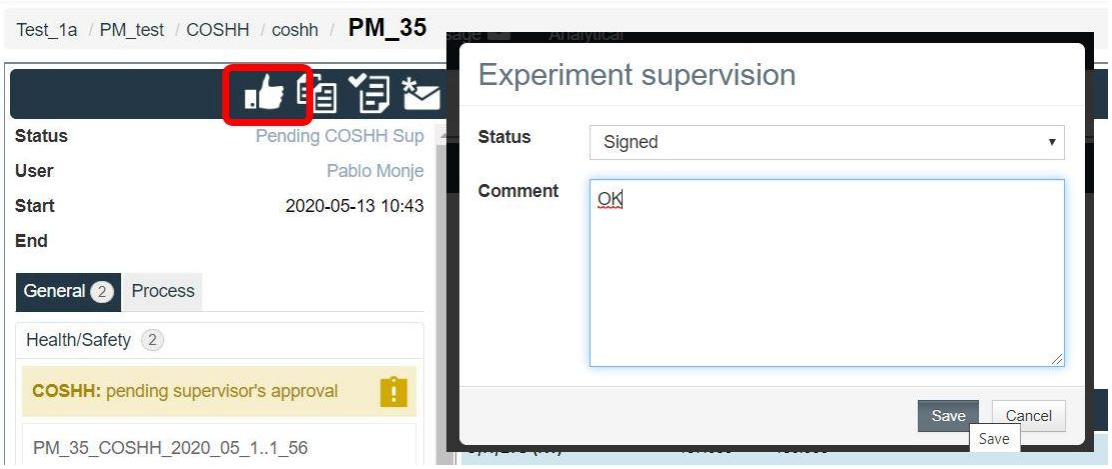


If the option to sign the COSHH assessment in every experiment is checked, a notification in red will appear after having added a compound to the experiment indicating that the assessment will need to be signed:



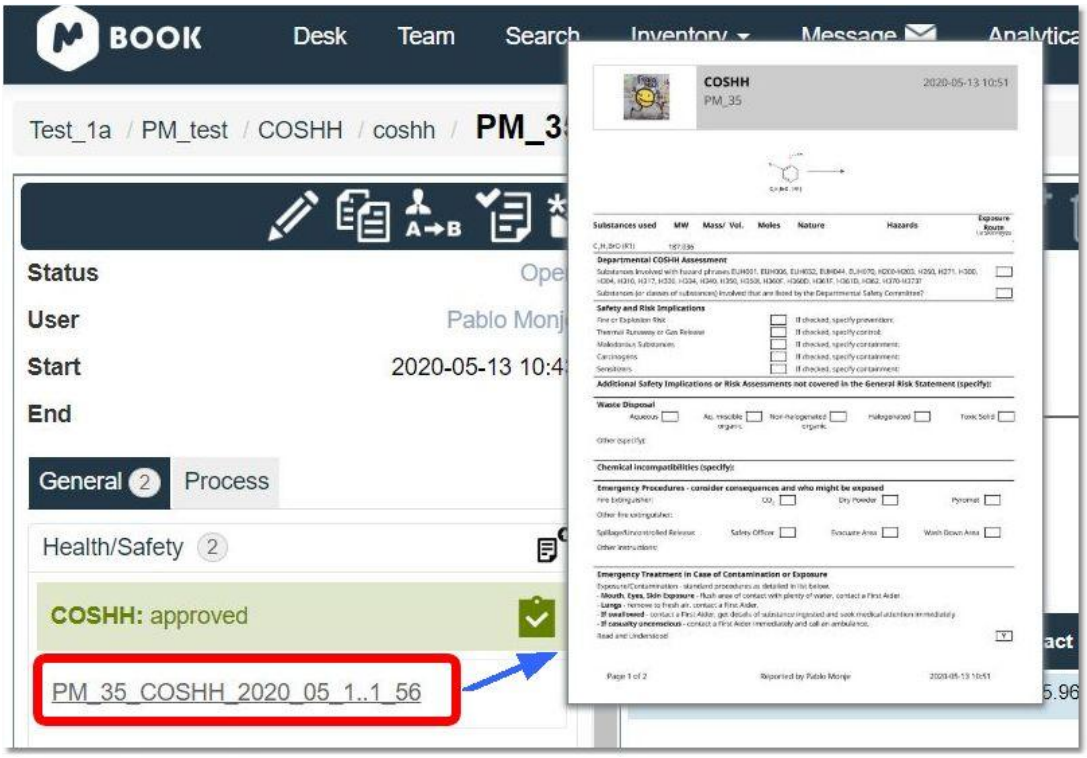
Fill the form with the relevant information, check the "Read and Understood" box and click on the Save button.

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

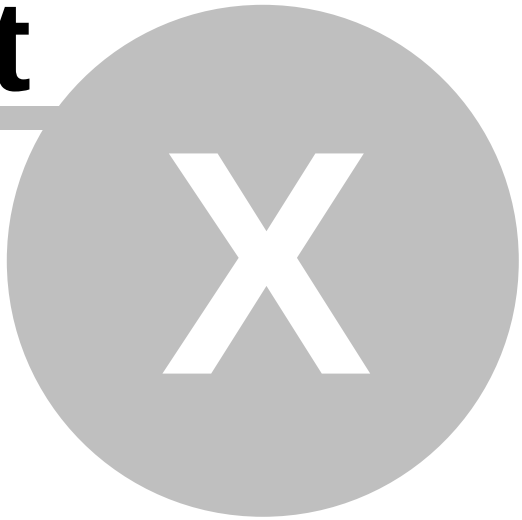


During this process, the experiment will remain blocked (the user, however, will be able to continue adding reactants, solvents, and products, but will not be able to edit the products in the stoichiometric table or to write the experimental section). If the user attempts to edit the product, a warning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

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 Mbook Analytical

This feature is included in the Mbook Analytical and Enterprise packages (it is not included in the Mbook Chemistry or Pro packages)

Mbook Analytical is an Electronic Laboratory Notebook (ELN) specially designed for analytical chemists.

As an analytical chemist, you can manage your entire workflow digitally with Mbook Analytical, including:

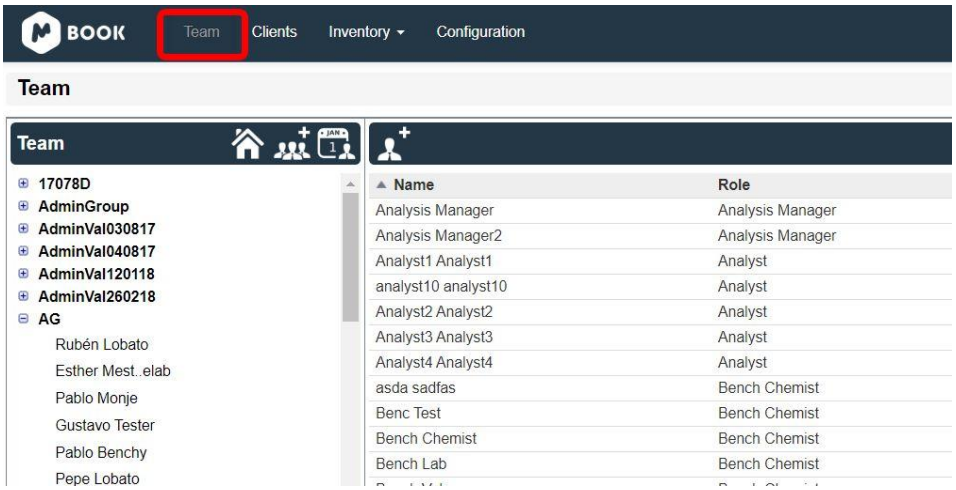
- Setting up your laboratory.
- Organizing your team.
- Scheduling and processing your analytical experiments.
- Recording and reporting the results of your analytical experiments.
- Developing an end-to-end customer experience by allowing your customers to request your analytical services and get real-time feedback via Mbook Analytical.

This guide will show you how to get started with Mbook Analytical, which is achieved in three main steps:

- First, you will divide users in two categories: those who request your analytical services, or clients, and those who provide your analytical services, or analysts.
- You will then set up your laboratory by defining which analytical instruments are available to your analysts and which analytical services are available for your clients to request.
- Finally, you will understand the complete lifecycle of a request of analytical services, namely how analytical services are requested by a client, how they are processed by an analyst, and how their results are reported in Mbook Analytical.

10.1 Create an analyst

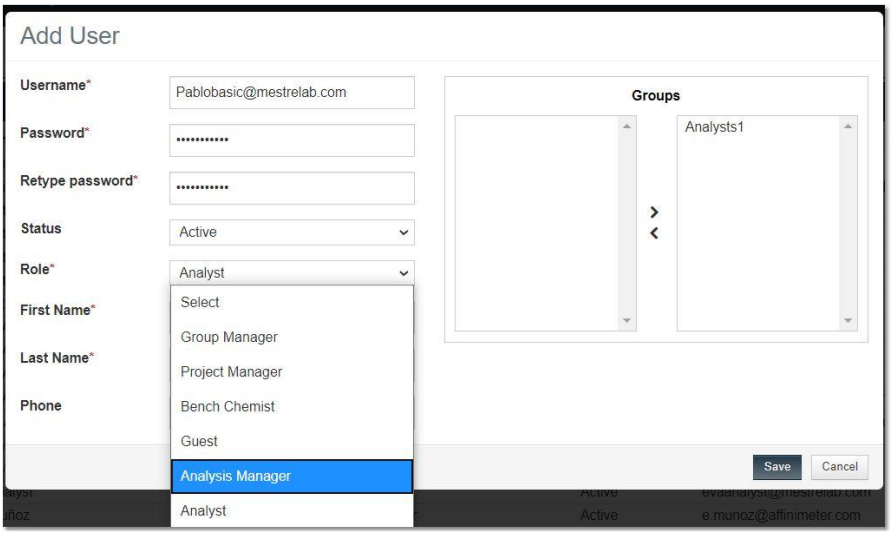
Open the Team panel with the administrator account by clicking on the Team button. There are two categories of users in Mbook Analytical: those who request analytical services, the clients, and those who provide analytical services, the analysts.



Analysts are organized into groups. You will find a list of groups on the left-hand side of the Team panel. Clicking on any group in the list will display a list of the analysts belonging to that group.
Tip: You can edit a group by double-clicking on it. You can configure analysis result visualization by clicking on the configuration button.

When creating new analysts in Mbook Analytical, you should consider two particular points:

First, you should assign your new analyst a role. Roles provide analysts with different levels of access to data.



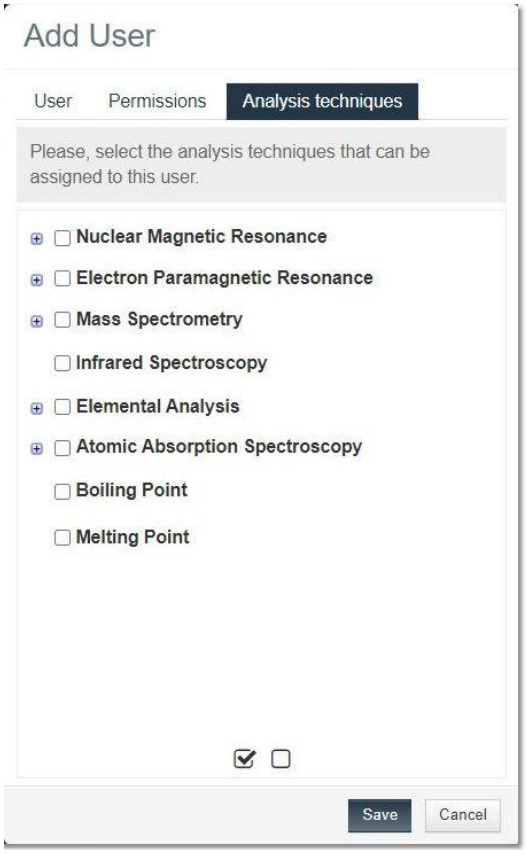
The main analyst roles in Mbook Analytical are listed below (from the highest to the lowest levels of access):

- Analysis managers, who can create users (both analysts and clients), set up the analytical laboratory (by defining the instruments and services available to analysts and clients, respectively), and manage the complete lifecycle of a request for analytical services.

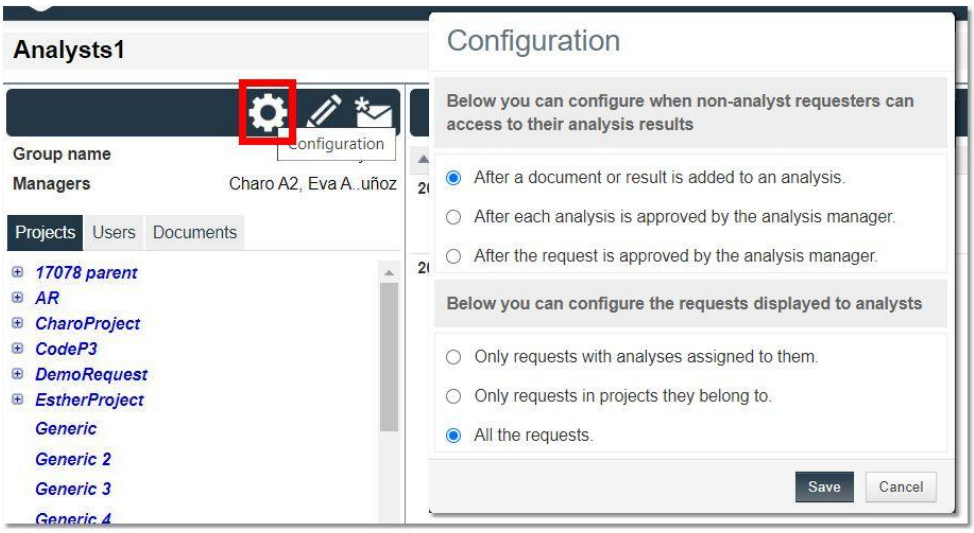
- Basic analysts, who can only process analytical services requested by clients.

Second, the **analysis manager** needs to authorize the new analyst to process a limited set of analytical services. Each analytical service requested by a client (e.g., NMR-1H) belongs to a particular type (1H), which is categorized under a technique (NMR). Analysts can only process those analytical services that belong to a type they have been authorized to deal with.

On the left-hand side of the Team panel, click on the 'Add user' button to create a new analyst and given them a basic analyst role and authorization to process any kind of analytical service from the 'Analysis techniques' tab:



The Analysis Manager can configure the requests that can be seen by the analysts (by double-clicking on the group name and selecting the configuration button):

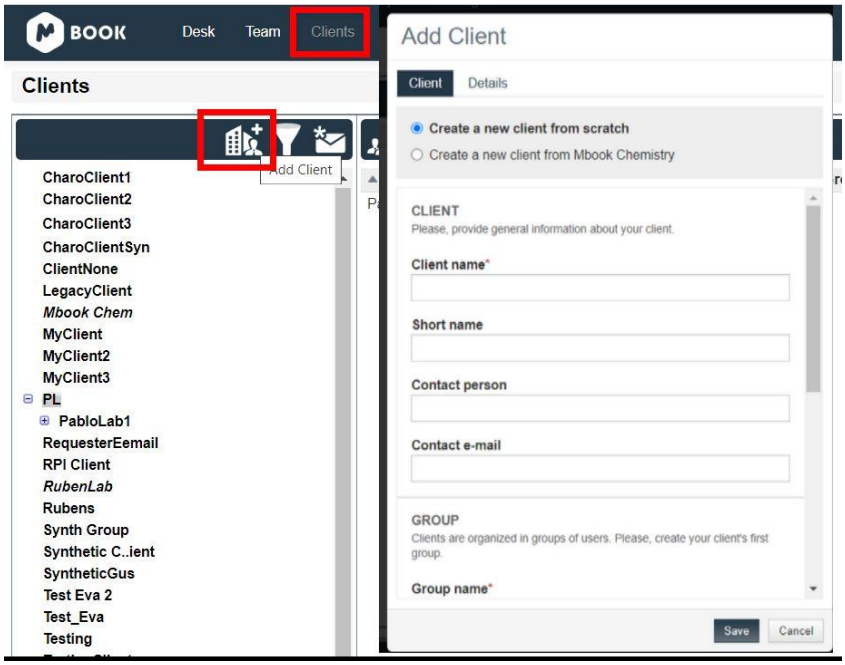


10.2 Create a client

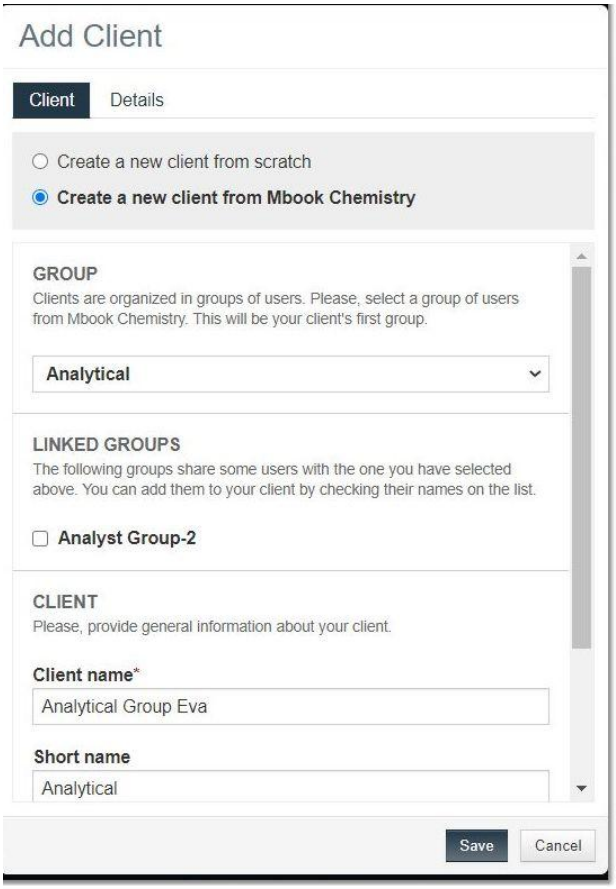
Every organization (company or institution) that requests the analytical services you provide is considered to be client in Mbook Analytical.

You can divide a client into groups (which can be created by the administrator) and include a set of users, also known as analysis requesters, in each group.

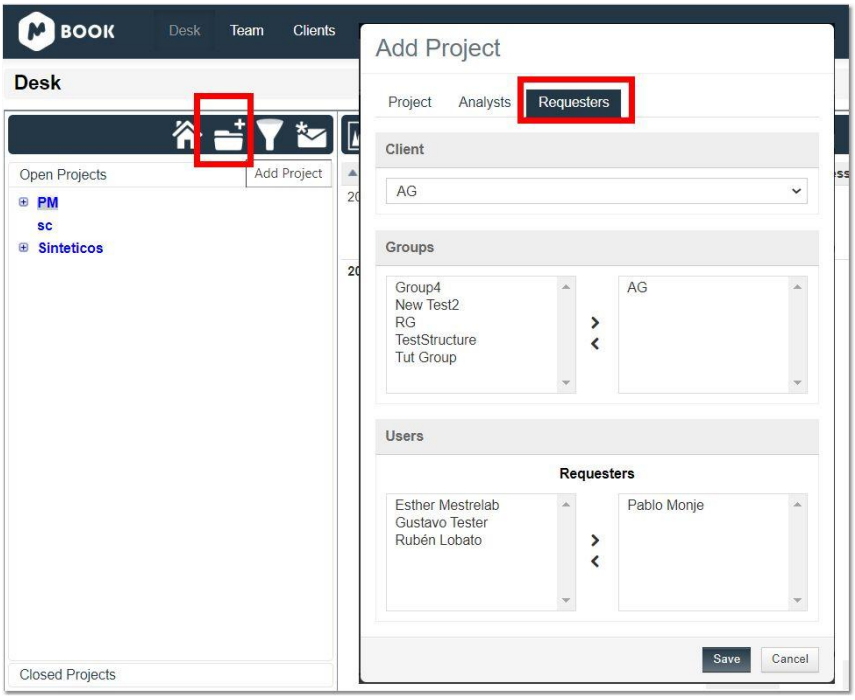
Open the Clients panel (from an Analysis Manager account) and click on the 'Add client button' to create a new client. Then, include a group, and then add a user (a.k.a. Analysis Requester) to that group:



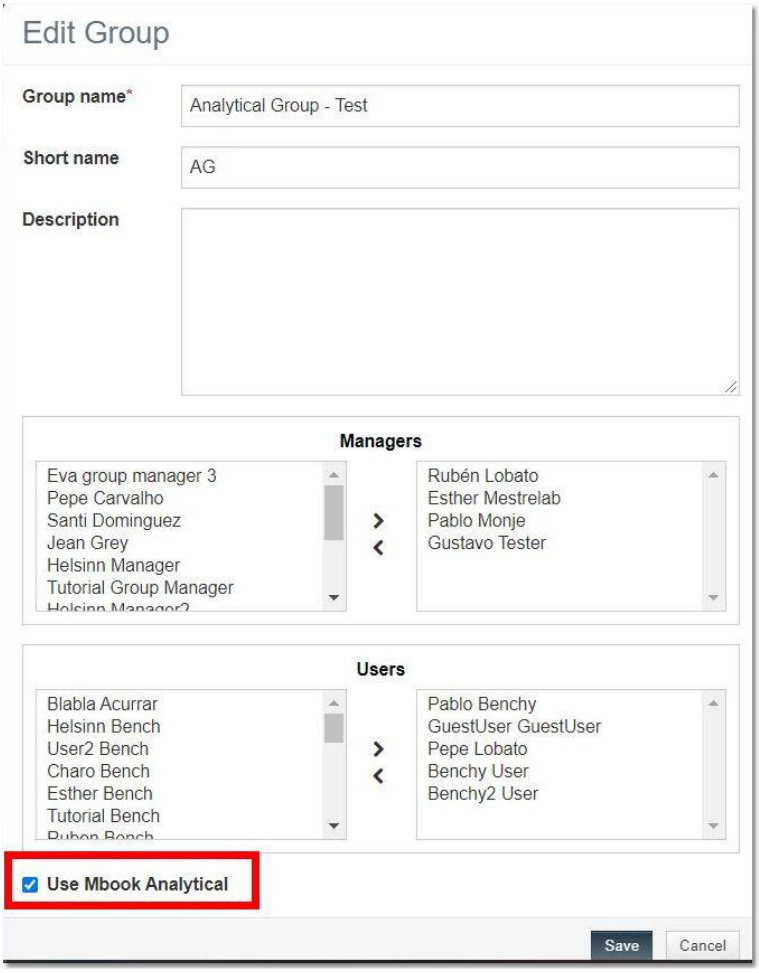
An Analysis Manager can create clients from synthetic groups with the check "Use Analytical Services" previously activated by a Group Manager. Only users within groups with "Request Author" permissions (also given by a Group Manager) will have access to the Analytical tab.



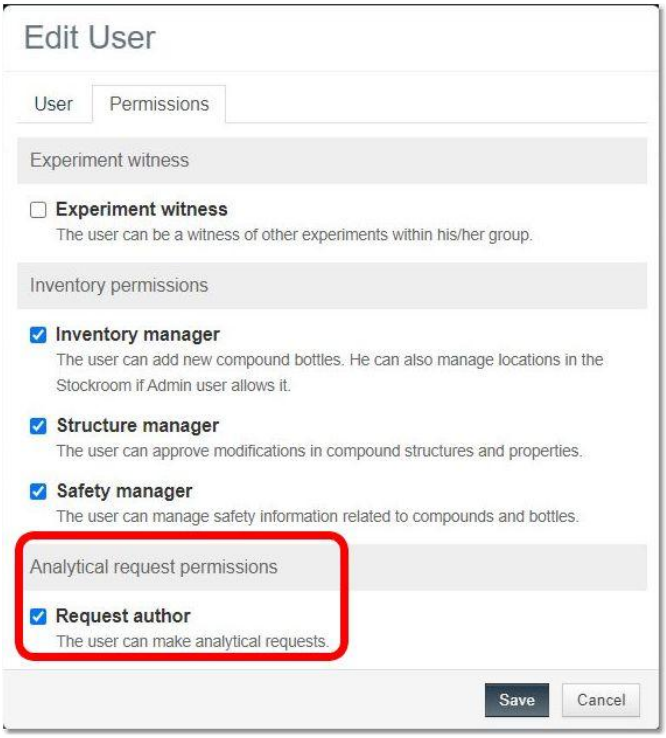
You will now need to create a new project (from the Desk panel) for the newly created client:



Ensure that the example user you created above belongs to a group with permissions to use 'Mbook Analytical':



The group manager will also need to give "requester author permissions" to each user within that group:

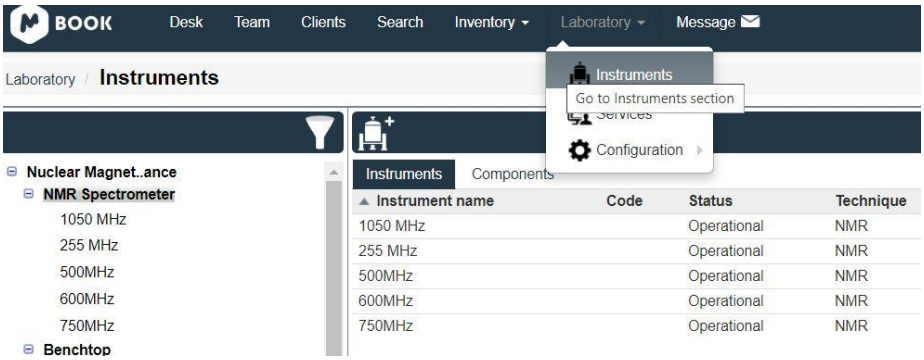


Once you are done, you will find your new client and the group it contains on the left-hand side of the Clients panel. Click on the plus button next to the group name to see a list of associated users: the user you have just created should be in this list.

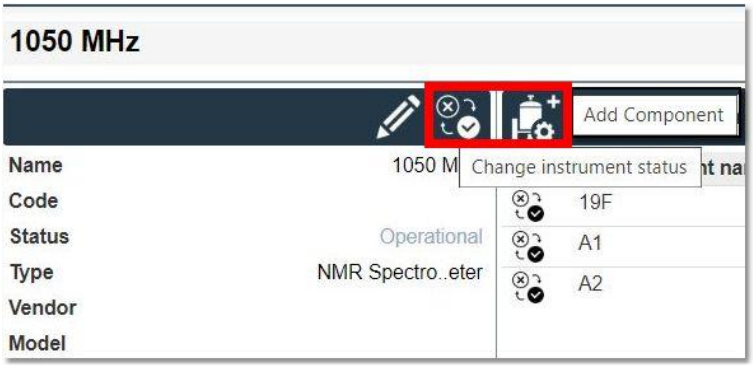
10.3 Create an instrument

You can use the Instruments panel to define which analytical instruments are available for use by your analysts. In Mbook Analytical, each instrument (e.g., a 200 MHz NMR Spectrometer) belongs to a particular type (NMR Spectrometer), which is categorized according to its associated technique (NMR).

You will find a list of analytical techniques on the left-hand side of the Instruments panel:

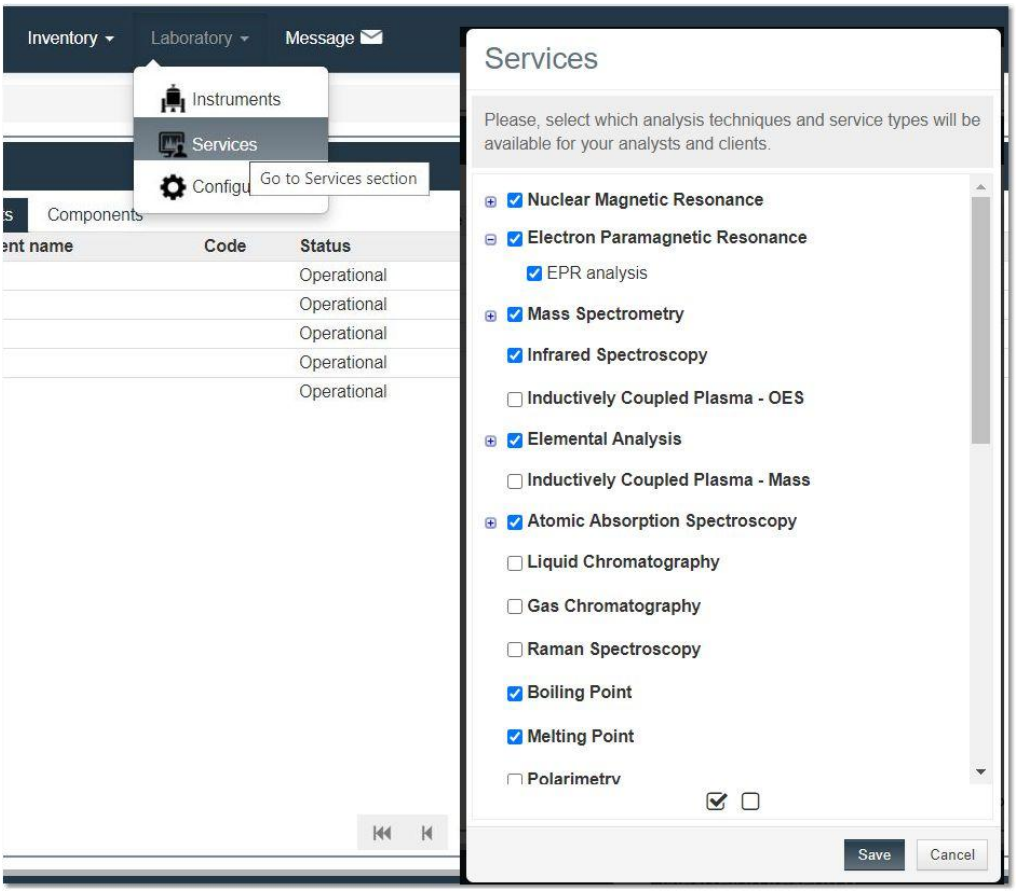


Clicking on any instrument will allow you to change its status and add components:



10.4 Define your service offer

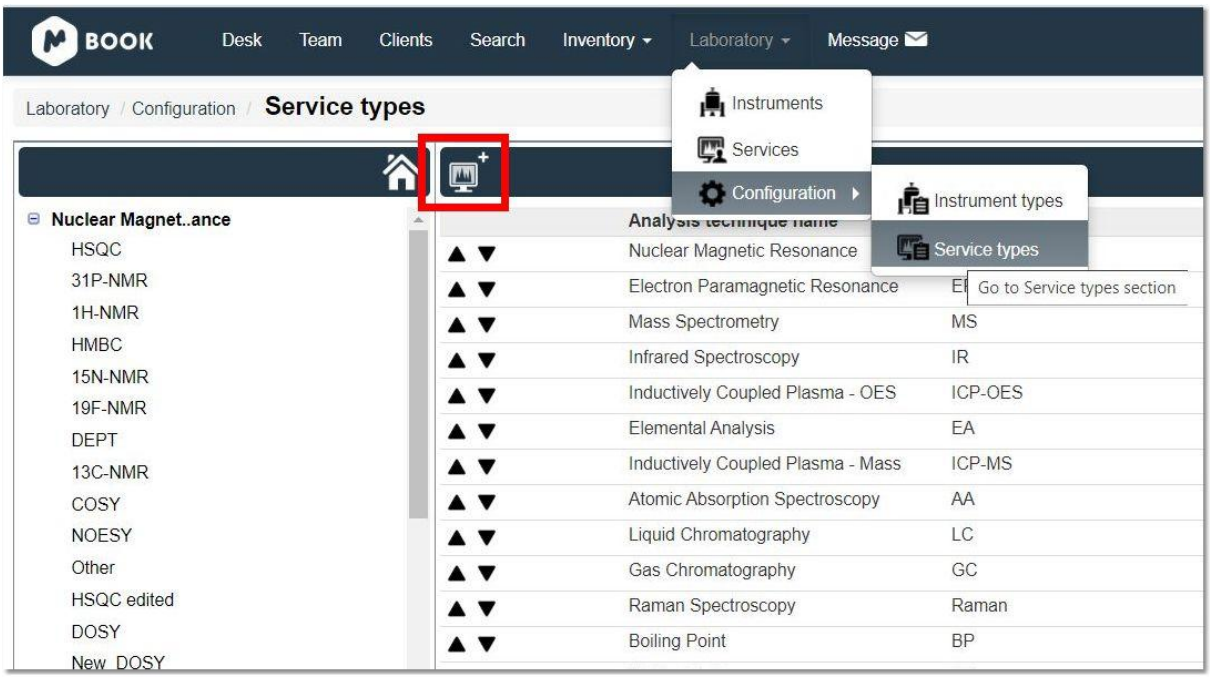
Select Services from the Laboratory scroll down menu:



You can use the Services dialog to define the range of analytical services that your clients can request from your laboratory. In this dialog, you will find a list of service types organized by analytical technique. As you may remember, each analytical service that can be requested by a client (e.g., NMR - 1H) belongs to a particular type (1H), which is categorized according to technique (NMR).

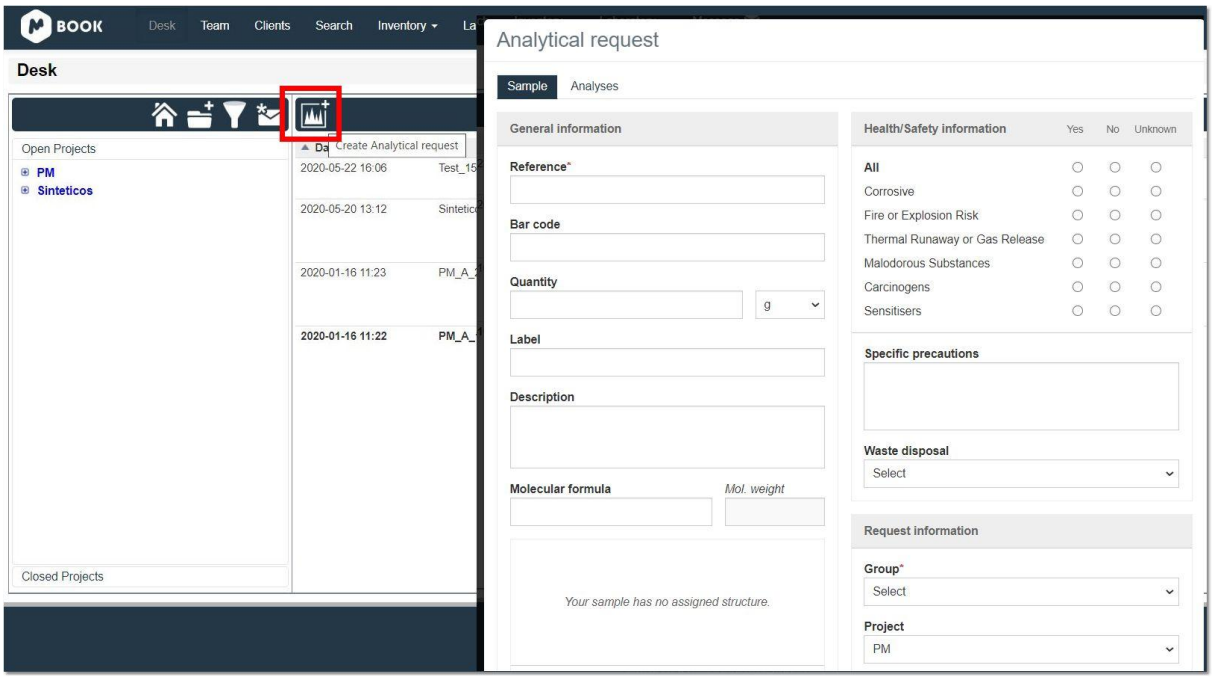
In the Services dialog, select the service types that your laboratory can provide. Your clients will only be able to request analytical services belonging to one of those selected types.

You can add new analysis techniques by selecting 'Configuration/Service Types' (from the Laboratory scroll down menu) and clicking on the 'Add Analysis technique' button:

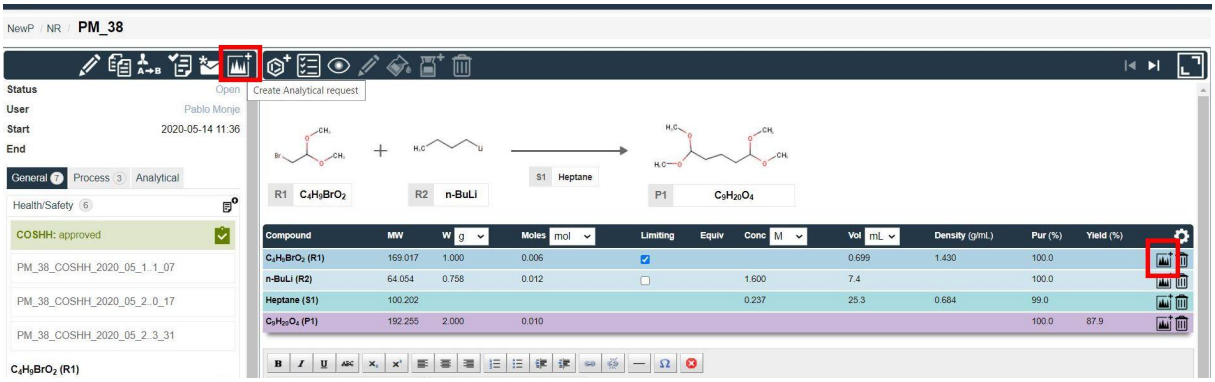


10.5 How to request a service

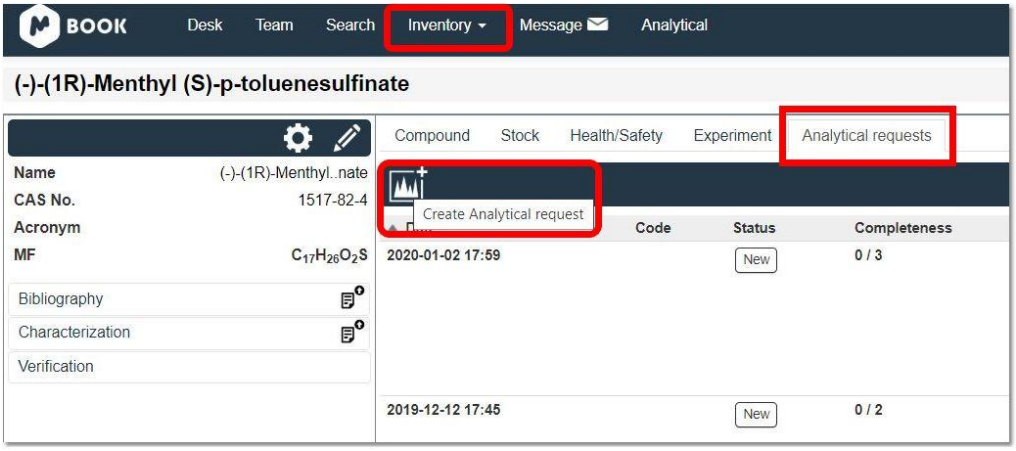
The Analysis Manager user can easily request a service from the Desk panel by clicking on the 'create analytical request' button:



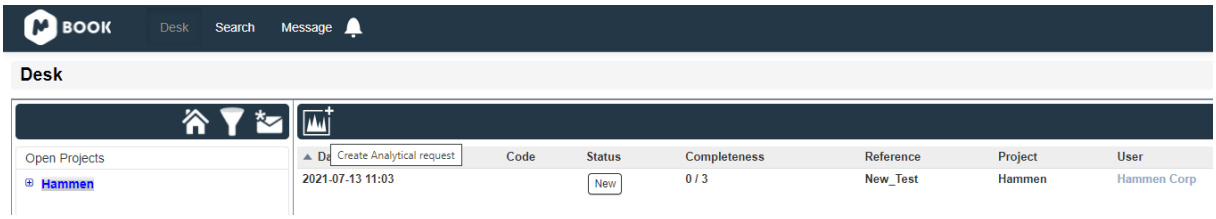
Any synthetic client with an "Analysis requester" role will be able to request a service from the experiment panel or from the stoichiometric table header:



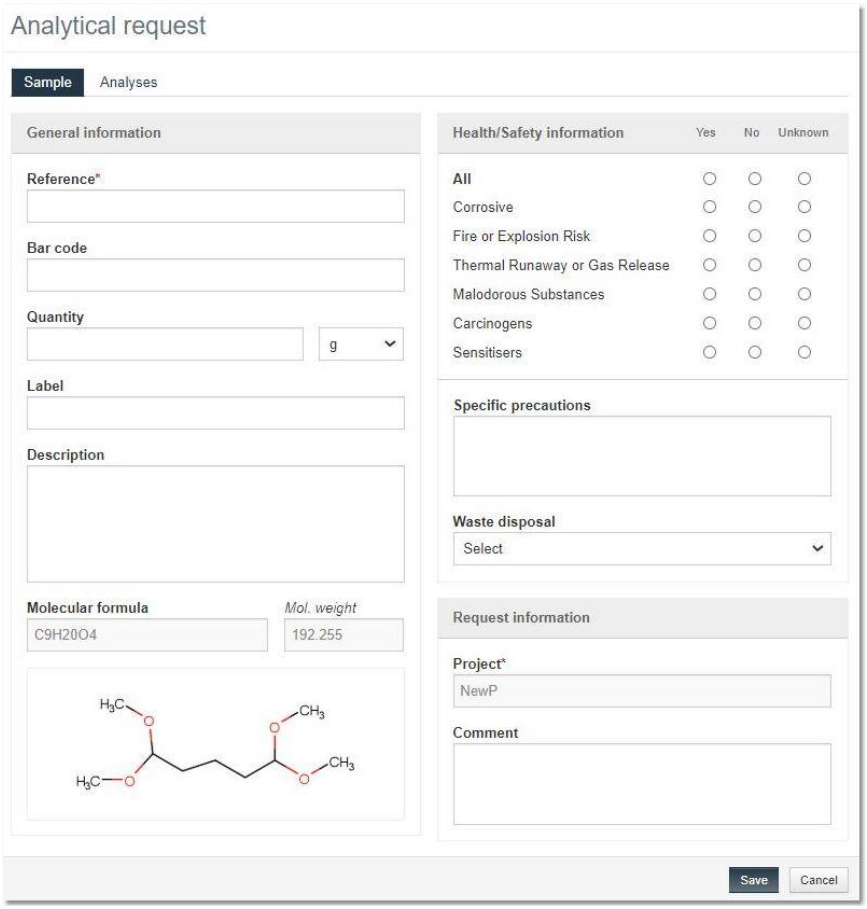
It will also be possible to request a service from the 'Inventory/Compound DB/Analytical Request' menu (after having selected the desired compound):



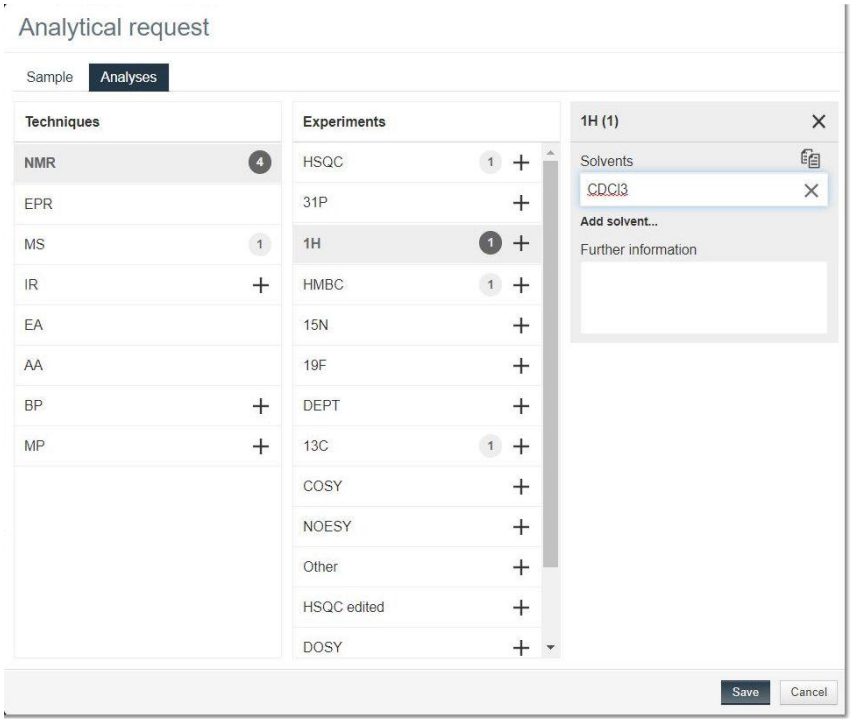
Any analytical client with an "Analysis requester" role will be also able to request a service from the Desk panel by clicking on the 'create analytical request' button:



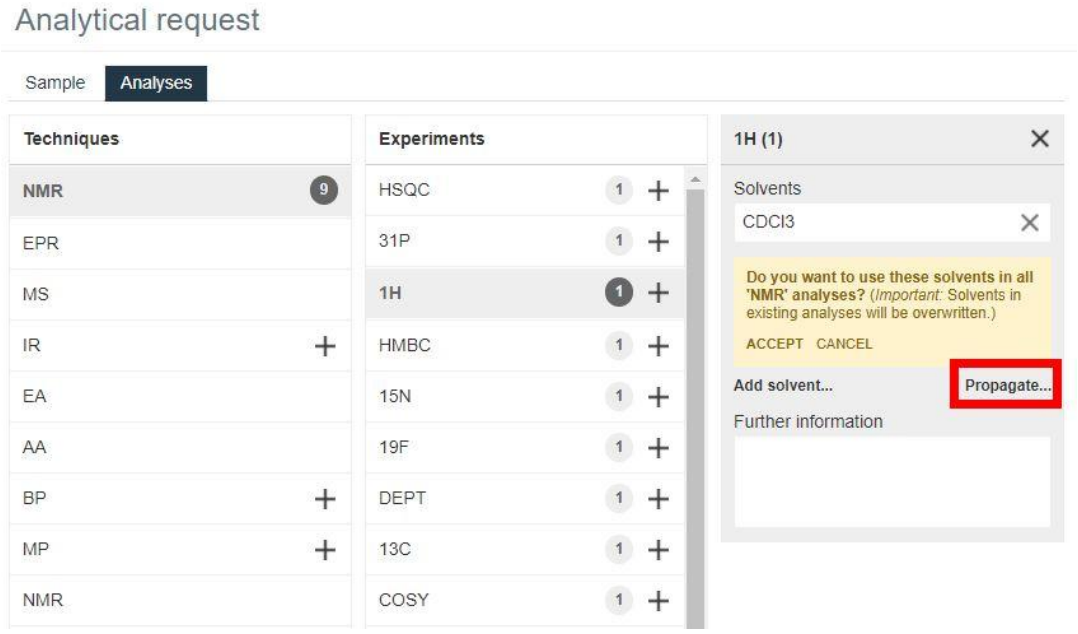
By clicking on the appropriate button, the 'Analytical Request' form will be displayed to allow you to include information about the sample:



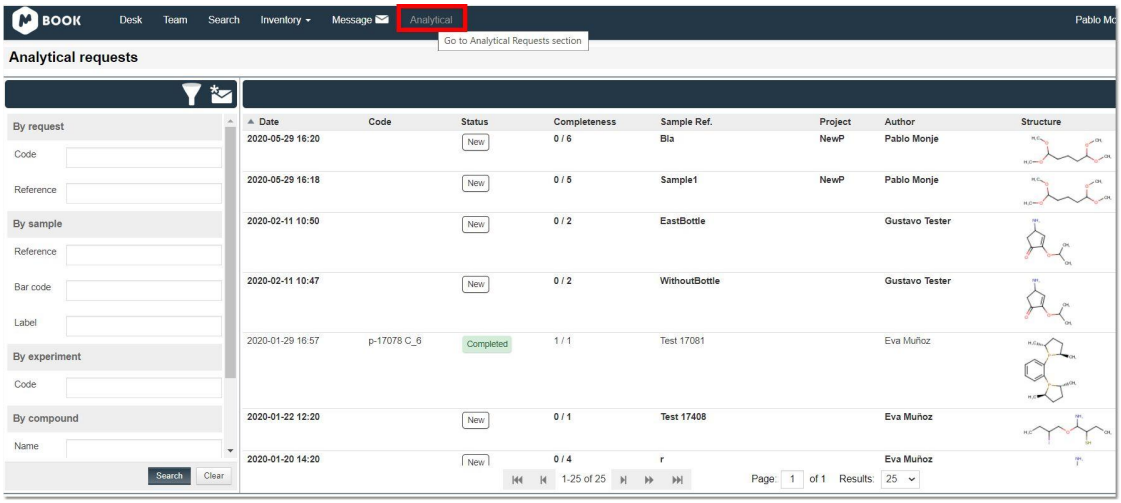
and to select the analysis that you want to request:



When adding one or more solvents to an analysis, the "Propagate" button will be displayed. By clicked on this (and accepting the warning dialog that appears), the solvent (or solvents) will be automatically propagated when adding a new analysis that uses the same technique.

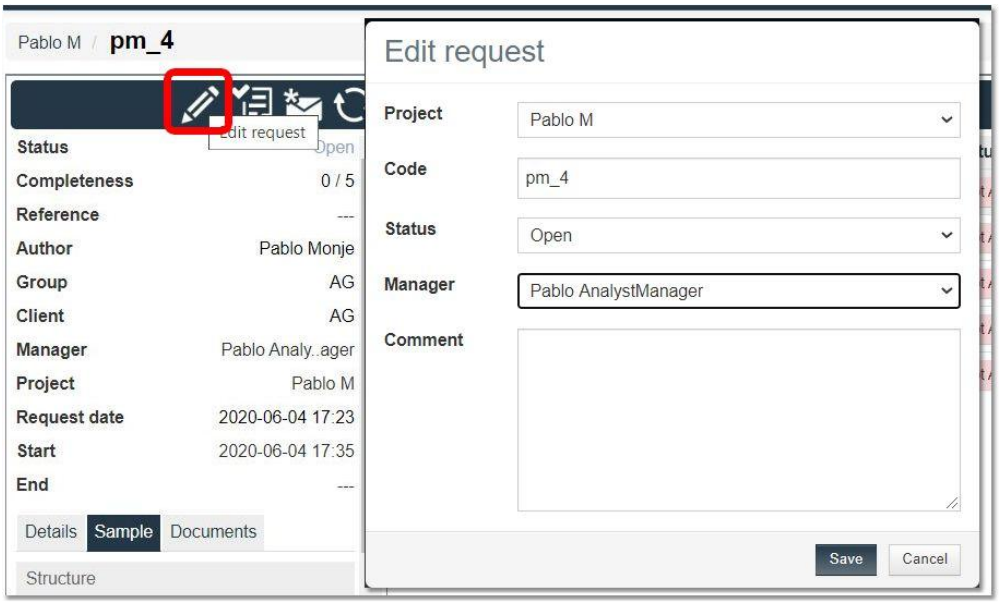


The request will appear under the Analytical menu. From this dialog box, you will also be able to search by request, sample, experiment, or compound:

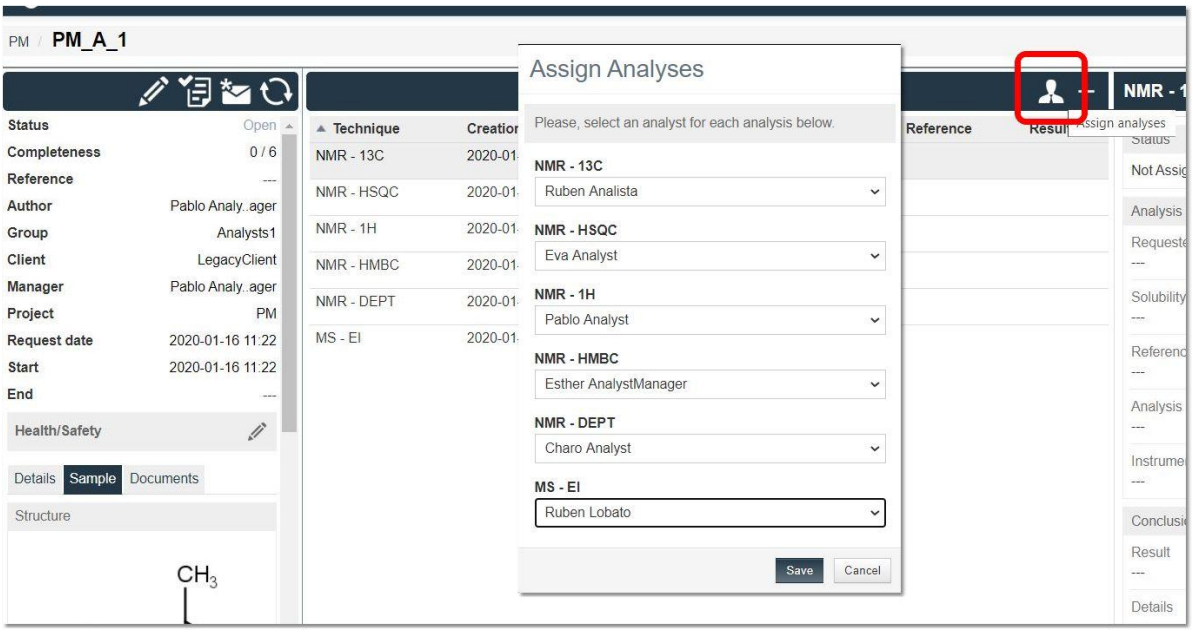


The Analysis Manager can create requests from the 'Inventory/Compound DB' tab, and from 'Desk'.

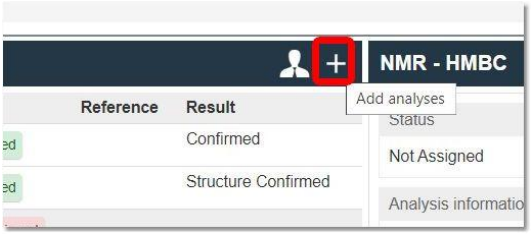
When an Analysis Manager receives a request, they will need to assign the request to a project and change the status to 'open' by clicking on the edit button:



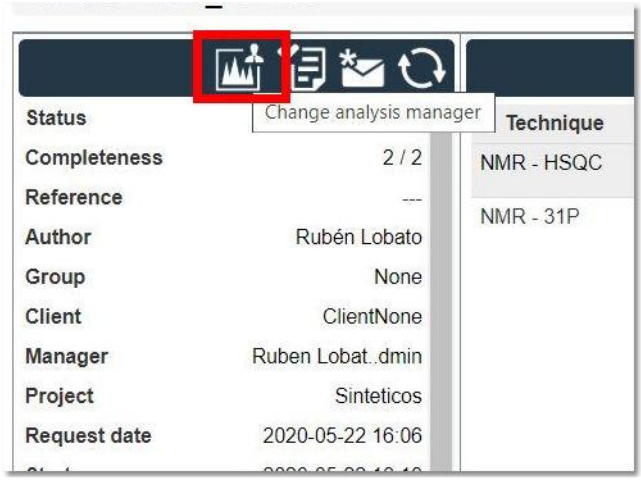
The Analysis Manager will also be able to assign each of the tests to other analysts:



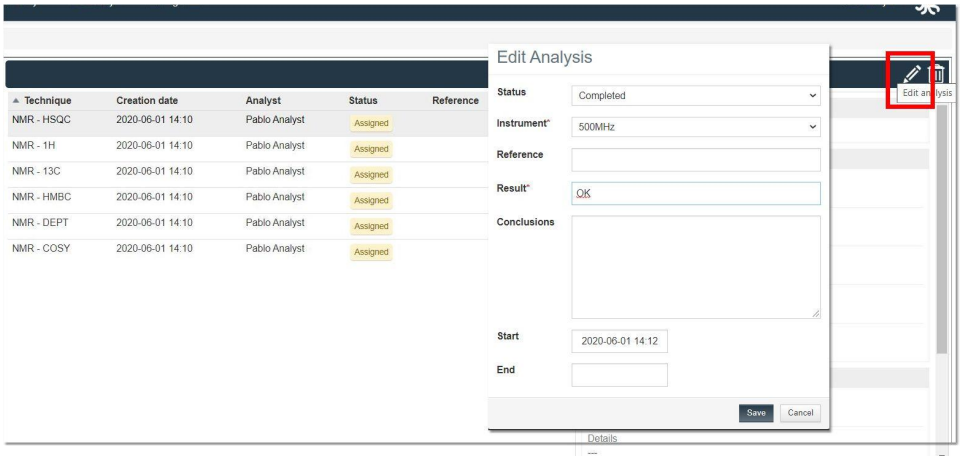
Clicking on the plus button will allow you to add additional analyses to the existing request:



The Analysis Manager associated with a particular request can be changed by using this button from the 'request panel':

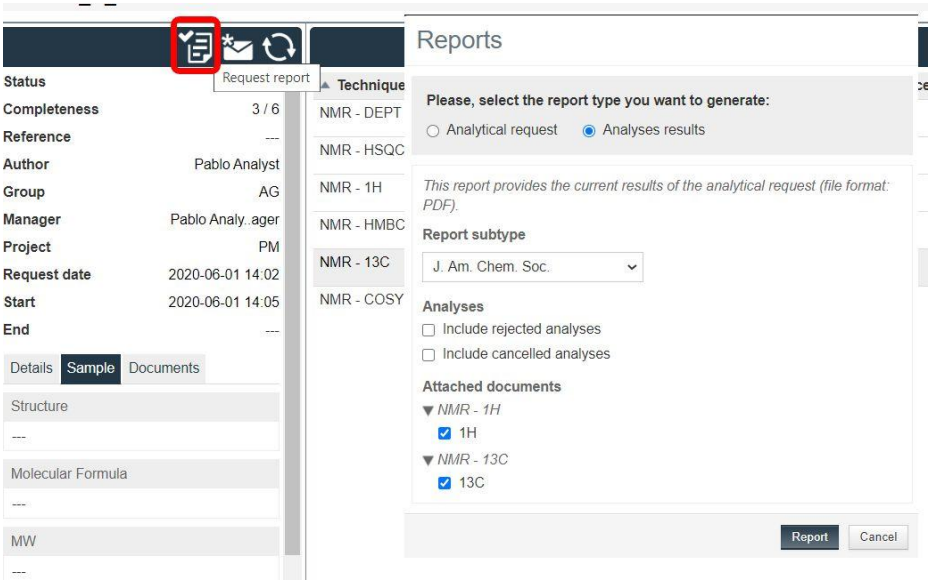


The analyst could edit the status of the request by clicking on the 'Edit request' button (clicking on the bin icon will cancel the request):

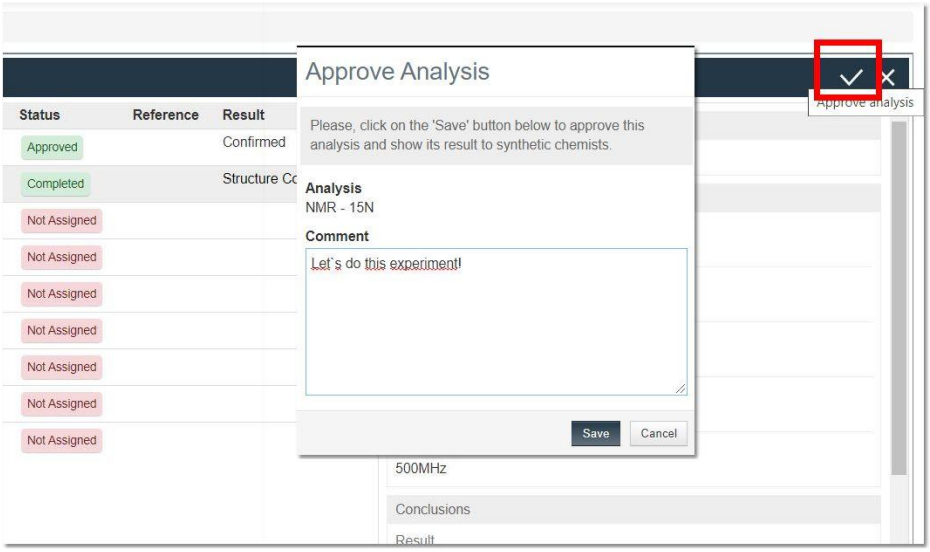


Scrolling down the panel will allow you to attach documents to the results:

Clicking on the 'request report' button will generate a PDF with the 'analytical request' or 'analyses results':

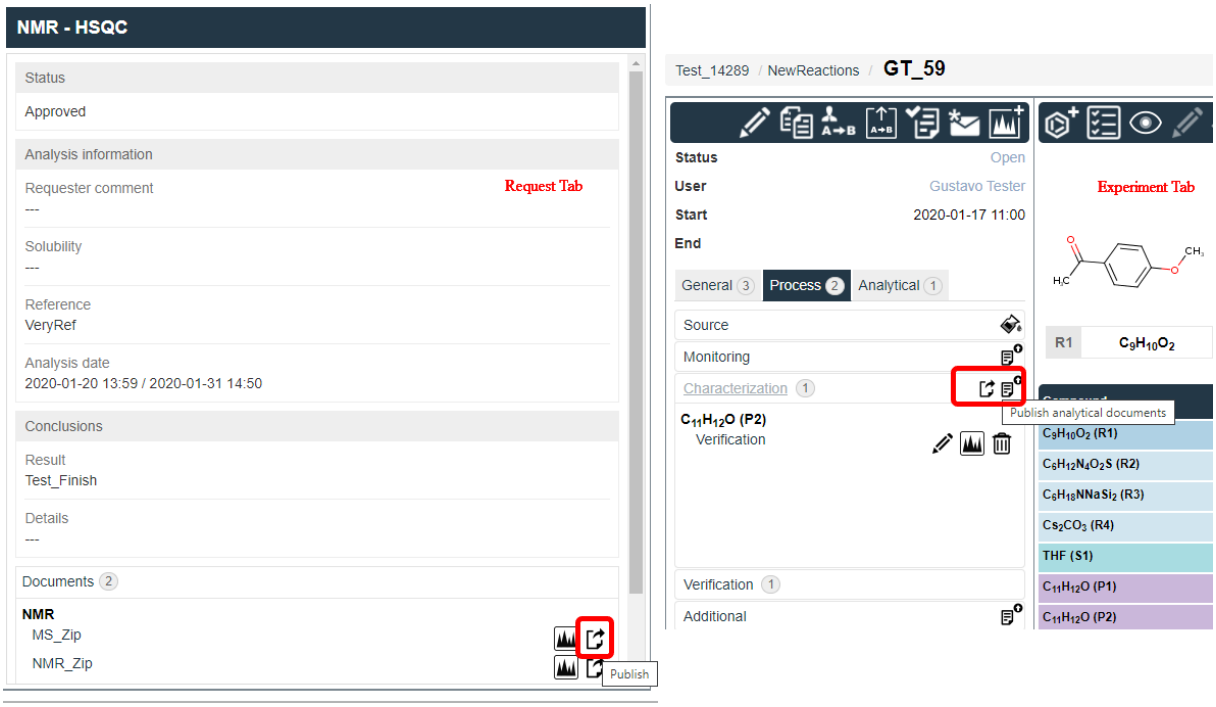


The Analysis Manager can approve or reject an analysis and include a comment after clicking the appropriate button:



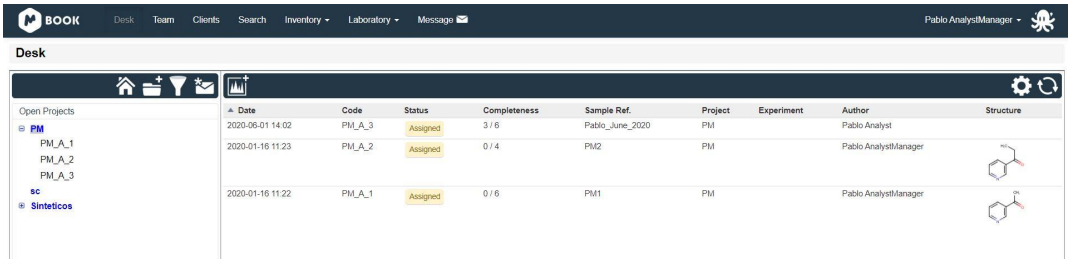
Once the request is approved by the Analysis Manager, a confirmation email will be sent to the request originator.

A chemistry user can decide to publish (or not) their analytical results under the process tab of their experiments by clicking on the button to Publish their analytical documents (Option available under experiment or request tabs):

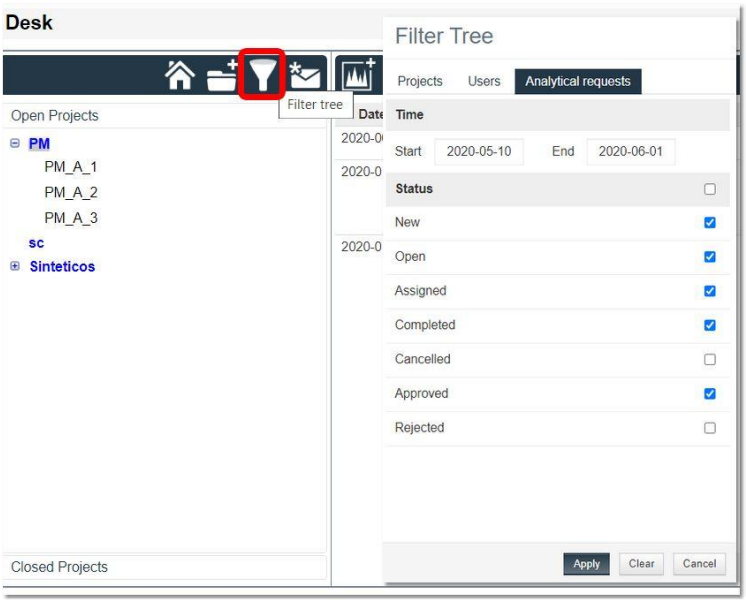


10.6 Search Requests

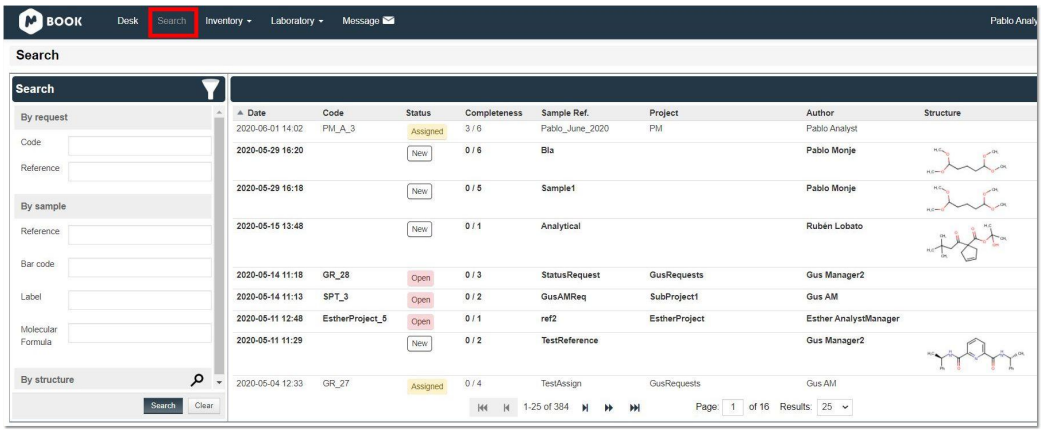
The Analysis Manager can use the Desk panel to display the requests for each project. Clicking on any of the projects will display the requests belonging to that particular project:



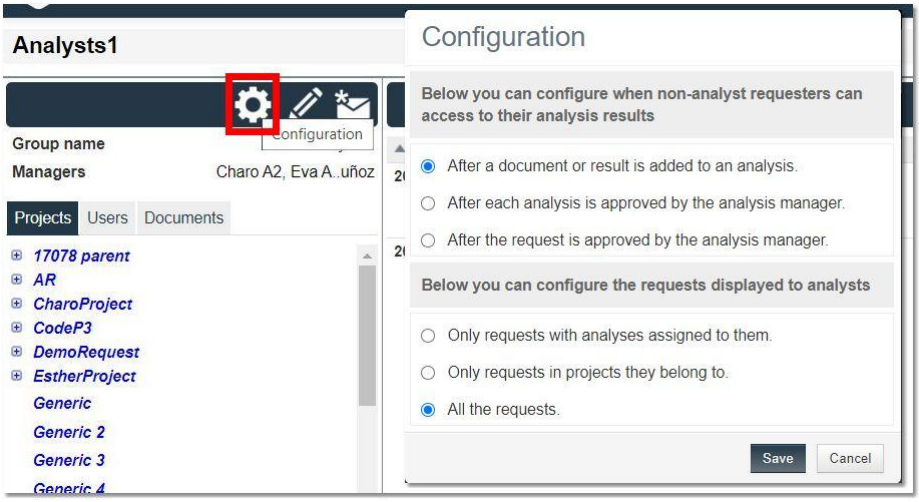
You can use the filter tree from the Desk panel to filter your analytical requests by time period or by status:



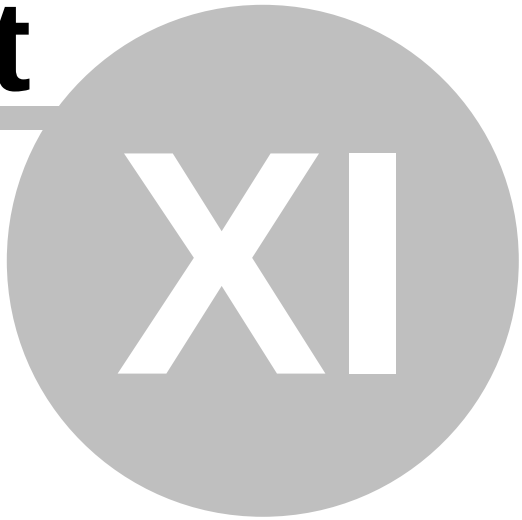
You can also use the Search tab to search the requests according to different fields:



You can configure the analysis result visualization by double clicking on the group name and selecting the configuration button:



Part



11 Further information

More information: http://resources.mestrelab.com/category/resources-by-product/resources-mbook-resources-by-product/
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