This is the manual of Mbook
Mbook Manual

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Part I
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 of any type of information related to your chemistry: reaction graphical representation, 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 set up 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 preexisting structures/information

1.1 Definitions

- **Groups**: Set of users which will carry out a project.
- **Projects**: Tasks created by privileged roles that contain a set of reactions.
- **Reactions**: Set of experiments inside a project.
- **Experiments**: Each one of the tests run generally by the Chemist inside 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 (in black) with the applicable reaction scheme:
- **Inventory**: Set of compounds, stockrooms and suppliers.
2 Starting with Mbook

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

After having typed the applicable username and password, you will enter to the GUI:
3 Users and Groups Configuration

Before you start creating users and groups we strongly recommend you to read below the description of the four types of users within Mbook ELN.

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

3.1 User Roles

Mbook provides several levels of access through user roles, limiting access depending on the position occupied by the individual user (Administrator, Group Manager, Project Manager, Bench Chemist and Guest).

Here you can find the list of permissions sorted by role:

<table>
<thead>
<tr>
<th>Role</th>
<th>Group Manager</th>
<th>Project Manager</th>
<th>Bench Chemist</th>
<th>Administrator</th>
<th>Guest</th>
</tr>
</thead>
<tbody>
<tr>
<td>Manage users</td>
<td>✓</td>
<td></td>
<td></td>
<td>✓</td>
<td>x</td>
</tr>
<tr>
<td>Manage groups</td>
<td>✓</td>
<td></td>
<td></td>
<td></td>
<td>x</td>
</tr>
<tr>
<td>Assign structure, inventory &amp; safety managers</td>
<td>✓</td>
<td>x</td>
<td>x</td>
<td>✓</td>
<td>x</td>
</tr>
<tr>
<td>Assign witness power</td>
<td>✓</td>
<td></td>
<td></td>
<td></td>
<td>x</td>
</tr>
<tr>
<td>Manage projects</td>
<td>✓</td>
<td>✓</td>
<td></td>
<td></td>
<td>x</td>
</tr>
<tr>
<td>Approve changes in structures</td>
<td>✓</td>
<td>✓</td>
<td>x</td>
<td>x</td>
<td>x</td>
</tr>
<tr>
<td>Assign users to projects</td>
<td>✓</td>
<td>✓</td>
<td>x</td>
<td></td>
<td>x</td>
</tr>
<tr>
<td>Approves experiments</td>
<td>✓</td>
<td>✓</td>
<td></td>
<td></td>
<td>x</td>
</tr>
<tr>
<td>Manage reactions &amp; experiments</td>
<td>✓</td>
<td>✓</td>
<td></td>
<td>x</td>
<td>x</td>
</tr>
<tr>
<td>Witness experiments</td>
<td>✓</td>
<td>✓</td>
<td></td>
<td></td>
<td>x</td>
</tr>
<tr>
<td>See projects, reactions &amp; experiments</td>
<td>✓</td>
<td></td>
<td>if part of the project</td>
<td></td>
<td>x</td>
</tr>
</tbody>
</table>

**Administrator:**

This role is for authorised 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 don’t charge a license for it). The administrator has all permissions granted to Group Managers, except it cannot create or work with projects, reactions or experiments. An administrator, however, can create groups that are completely independent from each other, something a Group Manager cannot do.

If your group is small, then this role is rarely needed. This is useful for organizations that have several sites or very distinct working groups within a lab, for example separated 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 authorised user to supervise them, like stockroom or the setting up of Audit trails.

- **Group Manager:**

The Group Manager role is for team leaders with management & lab responsibilities. The group manager can create users, groups, as well as Projects, reactions and experiments. In addition, it can assign extra permissions to other users so they are responsible for inventory, safety or structures.

Witness and approval of experiments are also part of the permissions granted to group managers by default, as well as designating other users that can witness and approve too.

**NOTE:**

When a compound has associated experiments, the user could 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 also to the associated project managers. In case of closed experiments (or equivalent), they will be opened again. No automatic modification in the experiment will be done. These modifications (if any) are 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 haven’t got 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.

- **Bench Chemist:**

This is a role designed to fit chemists that have neither management responsibilities nor ownership or projects. A Bench Chemist can create reactions and experiments, but not groups or users. They can also be witnesses of experiments.
By default, Bench Chemist users will only see their own experiments in the navigation tree of the Desk panel, but this can be modified.

- **Guest:**

This role was added to Mbook in version 2.1, following several requests from Contract Research Organizations (CROs). CROs wanted to be able to prove to potential clients their expertise in certain processes or to show existing customers progress on their projects with 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 customisation 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 we mentioned, an Admin user 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 is any existing one) for the new user:
The Prefix field will be used to automatically generate the experiments codes created by the user.

GROUP MANAGER - How to create a user?

A Group Manager can also create users and groups among other duties. As you can see in the screenshot below, the Group Manager has more active tabs.

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

Please note that a Group Manager can also give privileges to any user to be an Experiment Witness, an Inventory Manager or a Structure Manager (This is something that an Admin user cannot do).

ADMIN - How to create a Group?

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

Fill in the form and add any existing managers and users.
Once you have created some groups, you will find the list of them on the left hand side. You can click on any of them to see the users associated to 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:

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

GROUP MANAGER - How to create a Group?

The Group Manager can also create a group (as we described above for the admin role):
3.3 Managing groups

Double clicking on the group name, will display the reactions of the group and will allow you to send a message to all the users or edit the current group:

Going back to the ‘Team’ panel and clicking on the ‘filter’ button will allow you to filter the information by groups shown in the panel:

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 the user details (password, status, role, etc...):
4 Creating Projects

How to create a Project?

Once the 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 has access to see and search only in the projects in which he/she is involved, and these will be the projects 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, you will get the list of them in the left panel.

Sub-projects can be created just by selecting the applicable ‘Parent Project’ in the ‘Add Project’ dialog box:

For further information about creating Projects in Mbook, please follow this link.
Part V
5 Creating Reactions and Experiments

Highlighting from the left panel any of the available projects and clicking on the applicable button, will allow you to add reactions:

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

In the example below, we have created the experiment ‘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 will be to add the information about the experiment (reagents, products, amounts of reactant, solvents and products, reaction description, etc):

You will find a toolbar to Add, Edit, Show/Hide or Delete Participants (reactant, solvents and/or products) of the experiment. Create, or assign sources and also to select the experimental conditions (temperature, time, pressure, pH or other).

Clicking on the 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 input 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 in the database for that substance (this will be faster than drawing the molecule in the molecular sketcher, so we recommend you to try to find your reactants in the database). Clicking on the Save button, will add the participant to the experiment.

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

You can also copy&paste structures from Chemdraw to Mbook using the option “Copy As: MOL Text” (shortcut Alt+Shift+Ctrl+O).
Of course, you can draw molecular structure by using the sketcher (useful if your compound is not present in the Database) or just drag&drop the mol files into the sketcher window.

The ‘Move’ mode will allow you to move an atom or a bond just by clicking&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 draw 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 about it, please follow this [link](#).

Mbook incorporates Marvin JS Sketcher. For further information about it, please use 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 will be to add another reactant (benzoyl peroxide), just by typing the applicable name in the edit box:

The solvent (CCl₄) will be added in the same way.

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

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

The next step will be to add the product. If the structure of the compound is similar with any of the reagents, you can just click&drag the structure of the reactant to the 'Product' place:
After that, the sketcher will 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 that 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 the desired fields (internal code, description, acronym, etc) and clicked 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 Resin is added to an experiment, a column Loading (mmol/g) is added to the stoechiometric table.
- Enzyme: If a compound checked as Enzyme is added to an experiment, a column Activity (U/g) is added to the stoechiometric table. No automatic calculations are done for this participant (the amount used in the experiment must be manually added by the user).
- Supported reagent: If a compound checked as Supported reagent is added to an experiment, a column Loading (wt%) is added to the stochiometric table. No automatic calculations are done for this participant (the amount used in the experiment must be added manually by the user).

- Solution: If a compound checked as 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&dropping.

Once we have drawn the experiment reaction with all the participants, let’s select the applicable amounts of reagents and solvents in the stoichiometry table.

After having input all the necessary information and formatted all the experimental procedure, we will click on the Save button:

Clicking on the ‘Show Participant’ button will allow you to show/Hide the molecule structure in the graph experiment, and also to display the participant as structure, name or both of them:

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 created bottle:

You can create links in the experimental section with 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 between the table and description. The same will happen with the volume in the case of solvents and with the amount, number of moles and yield for the products:

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

From the same 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 ‘Files’ tab, will allow you to add other relevant documentation, such as Mnova documents, the raw NMR/MS spectra in zip files, images, etc:

Once you have added the attachments, they will be listed in the applicable panel. 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 big preview of the processed spectrum will be obtained by clicking on the Preview button.

From the Preview, you could use the toolbar to ‘pan’, increase/decrease the peaks intensity or zoom in the region of interest:
You can also display the ‘Multiplets Table’ or generate a ‘Mutiplet Report’ in the journal format selected from 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 the desired changes:

Both original raw files and Mnova docs are stored in the ELN. By default, when clicking on the link, the Mnova doc gets opened. But the original raw file can also be downloading by clicking Edit and selecting the raw file from that window.

Of course, you could also attach MS spectra to your experiments:
If you have a verification license, you could check if your datasets match with your structures. See this chapter for further information.

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

You can also add PDF files under 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, import, clone or report it and send a message with the report (to any member of the same group):
Clicking on the ‘Edit Experiment’ button, will allow you to rename the experiment code, change the status (from open to closed, pending of signature or discarded), modify the start and end dates and typing ‘descriptions’ and conclusions:

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

In the ‘Experiment panel’, you will also find a button to ‘Clone’ any experiment; a very useful feature to create new experiments using an existing one as starting point (if you run again the same experiment with different conditions or if you run a new experiment which is a modified version of an existing one).
When the "Clone data" box is checked; the weight, volume and mols will get filled in the table of 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 the existing experiments:

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

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

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

5.1 Import experiments from ChemDraw

You can import experiments in CDXML format just by clicking on the applicable button (highlighted in red in the screenshot below):

After having clicked on that button, the user will be allowed to load the reaction scheme as a CDMXL file:
Another option would be to Copy&Paste the experiment from ChemDraw by using the command “Edit/Copy As: CDMXL Text” (Ctrl+D).

If the file has other format or it does not have a reaction or a recognizable structure, a warning will be shown.

**Warning**

Failed to import: Arrow not found

The detected compounds will be searchable in the compound DB and if they do not exist, the user can decide to create them.
5.2 Column Configuration

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

- Choose which column to show between equivalents and mol% (default value: equivalents).
- 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 done, columns will be the same as in previous Mbook versions.

Column configuration can be done by the Group Manager, each Project Manager or each experiment’s owner:

- If the Group Manager defines the column setup of 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 done 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 done 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 below.

![Configuration icon](image)

The “Configure columns” window will show up.

![Configure columns window](image)

There are three types of available columns:
Fixed columns that cannot be removed from the stoichiometric table (Compound, Molecular Weight, Weight, Moles and Yield).

Default columns that will initially be shown in the stoichiometric table, but 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 (Limiting Reagent 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 is defining 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 done 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.

![Group or Project Manager Icon](image)

The following window will show up.

![Column Configuration Window](image)

By clicking on the “Stoichiometric table” tab, the Group Manager and the Project Manager will be 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 done by the experiment owner”).
5.3 Searching

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

You can also type any free text as keyword (experiment code, username, etc) in the search field box.

5.4 Verification

Mbook Verify is a new developing approach for structure verification by NMR and MS.

The pharmaceutical and biotechnology industries are currently facing very significant challenges which are resulting on major organizational and operational changes. The 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 on chemical entities used to have to be carried out at an internal company level, now these same functions need to encompass the entirety of the supply chain and all partners involved in the company’s R&D effort. In addition, it is desirable to standardize data formats and data handling as much as possible, to keep tight controls on quality, particularly when compounds are being transferred between organizations and to optimize the sharing of information to maximize productivity.

A further challenge, which affects, among others, the domain of Analytical Data, 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 very large amounts of analytical data in high throughput, a bottleneck is being created by the capability of Analytical Departments to get eyes on data. In this situation, overseeing also the data and proposed chemical structures proposed by partners outside the organization, and typically received in large numbers, is becoming harder and 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 useful for chemists who need to validate decisions as to the structure corresponding to their experiments, either in single or batch mode.
5.4.1 Running Verifications

To run a verification, you would only need to have a 1H, 13C, HSQC or MS (alone or combined) associated to a molecular structure of your reaction scheme. You could upload to the characterization section; raw datasets (in a zip file) or Mnova documents. In the example below, we have uploaded a 1H and HSQC 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 also the expected purity):
After having clicked on the 'Verify' button, you will get the result:

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

See also:
Further information about Structure verification tool

5.5 Generating Reports

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

You can include in the report the spectra used for the characterization and the image (with the description):
After having clicked on the 'Report' button, a PDF will be generated with the current experiment:

5.6 Report Footer

Footers can be added to the PDF reports generated for each experiment. Footers may contain one or two signature sections, as well as a text area where warning or informative messages are displayed. Mbook provides each Group with 5 configurable footer templates. The Group Manager can customize each template, and then select which of those customized templates are available to the Group's Project Managers. Each Project Manager can select, from the customized templates made available by the Group Manager, the specific footer that will be added to all the experiment reports of the project (and its eventual subprojects). Finally, each experiment owner can decide, when generating a PDF report, whether to include a report footer or not.

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 5 footer templates available in Mook.

**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 icon below.

The report configuration window will show 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 clicking on that icon, 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 option: “This text can be customized in every project” (see picture above). 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 later on.

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

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

**Project Manager**

Each Project Manager can select, from the customized templates made available by the Group Manager, the specific footer that will be added to all the experiment reports of the project (and its
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 show up. Only the report footers previously selected by the Group Manager will be available to the Project Manager. The Project Manager can decide which one, if any, will be included in the experiment reports of the project.

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

"eventual subprojects").
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 (People) to manage the groups and the users.

From the desk, you can search for experiments by molecular structure or 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:

Add new compounds to the database, just by clicking on the applicable button:

From the left panel, you will be able to search by name, code, batch number or structure. When “available in stock” option is checked the search will only take into account those compounds with bottles 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 available bottles of the compound:

The ‘Health/Safety’ panel will allow you to check and modify the hazards and precautions assigned to the compound:
Clicking on the 'Experiment' button will display the list of experiments where the compound was used:

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

The Supplier option of 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) of your inbox:

![Message panel]

The Message panel shows by default the complete list of experiments open and the list of messages related to a user. Clicking on the ‘Home’ button will restore this original view after navigating the trees.
Part VII
7 Inventory

Many organizations choose an ELN, deploy it, get it adopted, train their users, etc. After all this effort is done, they start again with an inventory solution. Mbook comes with inventory integrated, so you deploy and adopt one application, which fulfills 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 it to Mbook 1.1.

Preliminary step: Become an inventory manager!

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

The inventory menu

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

The safety manager will be able to add hazards and the applicable pictograms to any existing compound from the ‘Health/Safety’ tab:
A practical example

Let’s go to the main menu and select Inventory/Compound DB and search “heptane” as an example:

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

As an inventory manager you can add a new entry or edit the information of any of these bottles such as description, quantity, purity, ordering date, who ordered it, etc. Then just save any changes done.
You can add new compounds to the inventory, just by clicking on the applicable button (from the compound DB):

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

Any user can go to Mbook’s desk panel and use the inventory entries to link them to an experiment. Let’s click on a recorded experiment and check the entries for heptane (or the reaction participant you prefer) by clicking on the “Assign Source” icon.
Now you can set the amount you have used of each chemical on any of the source entries.

Besides the available amount on 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 on 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 very simple manner and everything integrated in your electronic laboratory notebook.

**Warning messages**

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

- If the quantity consumed value is higher than the amount available in your bottle, you will see the following error message:

- If the quantity consumed is lower than the required as per the stoichiometric table, the warning message 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.

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 the access as an administrator (or his permission if you are an inventory manager). To do that, the admin 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 admin will be allowed to add locations as explained below.

Under this mode the Admin 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 Admin 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 Admin user cannot change locations under 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 would be to 'Add a location'.
From here, you can enter the type (Level 1 in this example), location name, description, storage conditions (see above) and also manage the 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 more levels by clicking on the 'add location' button:

You can also edit a location by clicking on the applicable button:
In this case, we will create a location in the level 3 (coldroom). You could give further restrictions and permissions for this level:

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

NOTE: If the bottle is not included in the inventory, you would 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 together to the same location, just by clicking on this button.

See also:

Resources about Inventory tool
Watch a miniclip about this functionality at this link
Part VIII
8 Experiment Witnessing, Approval and Structure Managers

Experiment Witness

Mbook includes the capability to sign experiments as witness. The Group Manager will have the capability to create and edit users with witness power just by checking the applicable box:

The group manager can allow every user to be a witness of other user’s experiments; if those experiments are accessible by the specific user.

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

After having clicked on the ‘Save button’ and selected 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 Sign (or Pending Approval), the icon for Experiment Supervision will be displayed (both for the experiment owner and witness user).

The witness will be allowed to type any comment before signing the experiment (the comment will be mandatory if the experiment is not signed):

After having clicked on the Save button; the supervision icon will disappear and the status of the experiment will turn to 'signed'. Once the experiment is signed, it can't be edited by the owner.

**Experiment Approval**

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

The group managers and project managers, can have privileges to approve experiments and to give approval privileges to other users.

The Project Manager will have the capability to create projects with 'experiment approvals' just by checking the applicable box on 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 that there is an experiment 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 will not need to do anything else).

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

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

After approval, experiment state changes to "Approved", and the experiment owner will receive a notification. After the experiment is approved, it can't 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 that decided to check the experiment.

**Structure Managers**

By default, Group and Project managers will have the “Structure manager” permission.
Any user could modify a compound created by himself (if it was created by another user, it can not be changed) which is only present on his experiments. Only a message informing about that change will be displayed:

![Warning](image)

However, if the compound is present in experiments belonging to different users, the user will need an approval from the structure manager to modify the applicable compound. Once the user tries to edit the compound, an approval request (by message) to all the structure managers will be sent (only one approval will be needed):

![Warning](image)

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

![Structure](image)

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

![Entity Link](image)

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 also to the applicable project managers (informing about the approval).
In case of closed experiments, they will be opened automatically but no modifications in the stoichiometric table will be applied.

**Safety Managers**

This user can manage safety information related to compounds and bottles. The group manager will be allowed to assign this permission to any existing user (except guests):

**Inventory Managers**

This user can manage locations in stockroom (If administration user allows it) and also add or edit compounds bottles in **Stockroom** section:
9 Further information

More information: http://resources.mestrelab.com/category/resources-by-product/resources-mbook-resources-by-product/
Support: http://mestrelab.com/learn-support/
Thank you!

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

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

support@mestrelab.com

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