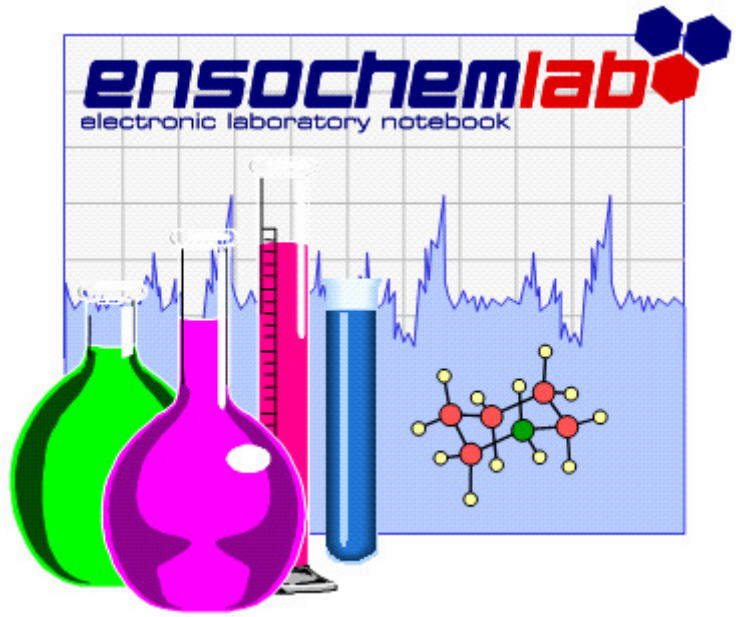
ensochemLab

Version 6.0

Tutorial
(Users Guide)



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Content

1. Overview

This user manual offers useful information concerning the daily use of the electronic laboratory notebook ‘ensochemLab’ to novices as well as to experienced users.

ensochemLab has been designed for the use in the professional area and enables you to work smarter and more comfortably.

This guide will show you how you can use the application as efficiently as possible and which features you can use to simplify your daily duties.

The manual has been written as a step-by-step introduction, but can also be used as a reference manual.

We recommend performing all steps explained herein once before you start your actual productive work with ensochemLab.

Each chapter is closed by a short summary that outlines the specific topic’s most important facts and can also be seen as an overview over the chapter. At some positions within the documentation, you can find “Remarks” sections in boxes. These sections are not indispensable for explaining the topic, however, can provide some useful information and help especially in case of problems.

When you are only interested in the new features of the current version, you can find a list containing the most important changes and new features in the “Release Notes” document or on our web page.

If you encounter a word or phrase from the world of computer software that you are not familiar with, you can look it up in the glossary (located in appendix A):

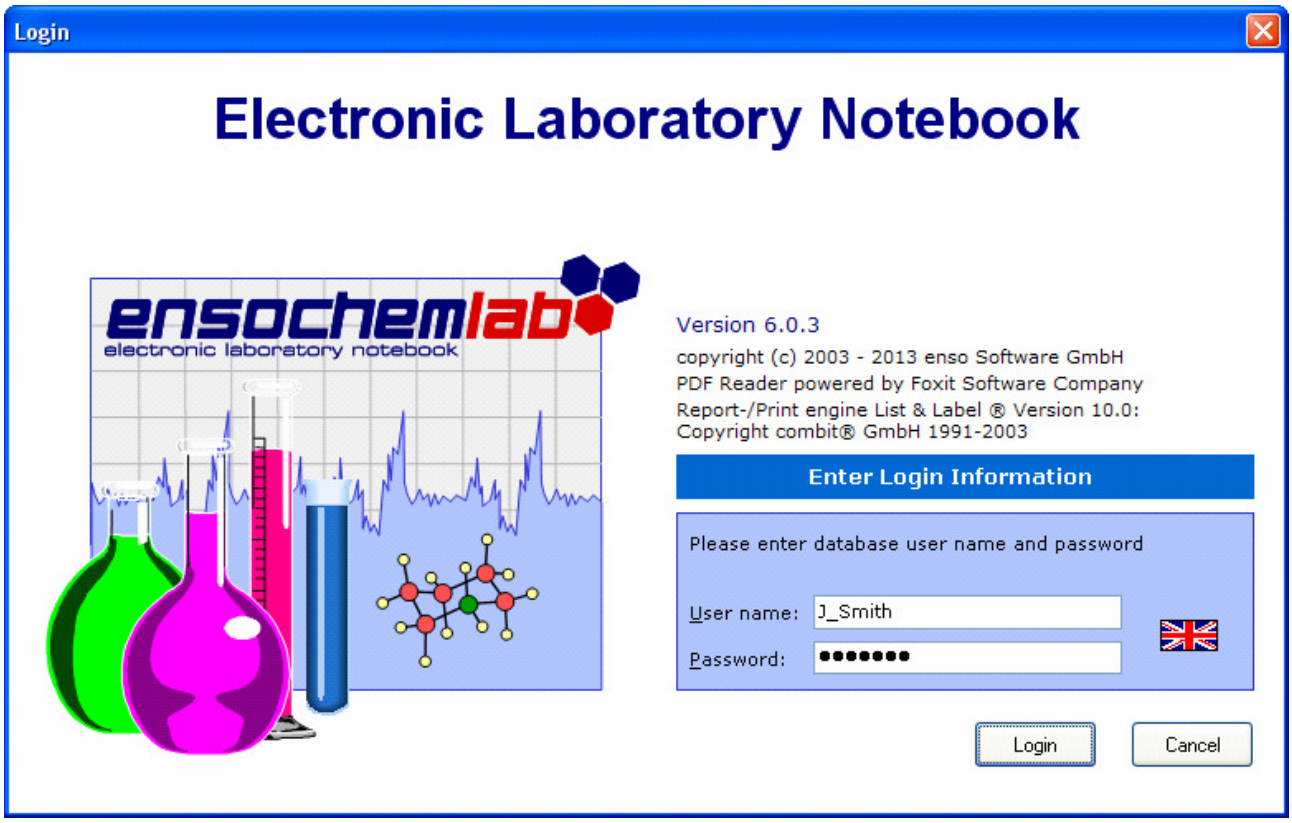
Thank you for choosing products from enso Software GmbH.

2. Login

To start the program, click on the Windows “Start” button in your desktop’s taskbar. Then select “Programs” \ “enso Software GmbH” \ “ensochemLab”, and last but not least, “Start ensochemLab”. Alternatively, you can do it even faster by double-clicking on the icon on your desktop.

Before you can use ensochemLab, you have to log in. This authenticates you against the database system and sets your privileges within the application.

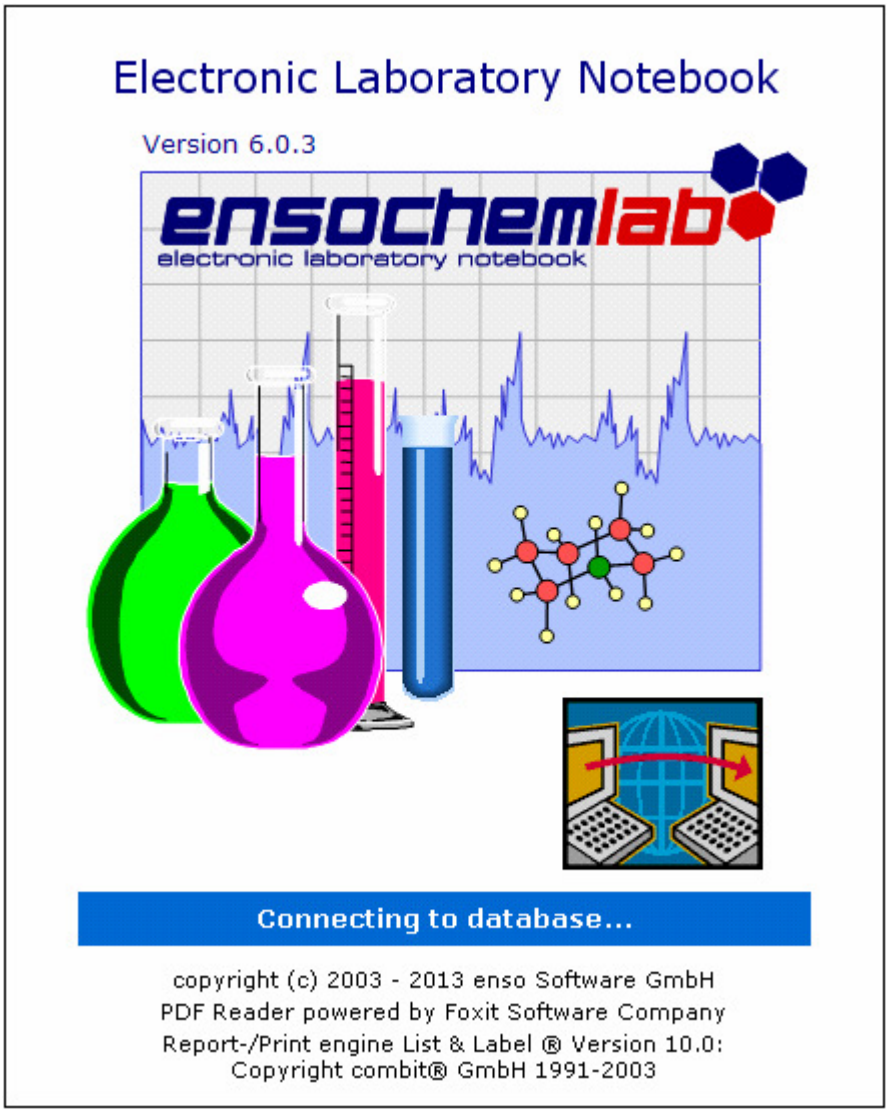
Directly after ensochemLab is started, it will check if your current database system requires you to enter username and password for logging in. If this is the case, the following window is displayed:



The “Username” field is predefined with your Windows login name. Check if this matches your database login name and change it if necessary. Having done so, just enter your password and click on “Login”.

Remarks:	If you are in doubt what data to enter, please contact your database administrator. Your login information does not necessary have to match your Windows account data.

If it's not necessary to enter login information, you are automatically logged in to the database with your windows user name. For this mode, you do not have to enter or confirm anything. The following window shows the current status:



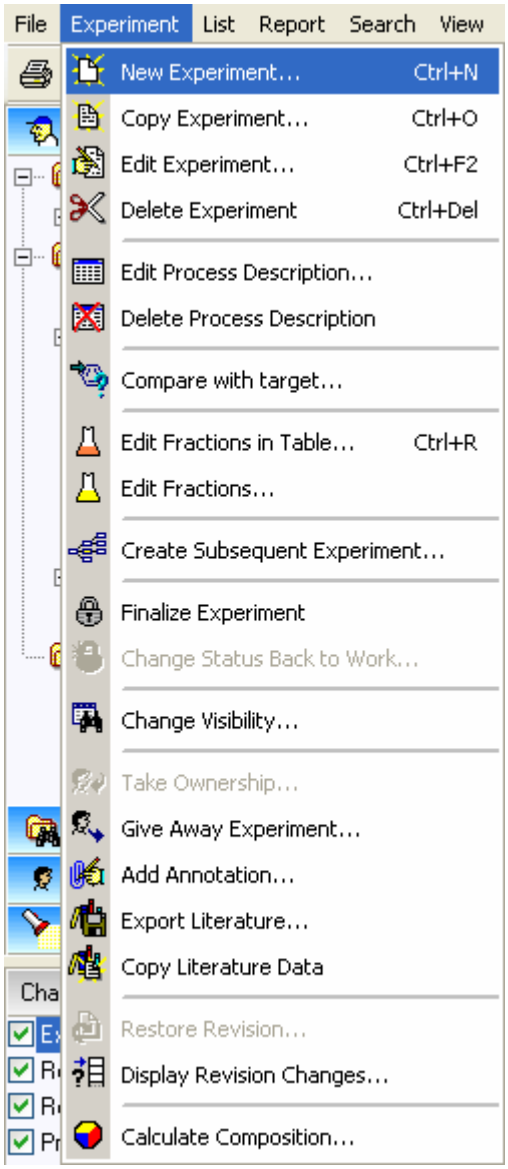
With ensochemLab Personal Edition or ensochemLab Workgroup Edition on MSDE, ensochemLab always performs an automatic logon.

Summary:	Before you can use ensochemLab, you have to log in to the database. This either happens automatically or you are prompted for username and password.

3. Create your first experiment

You are now connected to the database. This means that you can view and modify experiments. As there are possibly no experiments in your database yet, we will begin by creating a new one. Later, we will return to this position in the program and discuss the viewing options of the main window.

To create a new experiment, click on "Experiment“ in the main menu (you can find it at the top of the main window) and then on “New Experiment”:



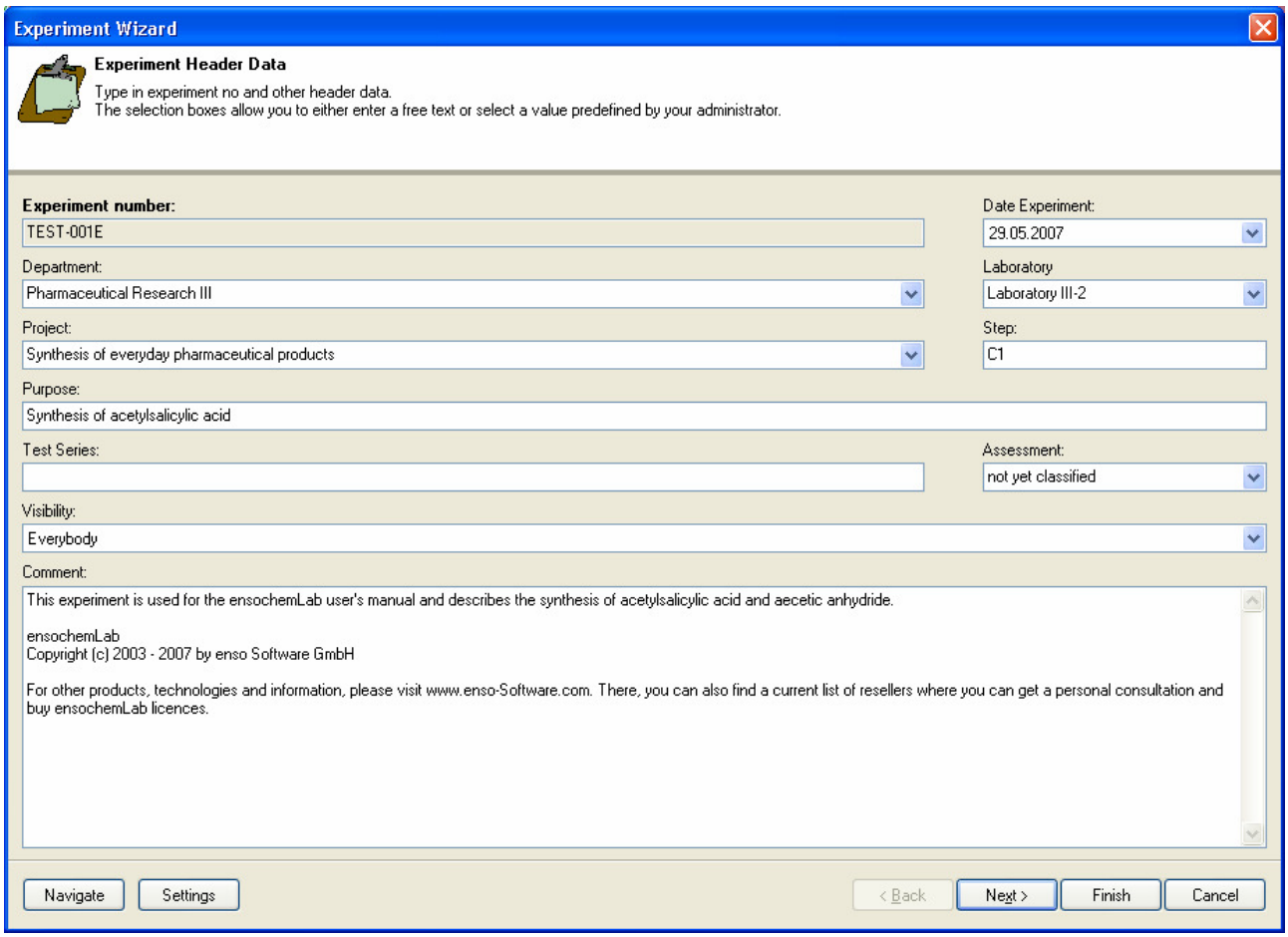
Alternatively, you can also click on the “New Experiment“ symbol ( ) in the toolbar.

ensochemLab will now open the experiment assistant that guides you through the creation of a new experiment. The assistant is divided into a number of pages that all handle with a specific topic. At the upper

side of each page, you will find a headline along with a short description that explains you what kind of data is requested below.

3.1. Header Data

The page “Header data” that is now visible is displayed first. Here you can enter general data for your new experiment.



The experiment number always has to be specified. You cannot save an experiment without an experiment number. Furthermore, it has to be unique, this means if you choose an experiment number that exists already, and you will get an error message when trying to save and cannot continue until you have changed it.
Depending on you user settings, the experiment number field may already be filled with a prefix to which you only have to add a unique suffix. We will discuss this setting and how to change it in a later chapter (see chapter “Customize your settings”).

Your administrator may also have configured the system for the fully-automated generation of experiment numbers. In such a case, the respective field within the experiment wizard already contains a value. If its background is displayed in gray, the number is directly assigned and cannot be changed anymore. Otherwise, it is only a recommendation.
Please note that an experiment number is regarded as “exhausted” once it has been generated. This means that if you, for example, cancel the assistant and start it once again, this number cannot be generated any more. The only way of using it is to manually enter it if you are allowed to do so. You can avoid this problem by saving the empty experiment as a template for future use.

The “Visibility“ setting is only available if your administrator has enabled the default ensochemLab user administration. With it, you can specify which users shall be allowed to view your experiment. The possibilities are:

Visibility	Meaning
Everybody	Every ensochemLab user can view your experiment without restrictions
Site	All users at your site may view the experiment
Department	All users at your department may view the experiment
Laboratory	All users at your laboratory may view the experiment
Cost Center	All users with the same cost center as you may view the experiment
Private	Only you may view the experiment

These restrictions also apply to ensochemLab users. Please note that “Department” for example also includes “Laboratory” as it is a higher organizational level.

As an example, please enter the experiment data that is displayed in the screenshot above.

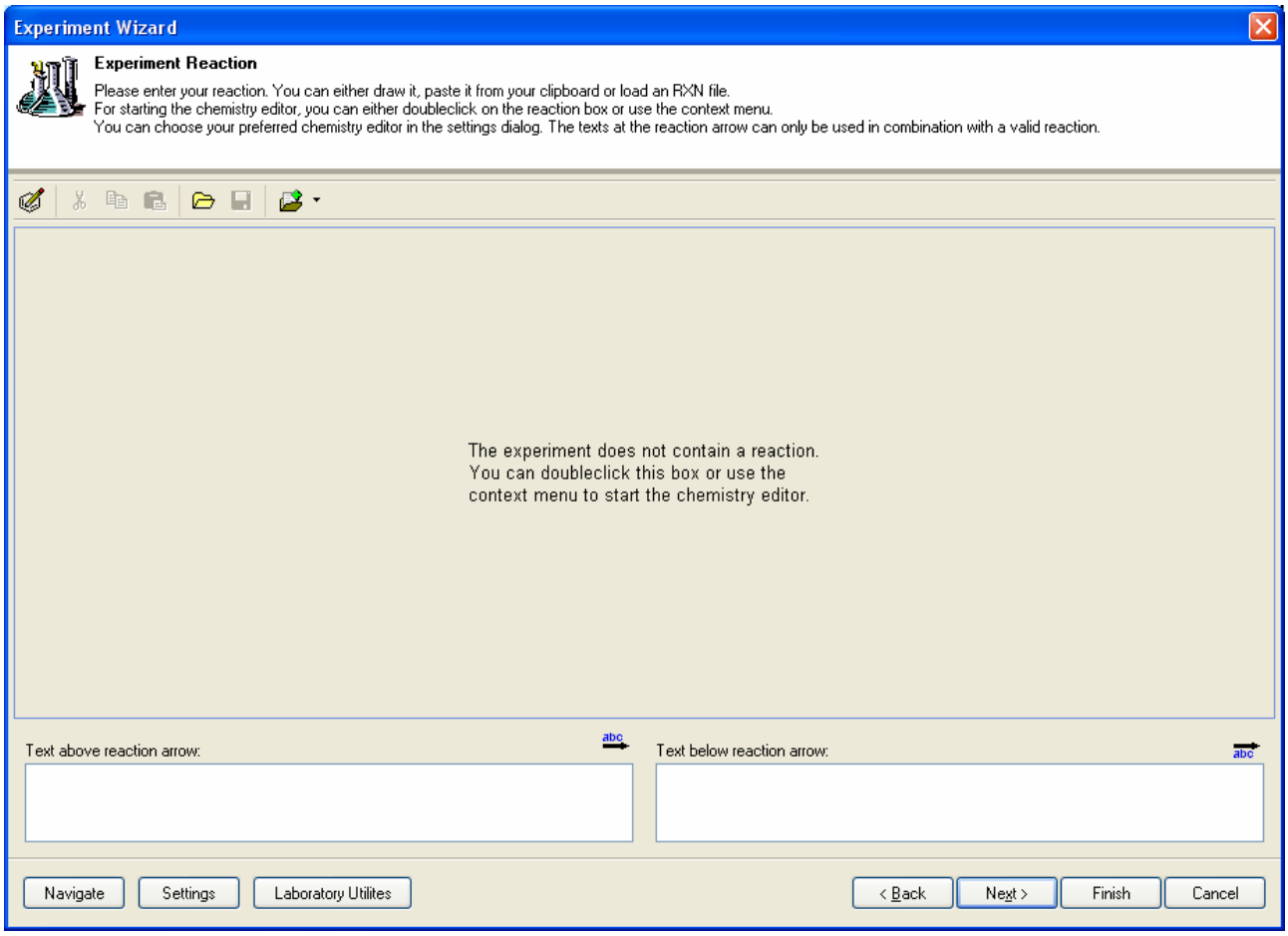
If you want to, you can also use other values. However, if you are new to ensochemLab, we recommend using these ones as we will need them again later in this manual.

Then click on “Next” to proceed with the next page in the assistant.

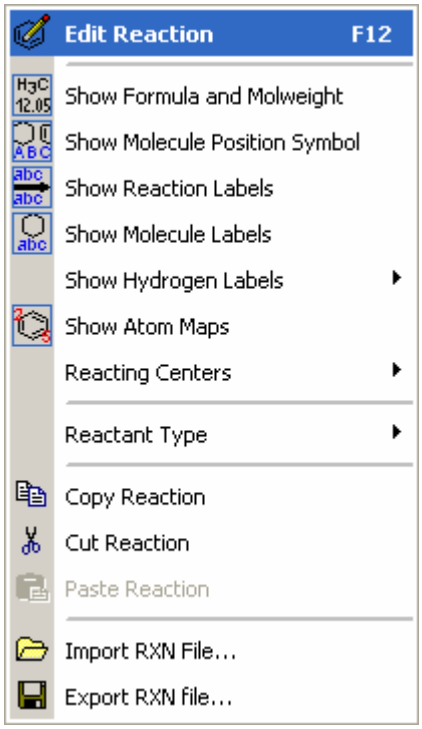
Remarks:	If you want to view a specific page, you don’t have to click on „Next“ until the page appears. You can also use the navigation box by clicking on the “Navigate” button in the lower right corner of the assistant. A window will appear where you can select the desired page.

3.2. Reaction

The next page in assistant mainly consists of a huge grey and empty field:

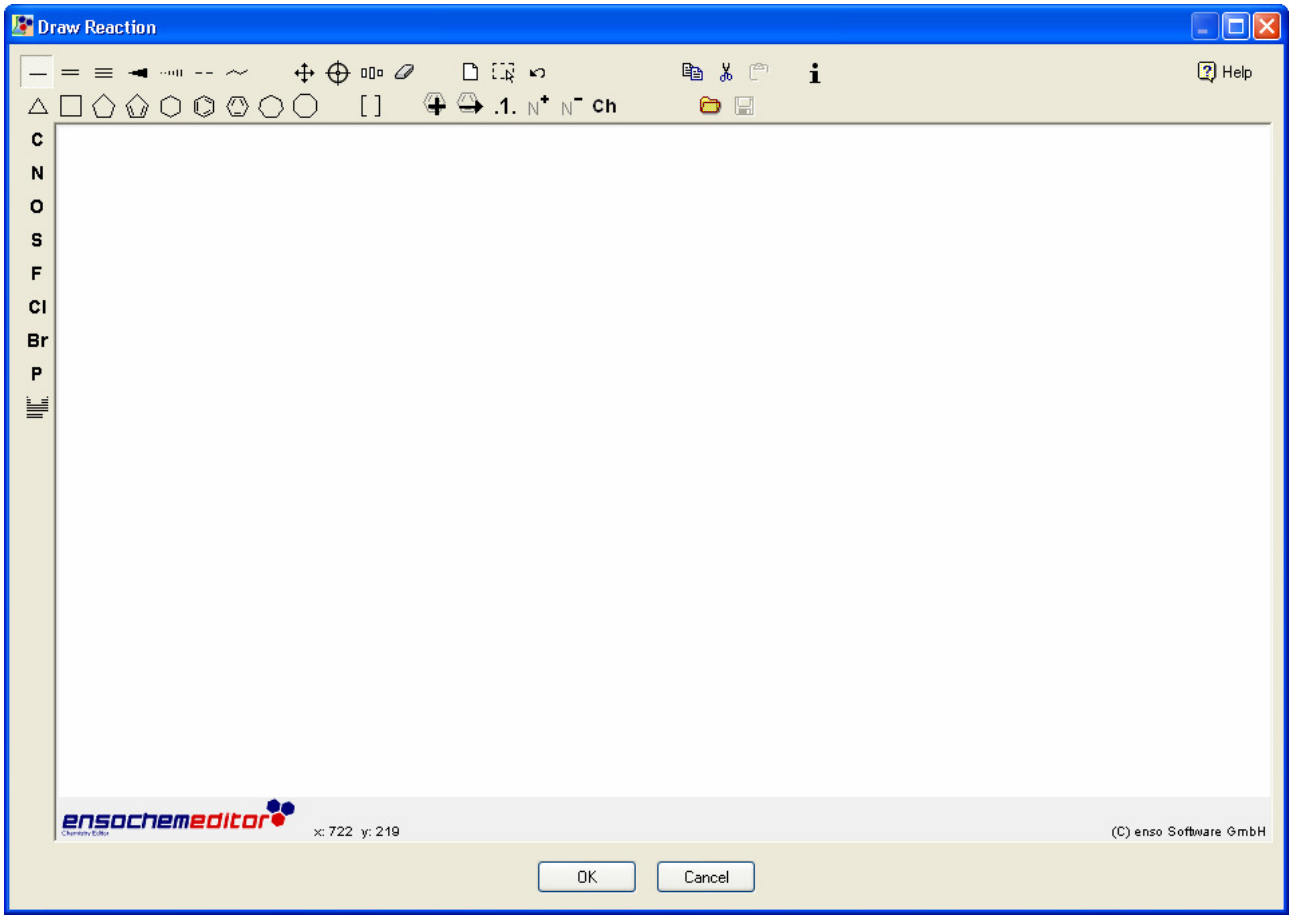


Later you will see your reaction in the place that is now empty. The reason, of course, is that you must enter your reaction first. This can be done by using a chemistry editor. The default editor is ensochemEditor Web Edition. Of course you can also configure one of the other supported editors using your personal settings. You can start the editor by double-clicking on the grey pane or using the context menu:



Of course, you can also use the respective toolbar button ().

A new dialog containing the editor will appear:



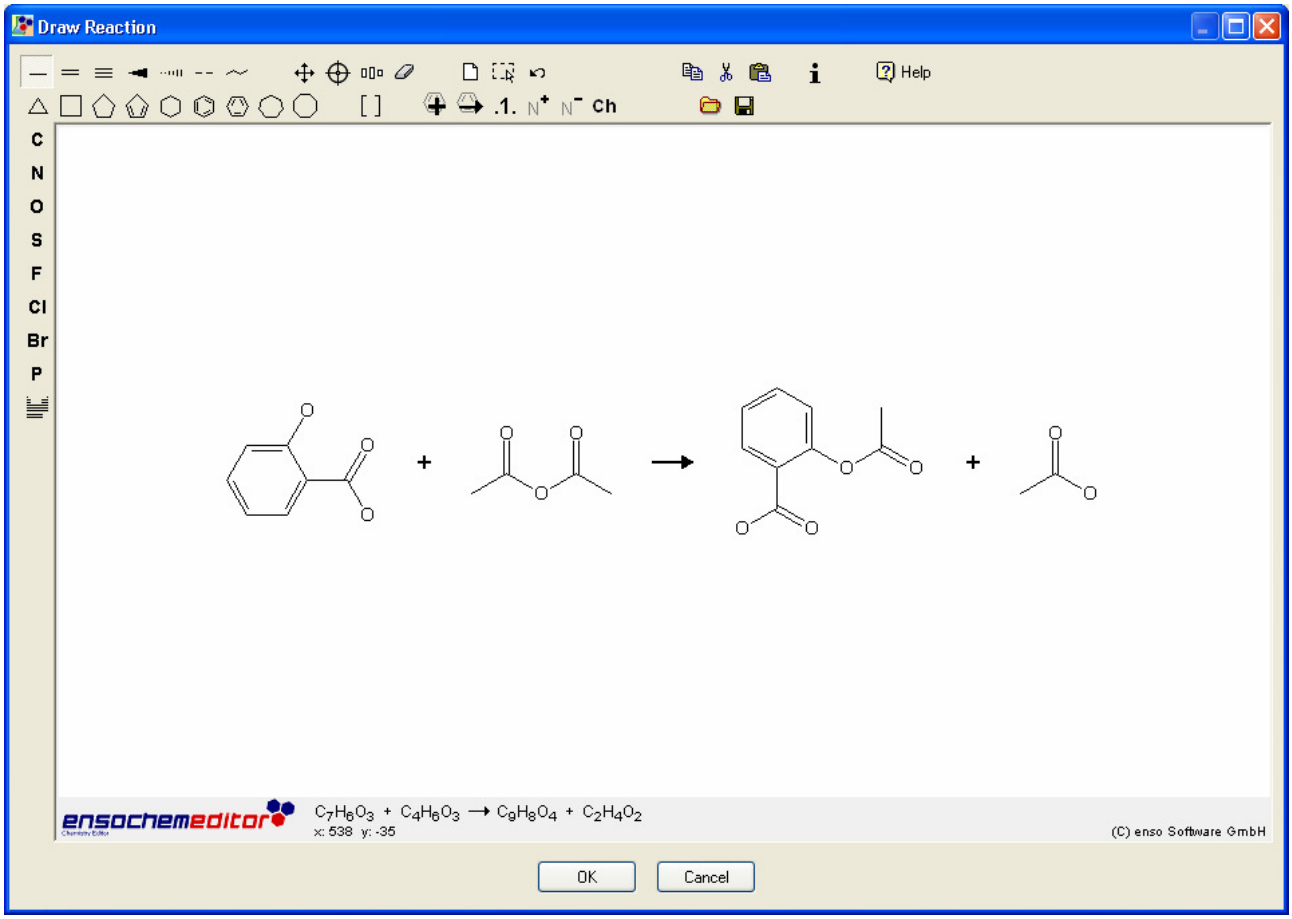
The toolbar is located at the upper side of the window. There you can find buttons for selecting templates, editing modes and the bond type to be drawn. A description of all features is included in the editor's help file that can be accessed by clicking on the "Editor Help" button in the upper right corner.

On the left side, there are the most common atoms that can be inserted in your reaction. If you want to draw another atom, just click on the "Atom List" button () which is the first button counted from the lower end of the toolbar. It will open a periodic system table where you can select the desired element.

The user interface of ensochemEditor Web Edition is very similar to the ones of the most common chemistry editors.

ensochemLab accepts all reactions that contain at least one reactant or product and a reaction arrow. This enables you to add your products later if you do not know them yet when entering the reaction. This can be the case if you first have to determine them by doing analytics jobs or something similar.

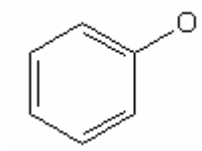
However, our sample experiment's reaction is known well and we can enter it fully right now.



Let's take a look at how the reaction in the upper screenshot has been drawn:

The editor helps us with templates which can be found in the toolbar. Select the benzene ring and then click on a free position on the drawing pane. It will be inserted there. Now click on a single bond and add it to the benzene by clicking on the C atom in the upper right corner of the molecule. Afterwards, select the element "O" from the toolbar on the left window side and then click on the end of the bond we have just created. It will be inserted there.

Our structure now looks like that:

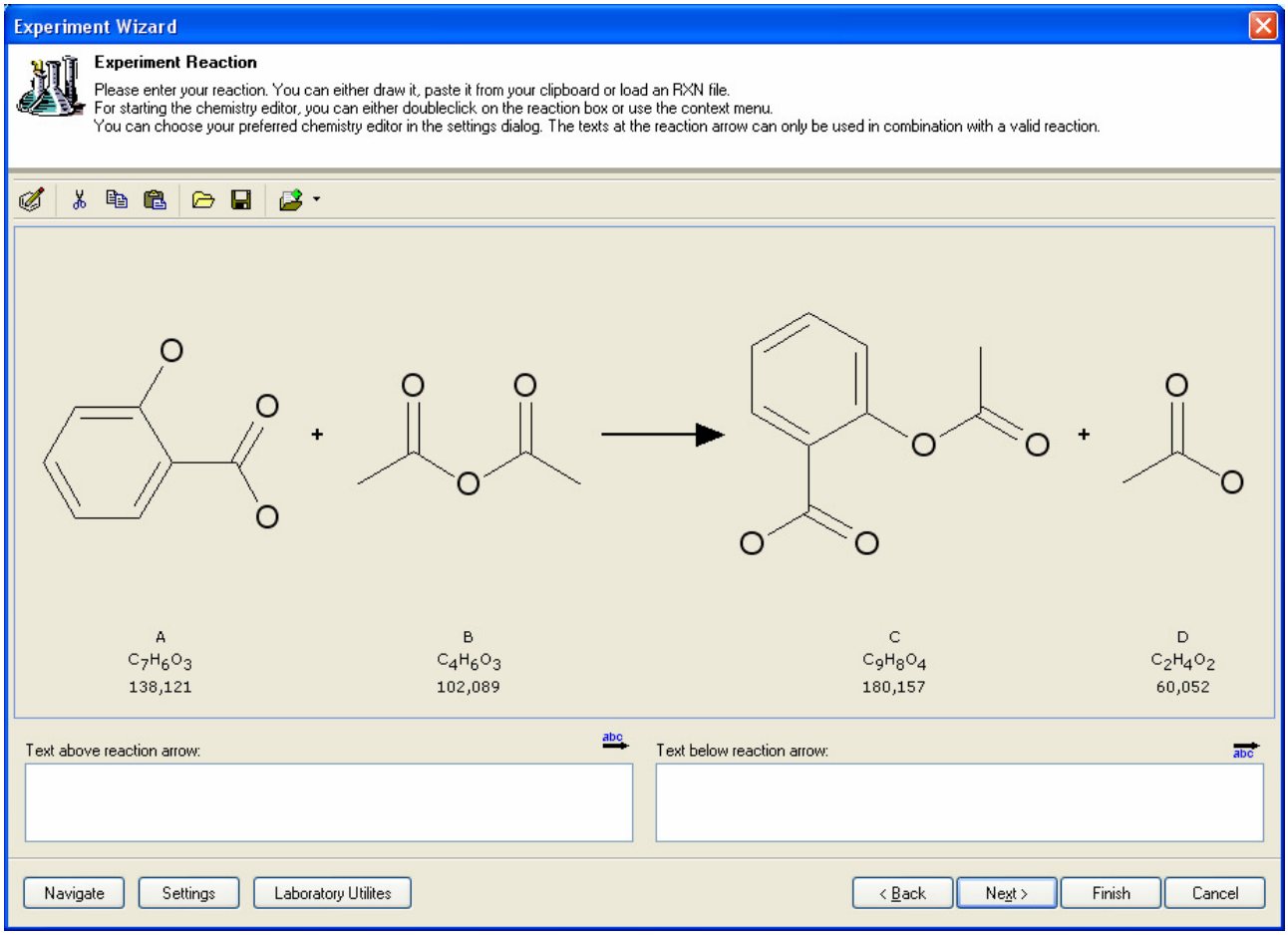


All other parts of the reaction can be created analogically. By the way: You should never draw hydrogen atoms directly in your reaction. ensochemLab can detect them automatically and show them if you have activated the corresponding function in your user settings. We will take a closer look at that later.

Click on "OK" to apply your reaction.

Remarks:	Beside ensochemEditor, you can also use a number of other chemistry editors to draw your reaction. We will discuss that in the chapter "Customize your settings".

When you return, the assistant will show the new reaction:



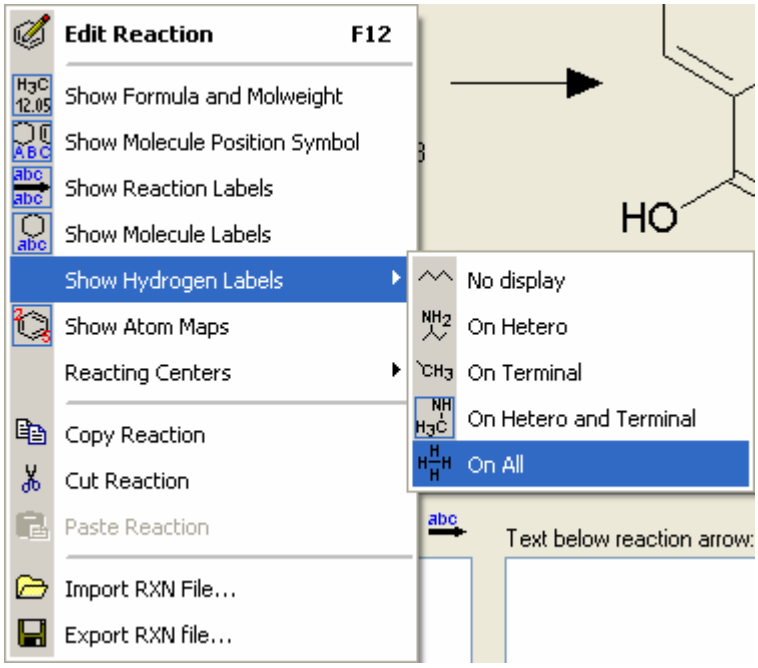
If you have already a reaction that is stored in a RXN file, you can import it directly into the assistant without having to start the editor. Just open the context menu by right-clicking on the structure pane and then select the “Import rxn file” entry or directly click on the toolbar’s “Import” button ( ).

You will see a “File open“ dialog that you are likely to know from many other Windows applications. Please select the desired file and commit the dialog by using the “Open” button. However, please note that this overrides the current reaction in the display pane!
A second way of importing a RXN file to drag it from your Windows Explorer’s display and let it drop on the reaction pane in ensochemLab.

You can also use the clipboard for exchanging reactions with other applications. For this purpose, ensochemLab offers you three functions: “Cut” ( ), “Copy” ( ) and “Paste” ( ) in the toolbar as well as in the reaction pane’s context menu. However, please note that your data has to be present in one of the supported chemistry formats for this operation to work.

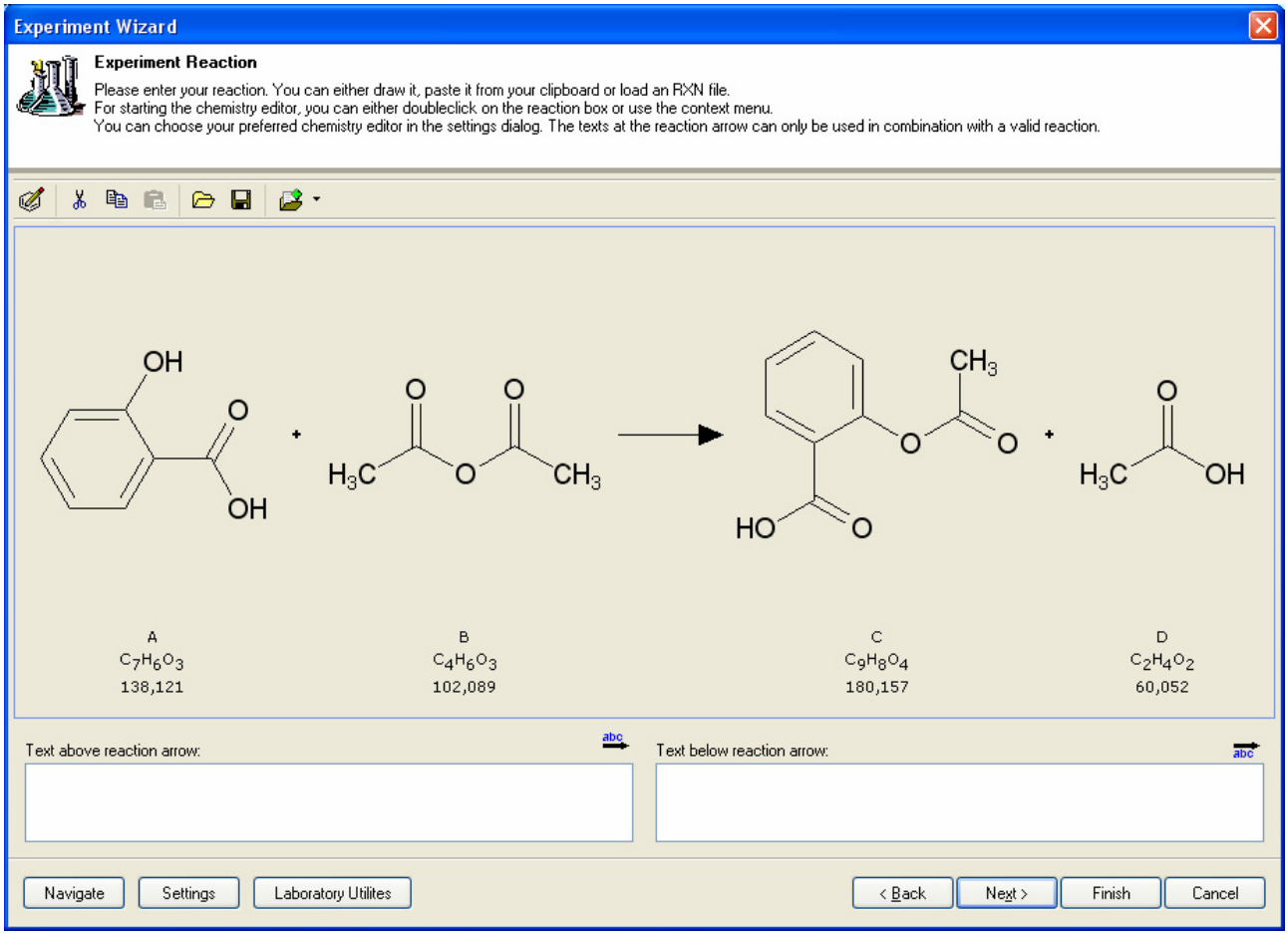
With the “Export” function ( ), you can save your reaction as an RXN file on your hard disk.

If you want to display your hydrogen atoms, open the context menu once again by right-clicking on the reaction. Then select “Show hydrogen labels” and a submenu with several options will appear where you can select the view mode you want to use:



The option you select here will be used for the whole program and therefore it is saved in your personal user settings. However, you can change you decision at all molecule / reaction display boxes in ensochemLab. Changing the setting directly will be explained in the chapter “Customize your settings”.

The experiment wizard with the hydrogen setting “On hetero and terminal” looks like this:



In addition to the chemical reaction, you can also enter texts which are to be shown beneath or above the reaction arrow. In order to use this feature, please just fill in the respective data into the text fields in the dialog. If you want to update the reaction display with this new data, please click on one of the update buttons (abc→).

We can now proceed to the next page.

3.3. Reactants

Here you can enter additional information for the reactants that you have defined on the previous page. Select a reactant from the list at the left side of the window and its detail data will be displayed in the details pane on the right side. Formula and molar mass are already predefined: They have been extracted out of the reactant's structure.

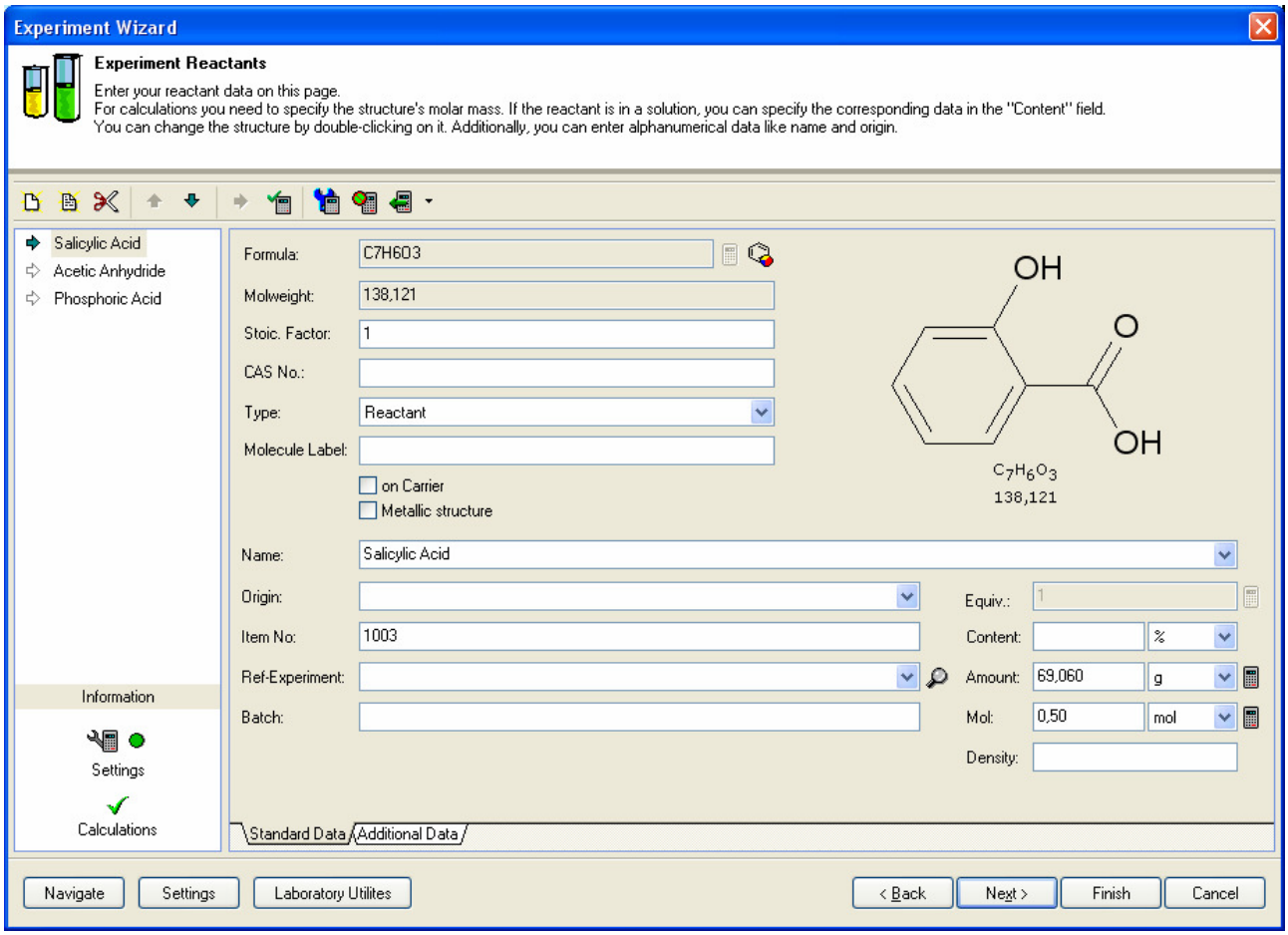
As an example, we enter some data into the description and amount fields which can be found beneath the structure. As origins, we simply choose "Supplier 1" and "Supplier 2". The item numbers are defined to be "10023" and "100563".

The "Origin" field is a selection field. You can either enter an own value (as we have done) or select one that has been predefined by your administrator. Your newly entered origin will be available as a selection with all reactants of the current experiment, but is not available for further experiments. To add an origin to the list of predefined ones, please contact your administrator.

The "Type" field is used to identify the type of your reactant. The default selection is "Reactant". Other possibilities are: Reagent, Catalyst and Solvent. Depending on your ensochemLab configuration, you may be able to select catalysts and solvents from a list predefined by your administrator. As an alternative, it may also be possible to apply the reactant data from a molecule database. ensochemLab can copy the chemical structure, the molecular weight, the density, the CAS number and the origin as well as other data fields.

The "Stoic. Factor" field can be used to enter a stoichiometric factor that shall be used in calculations.

The page now looks as follows:



If you have already synthesized the product once and then entered it into the database by defining it as a product of another experiment, you can enter the corresponding experiment number in the “Ref Experiment” field. You can also click on the lens at the right side of the field to search for it by its structure.

The reactant’s structure can be changed without having to return to the reaction page. Just double-click on the structure and it can be modified in the already well-known ensochemEditor (or the alternative editor you have configured in your personal settings). The changes you make here will automatically be applied to the reaction.

Using the green arrows in the toolbar ( ), you can change the order of your reactants. If you would return to the reaction page, you could see that the molecule order in the reactions has also been changed accordingly.

It is also possible to insert a new reactant by clicking on the “New reactant” button ( ). ensochemLab will then create a new, empty reactant and add it to your reaction. If you went back to the reaction page at this position, you would not see the newly created reactants as it does not have a structure yet. You can draw one by double-clicking on the structure box as already mentioned above.

By using the “Delete reactant“ button ( ), you can delete an existing reactants. In this case, ensochemLab also alters the reaction automatically.

If you don’t have a structure, you can also manually enter your formula and then click on the calculator symbol next to the data field. ensochemLab will then automatically calculate the corresponding molar mass.

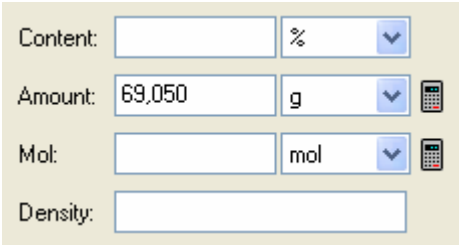
If the ACD interface has been activated on the server (you can contact your administrator for further information on this subject), you can automatically generate a chemical name for your reactant’s structure by clicking on the “Generate name for reactant” button ( ) at the right side of the name field.

Now it’s time to take a look at the calculation functions integrated into ensochemLab. We will use the example reaction we have just entered as a basis:

The experimental procedure tells us:

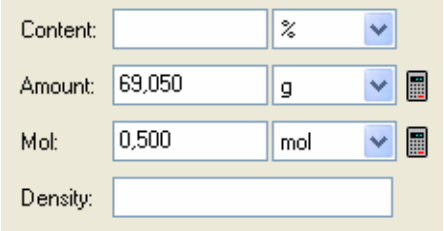
Mass of salicylic acid:	69.05 g
Mass of acetic anhydride:	51.05 g

At first, we calculate the mol amount:



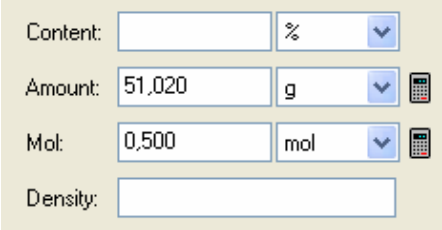
Enter the amount 69.05 and then select “g“ from the “Unit” field at the right side.

The small calculator symbol beside the “Mol” field has been activated. Click on it, and ensochemLab will automatically calculate the mol amount for you. The number of decimal places to be displayed can be changed in the program settings. Another chapter will explain this later.



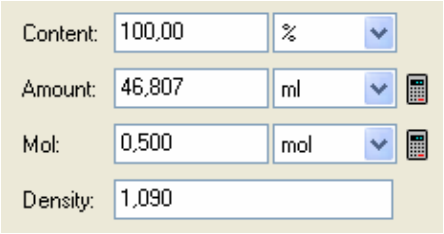
69.05g salicylic acid correspond to 0.5 mol

The mol amount for the second reactant can be calculated accordingly:



51.05g acetic anhydride correspond to 0.5 mol

If a reactant is in solution, the “Content“ field has to be regarded: You can specify the content either in [%], in [mol/l] or in [mmol/l]. If the content is entered in [mol/l], the amount is to be calculated in [g] and the “Density” field is empty, ensochemLab calculates using the density 1[g/l].



Enter a content of 100 and select “%” as the corresponding unit. This would be the pure substance. Keep the amount and mol values from the previous example, but change the density to “1.09” and then click on the calculator next to the “Amount” field. It will be recalculated to 46.807 ml.
On the calculation page, you will find the “Volume” field. There you will be able to use the volume as well as the mass.

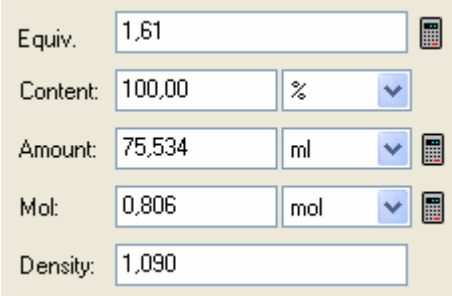
Remarks:	The amount does not quantify the amount of the dissolved substance, but the full amount of the solution.

Additionally, ensochemLab can calculate with equivalents. To use this function, you have to define one reactant to be the limiting reactant. To do so, select it in the reactant list and then click on the button in the toolbar. The limiting reactant will automatically be assigned an equivalent of 1. In our example, it is useful to specify the salicylic acid as limiting reactant.

For being able to perform calculations using equivalents, the corresponding option has to be enabled in your user settings. If this is not the case, a field for mol percents is displayed instead of the equivalent field.

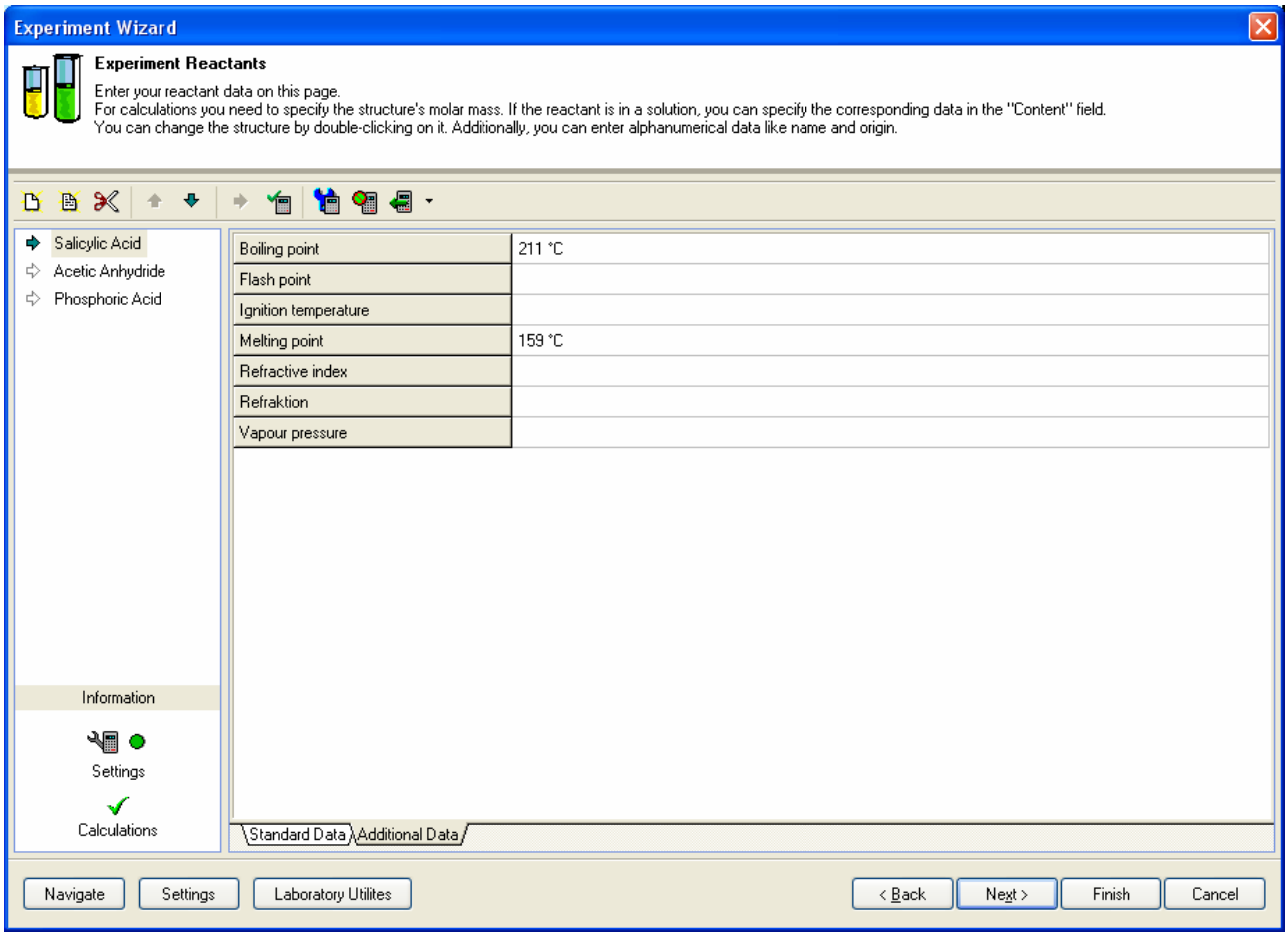
You do not have to leave the experiment wizard for changing your user settings. Just click on “Settings” at the bottom of the window.

Now select the acetylic anhydride and clear the “Amount” and “Mol” fields. Enter “1.48” as equivalent and then click on the calculator button:



As you can see in the screenshot above, ensochemLab has computed the fields “Amount” and “Mol” according to the equivalent you have entered. The calculations for examining the yield will be discussed with on the following page.

Until now, we have solely focused on the “Standard Data” page. Additionally, ensochemLab also supports entering other, supplemental data like chemical – physical information. To test it, please click on the “Additional data” tab in the data pane.



Here you can enter data for a number of additional data fields. To modify an entry in the table, please select the respective column by either clicking on it or navigating to it with the arrow keys on your keyboard. Then click into it or press “Enter”.
The possibilities for entering data depend on the field itself. ensochemLab supports the following types of fields:

- **Text fields**
  Text fields can contain arbitrary characters, numbers and special characters. It can be compared to a standard text file.

- **Exact number fields**
  These fields can only contain numbers and floating point values. Depending on the respective kind of field, it can also be possible to enter a unit and / or a condition (e.g. 12,5 °C at room temperature and 1 bar air pressure).

- **Range fields**
  These fields contain a range of numbers or floating point values. Like the exact number fields, conditions and units may also be possible.

- **Lookup fields**
  These fields allow you to select predefined values from a list. Depending on the specification it's possible to enter free text too.

- **Link**
  These fields allow you to enter data the same way as text fields. The only difference is that the given information is rated to be a hyper link which can be opened in a web browser by a simple click or an appropriate context menu item.

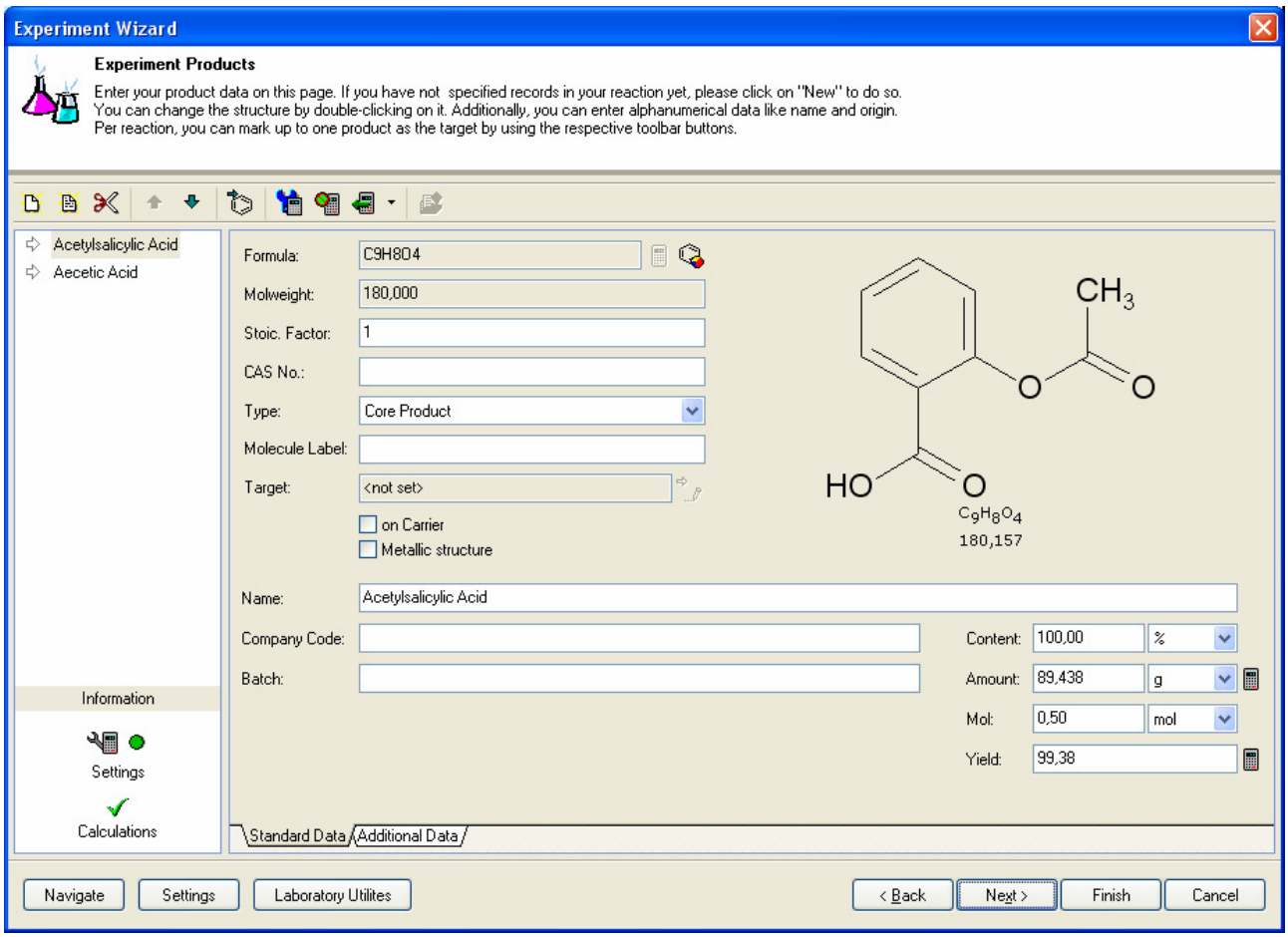
Please note that the language of the field names is defines by your administrator. He is able to add new fields, change the text or type of existing ones or set additional options. He may also enter language-dependent synonyms that will be used instead of the ones predefined by the database installation language.

At this position, it is not possible to add more data fields. If you need additional data fields, please contact your administrator.

By the way, if you want to create a new reactant that only slightly differs to an existing one in just a few data fields you do not have to enter all your data again. With a click on “Copy” (), you can create a duplicate of the currently selected record.
However, please note that this function has nothing to do with copying data to your clipboard which means that you cannot paste them elsewhere either.

3.4. Products

Click on “Next“ to proceed to the product page. This page is used to enter the product data and is very similar to the reactant page:



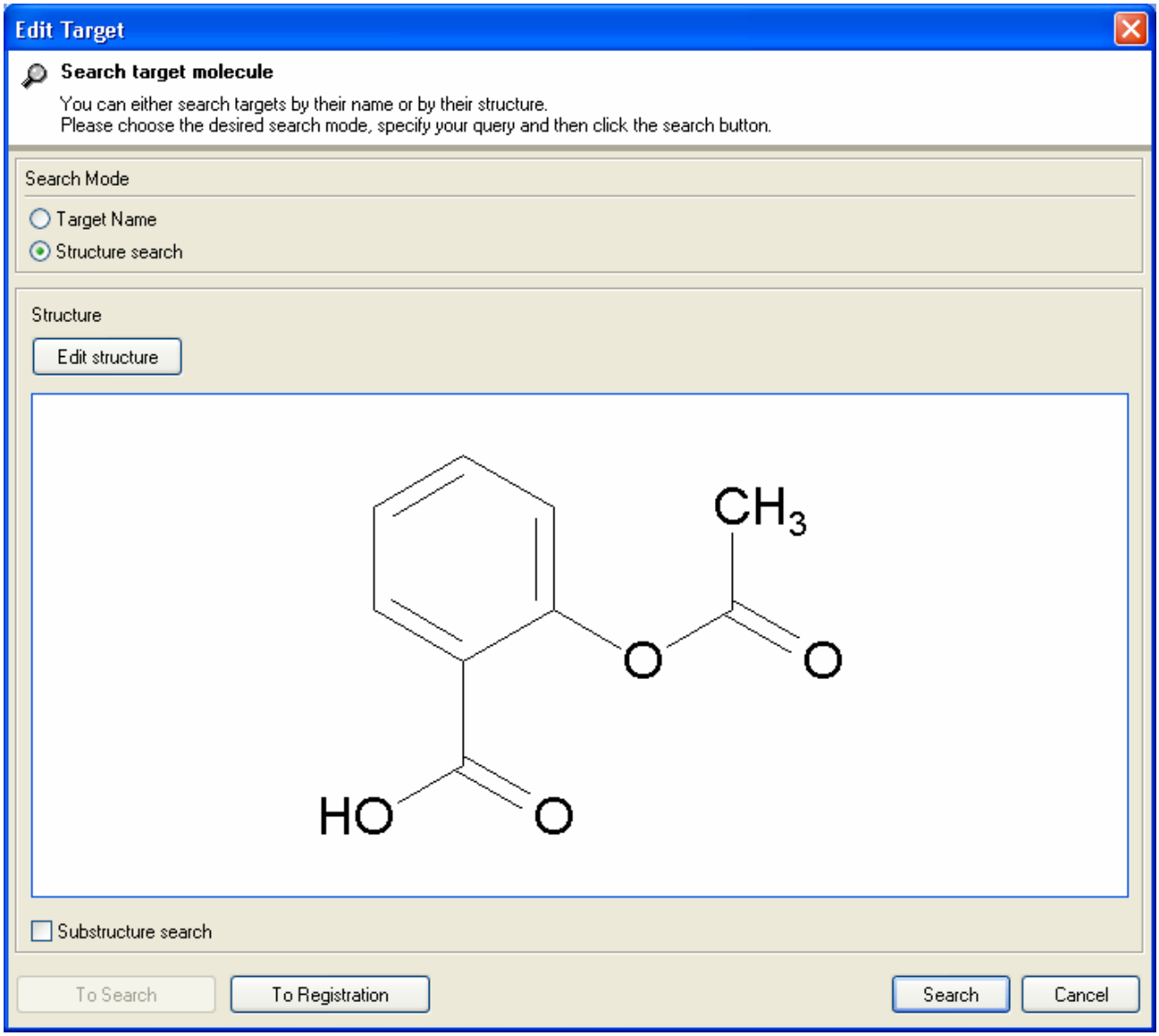
In this dialog, the product can be selected at the left side, just like the reactants on the reactant page. The data entry is also done on the right side of the window.

The field “Type” can be used to select the product to be either a core product or any kind of byproduct. In this example, we define the acetylsalicylic acid to be the core product and the acetic acid to be the byproduct.

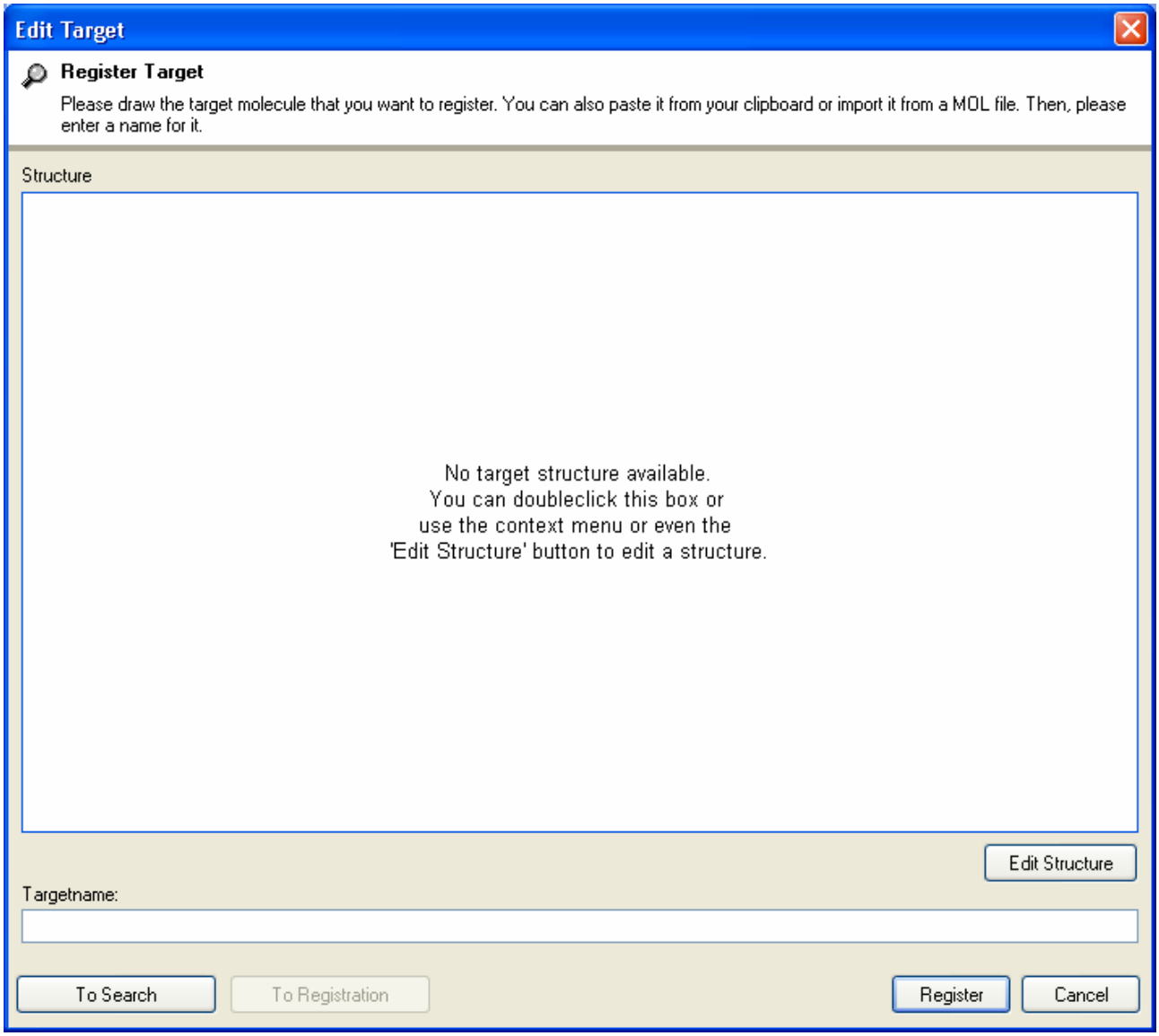
Next, we select our core product to be a target molecule. In order to do so, please click on the “Set as target” button ( ) in the toolbar.

ensochemLab will now automatically perform a structure search for the product structure. If it’s not found, you can either do a manual search in the list of existing target molecules or register a new one.

If you decide to search, please select whether you want to search for a target name (or one of its assigned synonyms) or for the product structure. Then please enter the name or draw the desired search structure. You can enter the chemistry editor by either double-clicking on the structure pane or clicking on the “Edit structure” button. Using the context menu, you can import your query from a MOL file on your local hard disk. When you are done, please click on “Search”:



This manual however assumes that there are no target molecules in your database yet. Thus, please click on “To Registration”. Before ensochemLab is able to register the current molecule as a new target, you have to enter the first name for it. We will have a look at the function for entering an arbitrary number of synonyms at a later time within this manual.

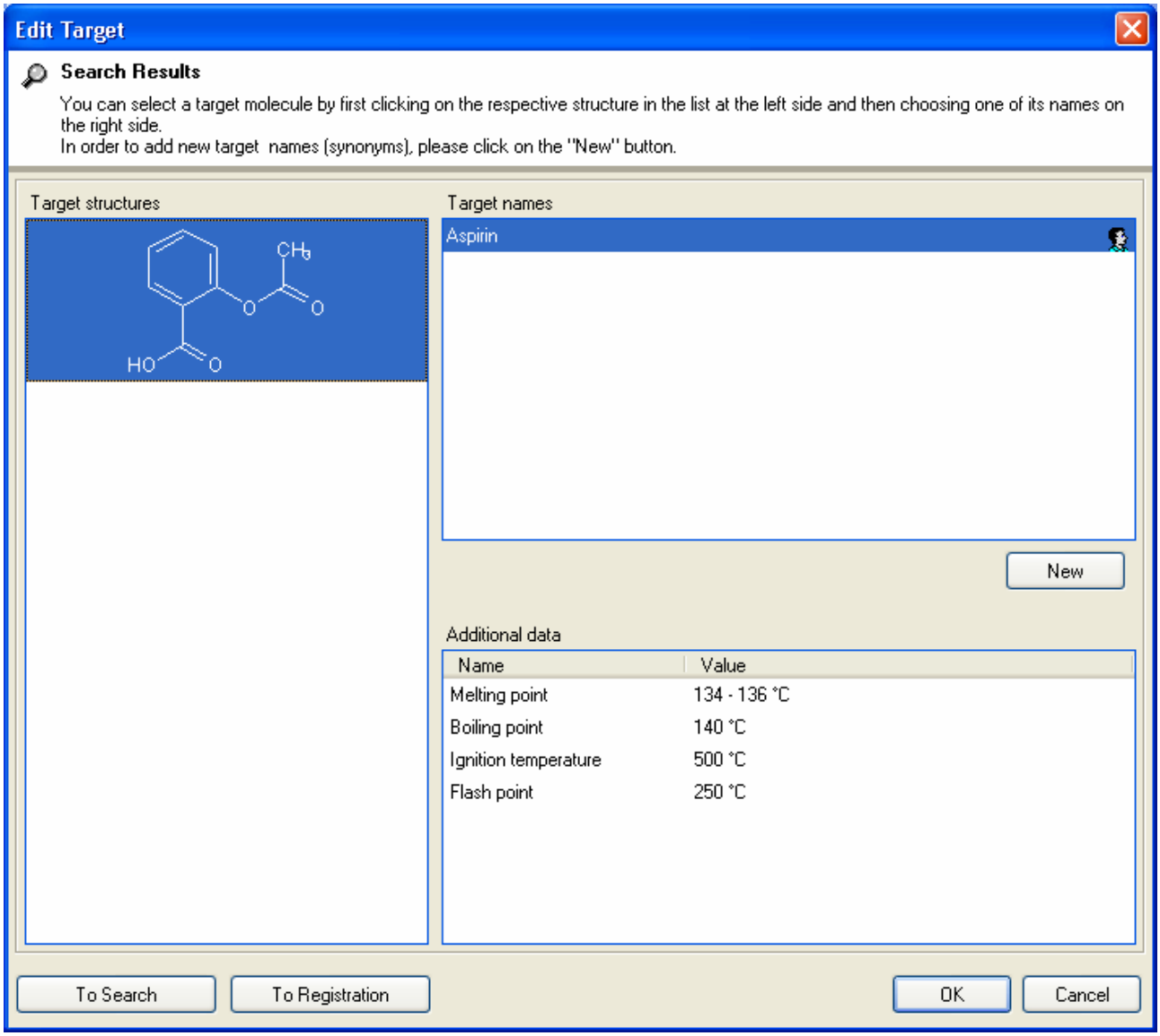


If you decide that you would prefer doing a search instead, please just click on “To Search” and you are comfortably redirected to the previously explained search page.

You can still change the structure on this page. Opening the chemistry editor is the same as it was on the previous page. Importing a MOL file is also possible likewise.
When you click on the “Register” button, ensochemLab will save the new target molecule and apply it to your experiment.

The registration or selection of a target molecule is of course optional. You can save experiments without doing so, too. This is meaningful whenever you are about to enter an interim step for an experiment queue or something similar to that.

Sooner, we have already hinted at the fact that a target molecule may have an arbitrary number of names (synonyms) in ensochemLab. Due to this fact, you have to select one of them which shall be applied to your experiment. In order to change the current display name, please click on the “Edit target data” button ( ) right beside the current target name.
Using this button, you can also select another target molecule for your reaction. The following dialog will be shown:

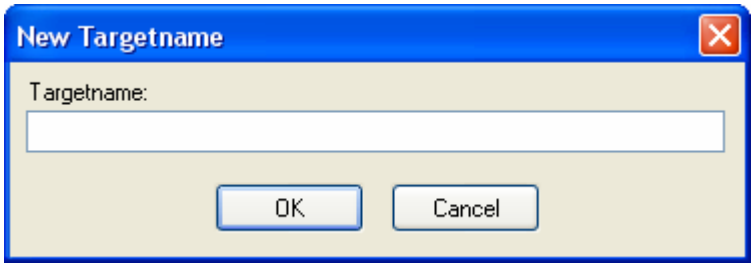


If you want to select another target molecule at all, please click on the “To Search” button which will take you to the search page that has already been discussed earlier. After you have performed the search, you will return to the current page. All structures that have been found with your query will then be display in the list at the left side.

If you do not perform a search, the list on the left side contains only your current target molecule. After you have clicked on a list item, you will see all corresponding names in the list on the upper right side of the window. The list on the lower right side contains additional data that your administrator has defined for the target molecule. Please note that the additional data does not only belong to the target molecule itself, but rather to the molecule and its corresponding name.

For every target molecule name, you can also find a small information symbol ( ) at the very right side of the list. If you move your mouse cursor over this symbol, a hint window containing the respective record’s owner and creation date is displayed.

With the “New” button, you can enter a new synonym for the target:

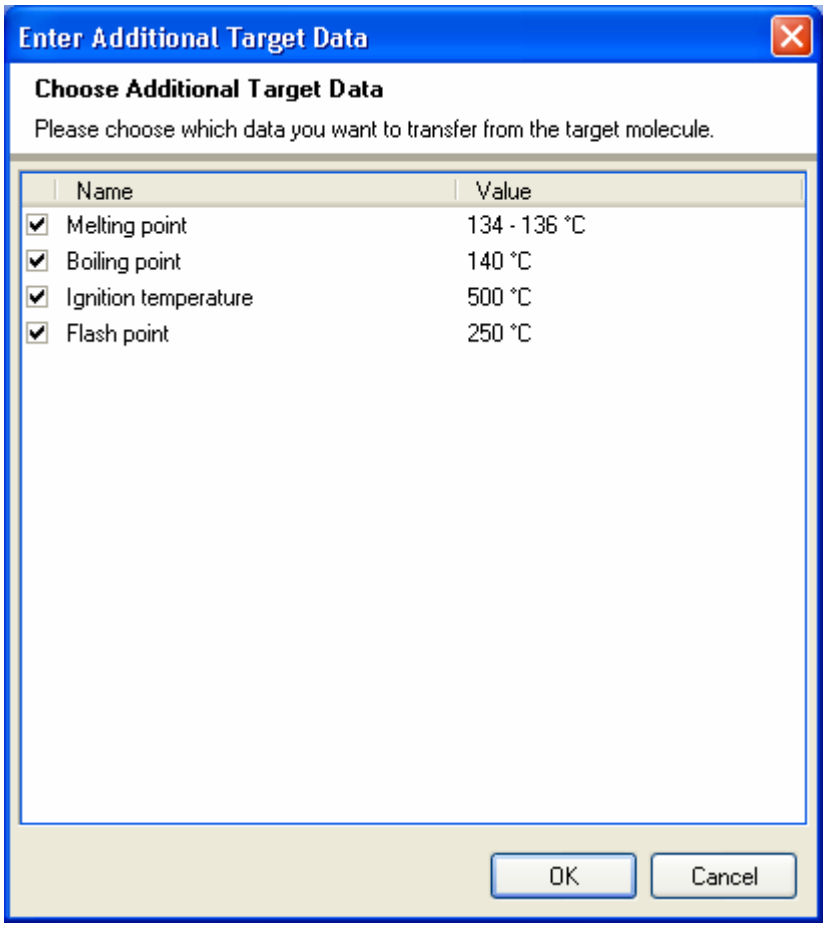


Please enter your new name for the target molecule and then click on “OK”. It will be added to the list on the right side. As soon as you close the target selection dialog with “OK”, the currently selected target molecule will be applied to your experiment using the name that is active at this time.

Remarks:	Due to security reasons, target molecules and synonyms can only be edited and deleted in a separate administration dialog. If you want to remove a record, please contact your administrator.

You can also add a completely new target molecule within this dialog by clicking on the “To Registration” button which will redirect you to the registration page we have seen earlier.

If your target molecule contains additional data, you can transfer them into your experiment when returning to the experiment wizard. Therefore, the following dialog is automatically displayed in such a case:

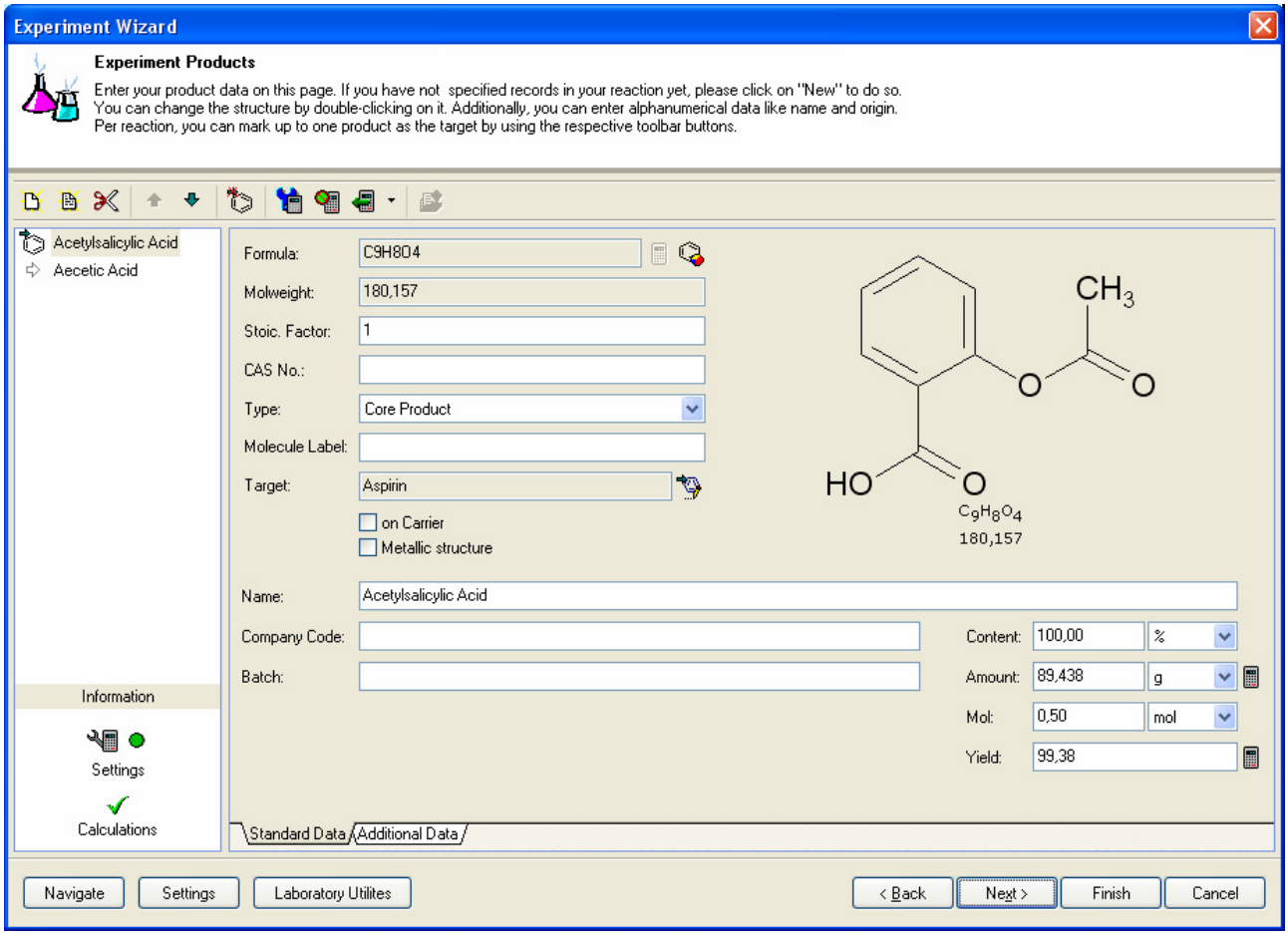


In the list, you can once again see the target molecule's additional data. In order to select an entry for transferal, please mark the corresponding checkbox. If you do not want a data field to be applied, please remove the respective check. By default, all entries are selected.

Please note that you cannot change any data within this dialog. Changing the target molecule's additional data is only possible for administrators in a separate dialog. After application, however, you can normally change the product's data within the experiment wizard.

If you click on "OK", the selected data is transferred. After a click on "Cancel", no additional data is applied, but the target molecule is nevertheless set.

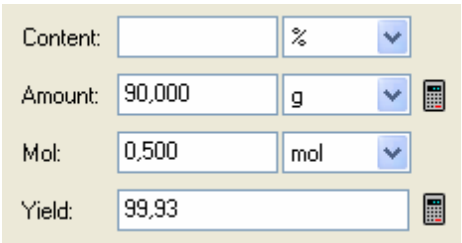
When you return to the experiment wizard, it will look like that with its newly set target molecule:



If you want to delete the current experiment's reference to the target molecule, please click on the "Deselect target" button (). The actual target molecule itself will persist.

At this position, we can also calculate the yield. Of course, this is only possible if one reactants works as a reference and distributes the necessary data (Amount …).

For our example, please enter to value "90" in the "Amount" field, select the unit "g" and then click on the calculator symbol next to the "Yield" field.



0.5 Mol salicylic acid + 0.5 Mol acetic anhydride react to 0.5 Mol acetylsalicylic acid + 0.5 Mol acetic acid.

You can do the same for the second product (Resulting amount: 60g).

Remarks:	If you want to work with carries, just select the checkbox "on Carrier"

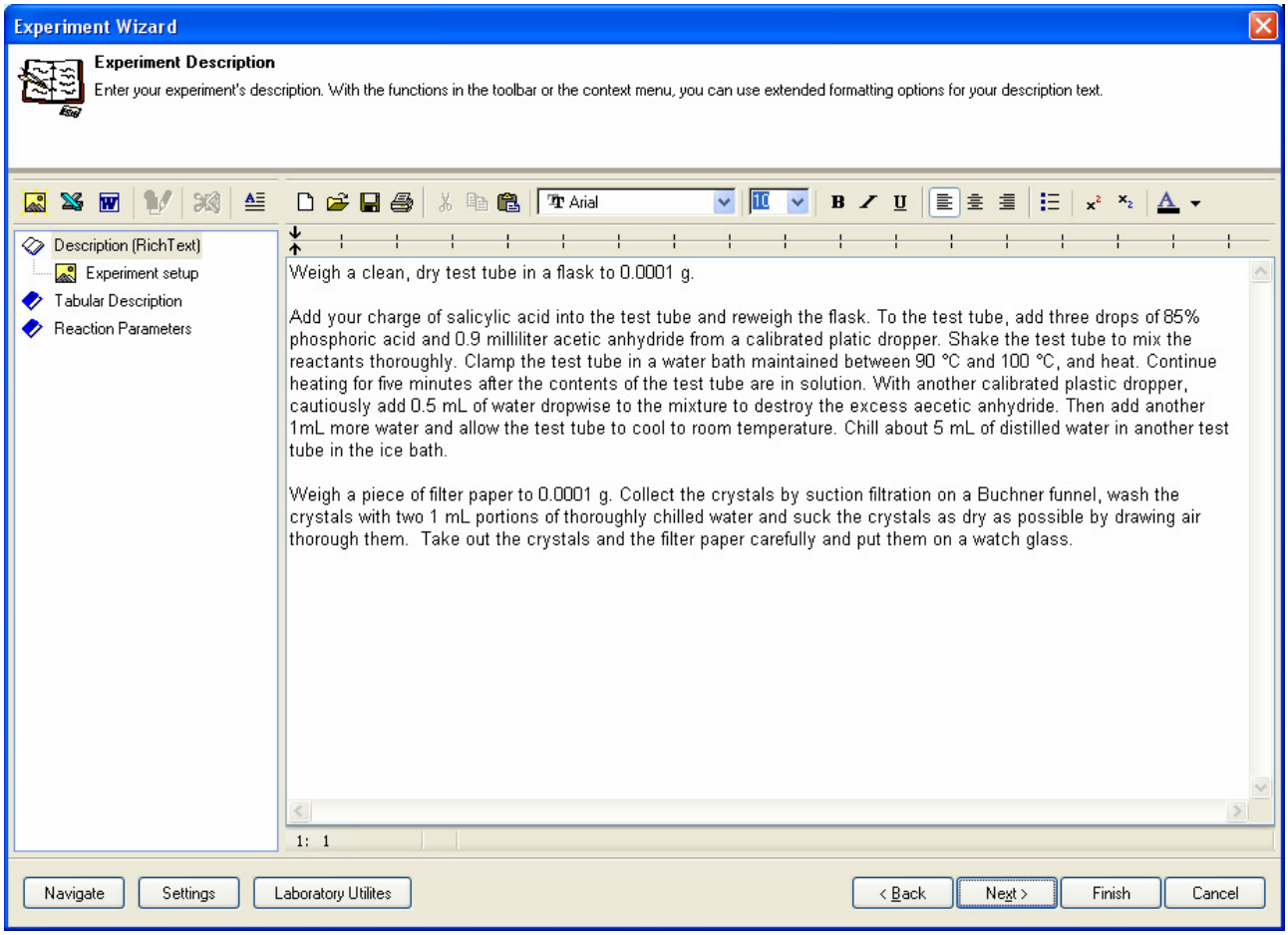
	and ensochemLab will display some additional data fields where you can enter your carrier's data.

Now click on "Next" to proceed to the next page.

3.5. Description

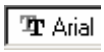
3.5.1. Description (Rich Text)

The following page is used to enter the experiment description. On the left side, you can select the desired type of the description.



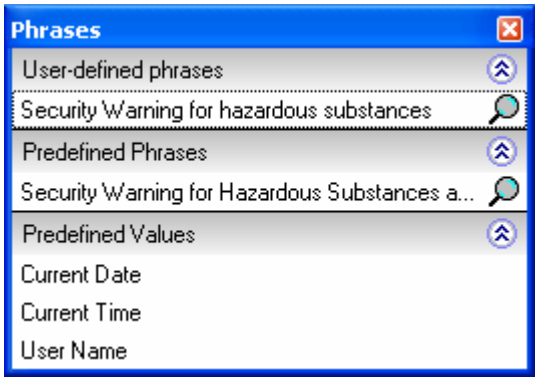
Select “Description (RichText)” to enter text just as you know it from other text processing software like Microsoft WordPad, OpenOffice and others. The toolbar offers you a number of functions to format your text. For the rich text description, the functions are:

	New document	This deletes the content of the current document
	Open File	Imports the text from a rich text file (*.rtf) on your hard disk. Please note that some programs include extended information in RTF files that ensochemLab either does not display (images for example) or depicts differently.
	File save	Saves the text to rich text file (*.rtf) on your hard disk
	Print file	This prints the experiment description. The current default printer is automatically selected for the printout.
	Cut	This function is only enabled when you have selected some text. It copies your selection into the clipboard and then deletes it from the experiment description.

	Copy	This function is only enabled when you have selected some text. It copies your current selection into the clipboard.
	Paste	This function inserts the current content of the clipboard into your experiment description. Your current selection (if you have one) will be overridden.
	Font	You can select the font you want to use from this list. Different parts of the text can have different fonts. If the experiment is displayed on a computer on which this font is not installed, a default font will be used instead.
	Font size	You can select the desired font size for the selected text passage from this list or enter an own value. Just like in text processing software, this value is specified in “point”.
	Bold face	Displays the selected text in bold face
	Italic	Displays the selected text in italic letters
	Underline	The selected text will be underlined
	Align left	The current paragraph will be aligned to the left side
	Center	The current paragraph will be aligned to the center
	Align right	The current paragraph will be aligned to the right side
	Enumeration	This function adds an enumeration to the experiment description
	Superscript	The selected text will be formatted as superscript
	Subscript	The selected text will be formatted as subscript
	Apply font color	Via color selection the text will be changed according to your choice out of the standard palette or by creating a user defined value.

Using the context menu, you can also insert data from your reactant and product records into your description text. Just look at the “Reactant Data” and “Product Data” submenus. Current values like date and time can be inserted via the “Predefined Values” menu. Please note that this data is copied, not referenced. If you change your reactants and products later, the description will not be updated.

Another handy feature is the support of phrases. A phrase is a piece of text or a sentence that you often use and that you have saved for comfortable access. With ensochemLab, you can insert these texts without having to enter them again every time. Click on “Show phrases window” ( ) to open the respective dialog:



In the upper part, you can find your personal phrases, regardless whether they have been configured as private or public ones. The next section contains the phrases predefined by your administrator.

In order to insert a phrase at your current cursor position, please either double-click on the respective entry in the list or select it and then click on the “Insert phase” entry ( ) in the context menu. Inserting it via drag & drop is also possible.

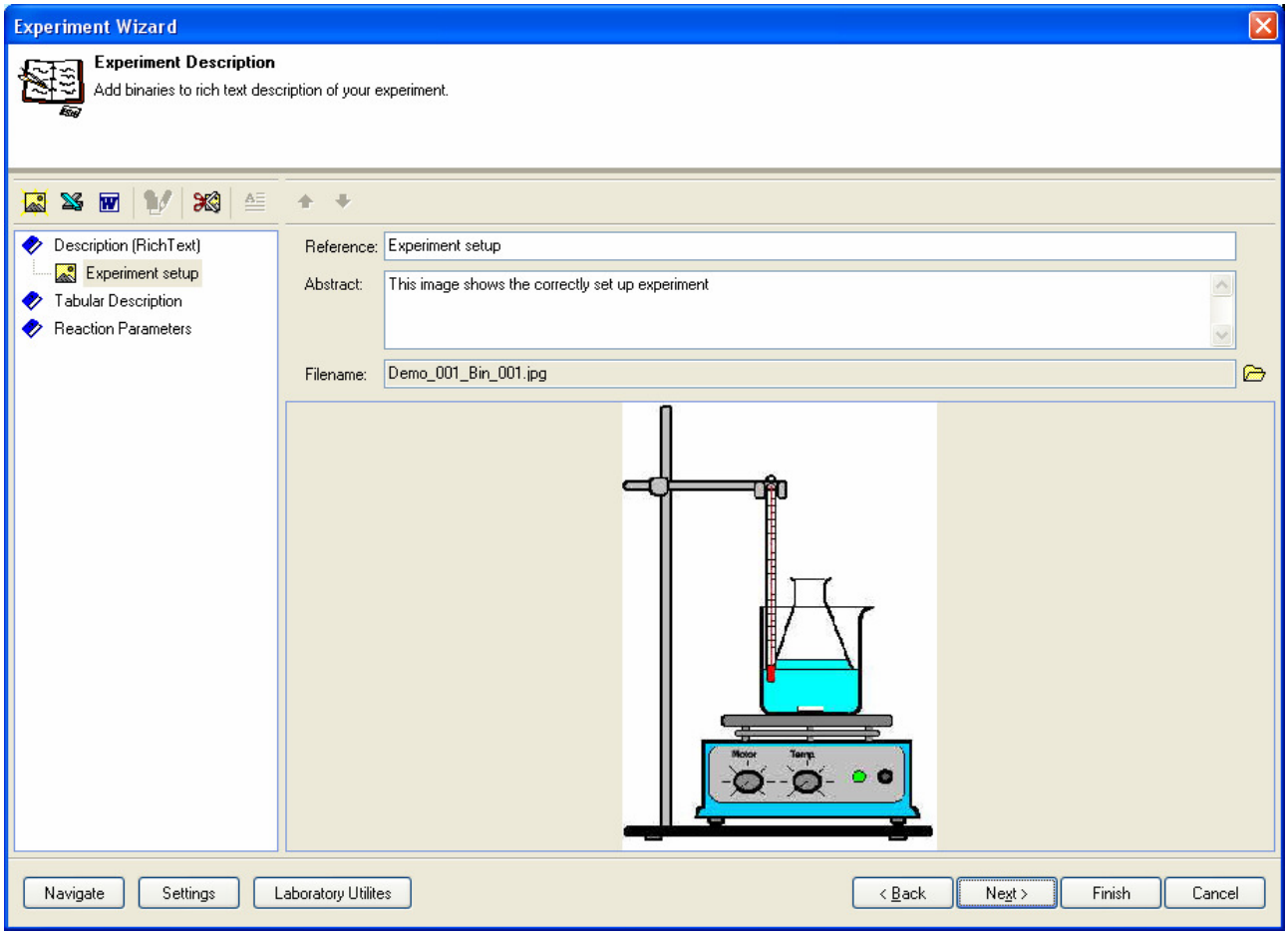
For changing the phrase category order which means for moving up the “Predefines Phrases” section for example, you can use the “Exchange phrase categories” function ( ) from the context menu.

With the ”Edit phrases” ( ) function, you can open the dialog for managing your personal text phrases. The current selection will directly be chosen for editing there. This functions is only available for own phrases. The management dialog is thoroughly explained in the “User defined phrases” chapter later in this tutorial

Besides the normal text phrases, the phrases window also contains additional data. This includes not only general values like the current date, but also experiment-related ones for the various reactants and products (name, amount, etc.) which are available in a grouped list in the very lowest category. You can work with these values just like with phrases.

If you want to directly create a new phrase using text in the current experiment description please select it and then choose the “Selection as New Phrase” ( ) function from the context menu. ensochemLab will now prompt you for a name. After you click on “OK” the new phrase is saved to the database.

Using the button “New Binary” (), you can attach files to your experiment’s description just as you know it from your E-Mail or collaboration program. This attachment can be any kind of file, for example an image, a PDF document or others. You can create an arbitrary number of attachments for your description.



For every attachment (binary data), you can enter a short description text and a reference. You always have to select a file from your hard disk. Just click on the “Open File” button () and ensochemLab will then show a dialog where you can select the path and name of your desired file.

If the file you want to attach is not displayed in the list, please select the entry “All files“ in the „File type“ section of the open dialog. However, these files might not be displayed directly by ensochemLab and have to be loaded into an external viewer application. If a preview image is displayed in the experiment wizard, an internal display is possible. If there is just a short text, the file format is not supported.

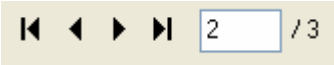
To save an imported file to your hard disk again, please right-click on the preview image and then select “Save binary”:

You can directly create Word documents and Excel spreadsheets with the respective buttons in the toolbar (and). These files are also displayed as preview images in the various experiment display modes. When printing, they are embedded into your document just like images. Of course, you can also import Word or Excel files from external sources.

By double-clicking on the preview image in the experiment assistant, you can directly change such Office documents without having to manually re-import them every time.

Please note that the respective Microsoft Office applications need to be installed on your local computer for using this feature. If they are not available, you can attach Office documents only as normal attachments of unknown type.
If no office documents are displayed and the functions for creating new ones are not available either, the respective feature may be disabled in your personal settings. For further information, please refer to the "Customize your settings" chapter in this manual.

If you select a PDF or Word document or an Excel spreadsheet, you can browse through the pages of your file with the special navigation toolbar that ensochemLab displays at the top side of the preview pane:



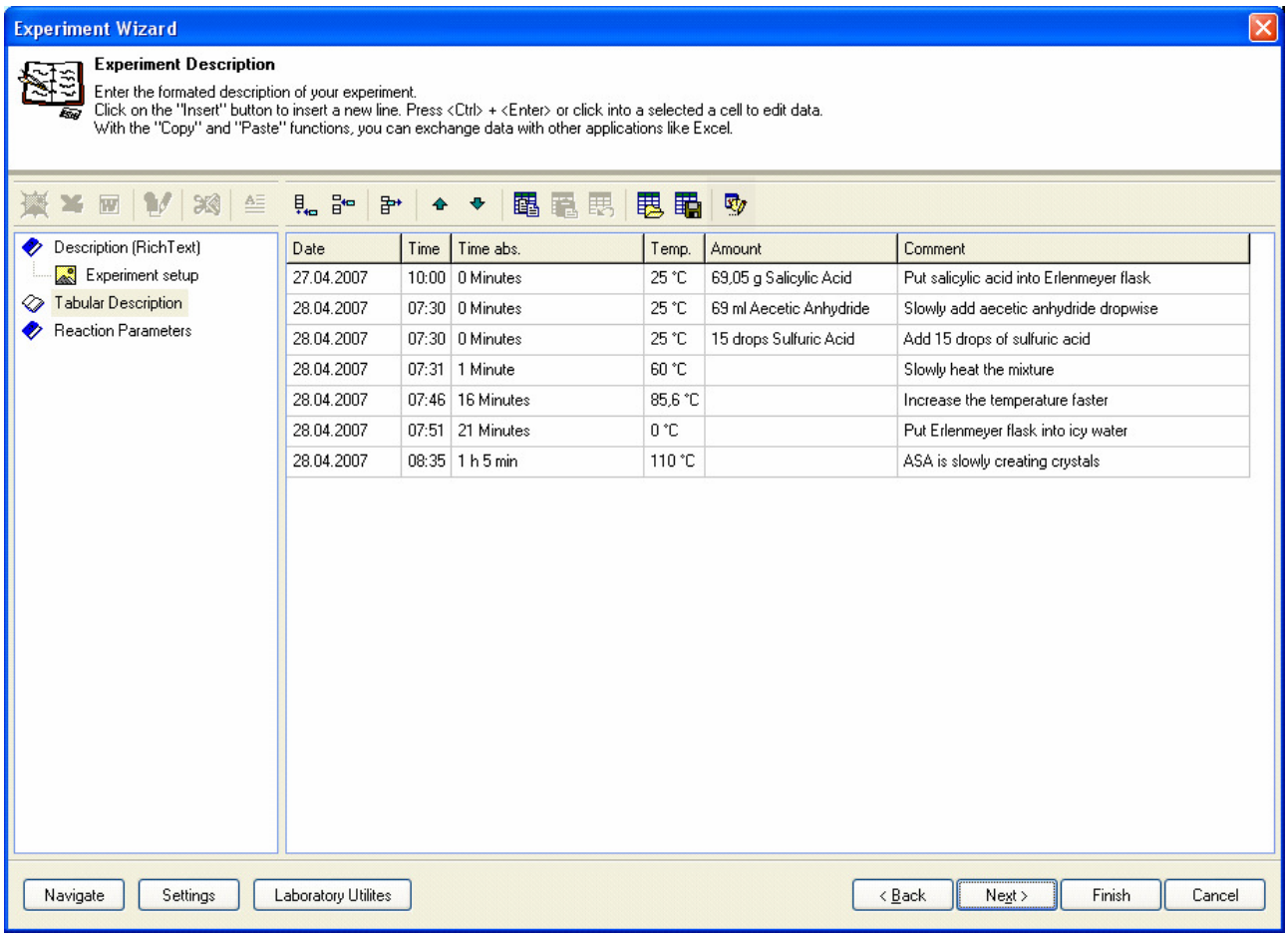
The text field always displays the number of the page that is currently visible. For directly jumping to a specific page, please just enter the corresponding number here and press the "Return" key. In the example, page 2 of 3 is currently visible. The buttons are:

- Displays the first page in the document
- Displays the previous page
- Displays the next page
- Displays the last page in the document

Using the button „Delete binary" (), you can delete an attachment. Please note that there is no limitation for the number and size of binaries files for an experiment description.

3.5.2. Tabular Description

In common, the tabular description on the next page in the wizard is used to document the progress of the reaction including temperatures, amounts and comments of any kind. Of course, you can also create any other headword documentation that you regard to be useful in connection with time stamping the experiment. In this example, we will document the addition of the reactants and the most important changes of the temperature.



You can directly start with entering your data in the first row which is automatically created by ensochemLab. The “Add row“ button () can be used to insert a new row into the listing which will be added below the current row. This is also possible by pressing the “Tab” key when the cursor is positioned in the last field of the end row. With the tabulator key, you can also jump to the next column. For inserting a row above the current one, please click on “Insert row” ().
The “Delete row” button () deletes the current row and all the data in it.

Per experiment, you can create an arbitrary number of rows with tabular description data, but you cannot attach any data files to it.

To change the data in a grid cell, just select it either by clicking on it with your mouse our moving to it with the arrow keys on your keyboard. Then either click into it or press the return key. Both possibilities will start the integrated field editor that you can use to enter your data.

Please note that row breaks within one cell are only possible in the “Comment” column. For other columns, you should consider creating a new data row instead.

If you enter a text that is too long (e.g. exceeds the column size), the wizard will only display the beginning and a … abbreviation. However, your data is not really truncated; it is only displayed in a truncated way within the assistant. The main experiment display and the printout processor will automatically insert line breaks to display all data.

ensochemLab automatically fills the first row with the current date. For all following lines, the date that has been selected in the row directly above is copied. The enables you to, for example, belatedly document an experiment you have done last week without having to change the date in every single row.

With the “Move up” button (), you can move the current row one position up in the table. The contrary function, “Move down” () enables you to move a row down in the grid.

ensochemLab also supports the easy data exchange with other applications. For example, you can continue your work at a tabular description in Microsoft Excel and then re-import your work results back into ensochemLab.
The “Copy” command () stores your complete description table in the clipboard.
With “Paste” (), you can insert the current contents of your clipboard in ensochemLab. Attention: This operation completely replaces your current data. Thus, a warning will be displayed. If you do not want to see this warning anymore, please check the “Do not show this message anymore” checkbox. In your personal settings dialog, you can change this decision at any time. If you leave the warning dialog with a click on “Cancel”, the checkbox state will not be saved and the warning will be displayed next time in any case.
If you have inserted data that you do not want to keep by accident, you can undo your last insert operation by clicking on “Undo” ().

If the new data you have created or modified outside ensochemLab are contradicting the data format required by ensochemLab (since it contains a different number of columns or the date field does not contain a valid date), an error message is displayed. You can then decide whether you want to continue (and maybe lose data) or whether you want to cancel the operation.

In this module, you can also export the tabular data into a local CSV file () or import it from such a file (). A detailed description of these functions can be found in a separate chapter called “CSV Data Exchange”.

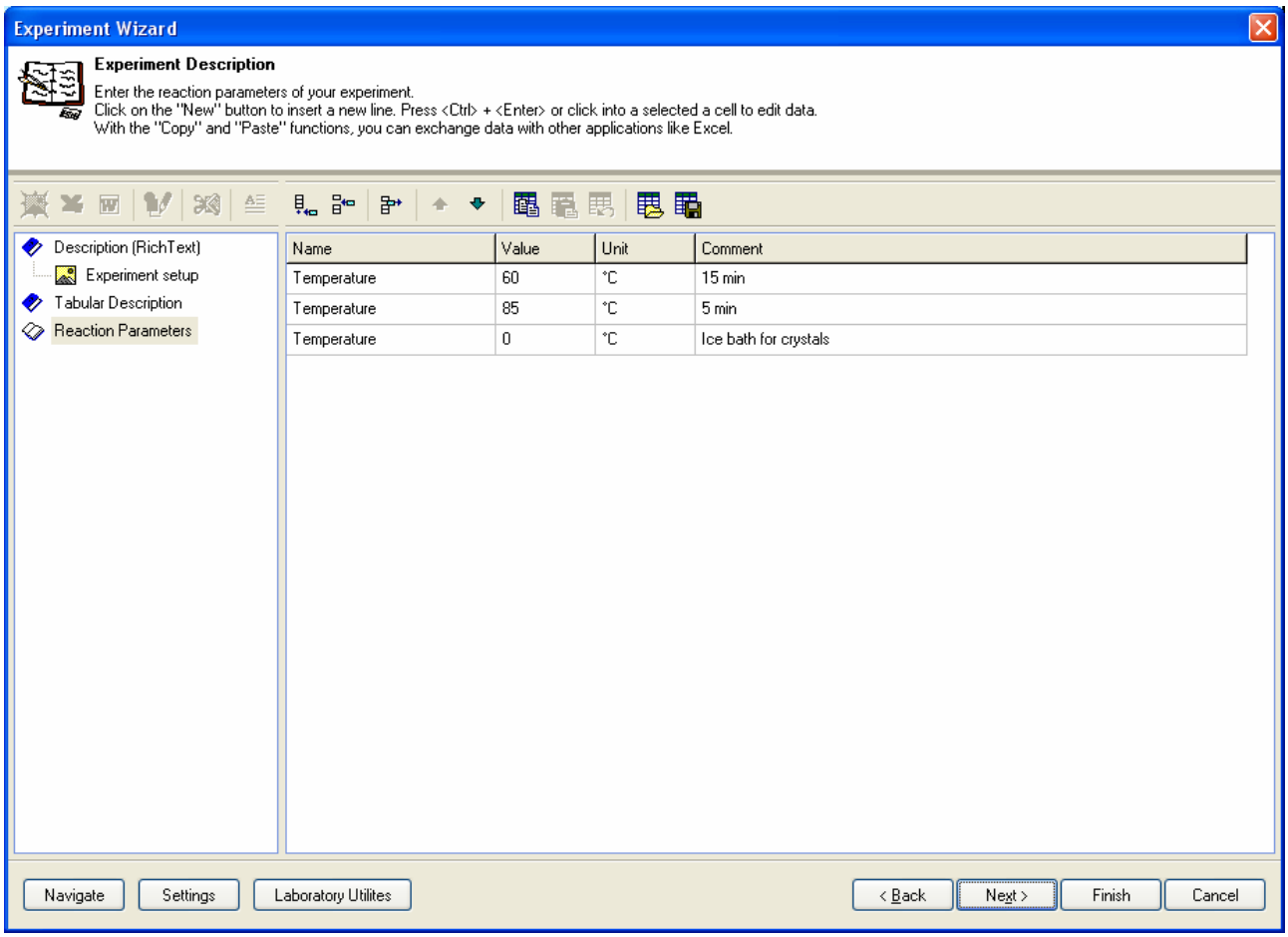
In case you need to adapt date / time values, which are e.g. the result of using another experiment as a template, to meet the actual synthesis execution, a wizard is available () to assist you in doing so. By providing a new date or time reference respectively the corresponding values are calculated automatically.

3.5.3. Reaction Parameters

The reaction parameters page can – just as its name says – be used to enter the reaction conditions in a tabular form (Have you worked under pressure? What was the room temperature?).

The “Name” field is a selection field. Every name you enter will be saved into the selection list temporarily for this experiment. Thus, you can use it in all rows without having to reenter it every time. However, this list is not adopted when creating another experiment.
The “Unit” field is very much alike; however, its selection list also contains the units predefined by the administrator.

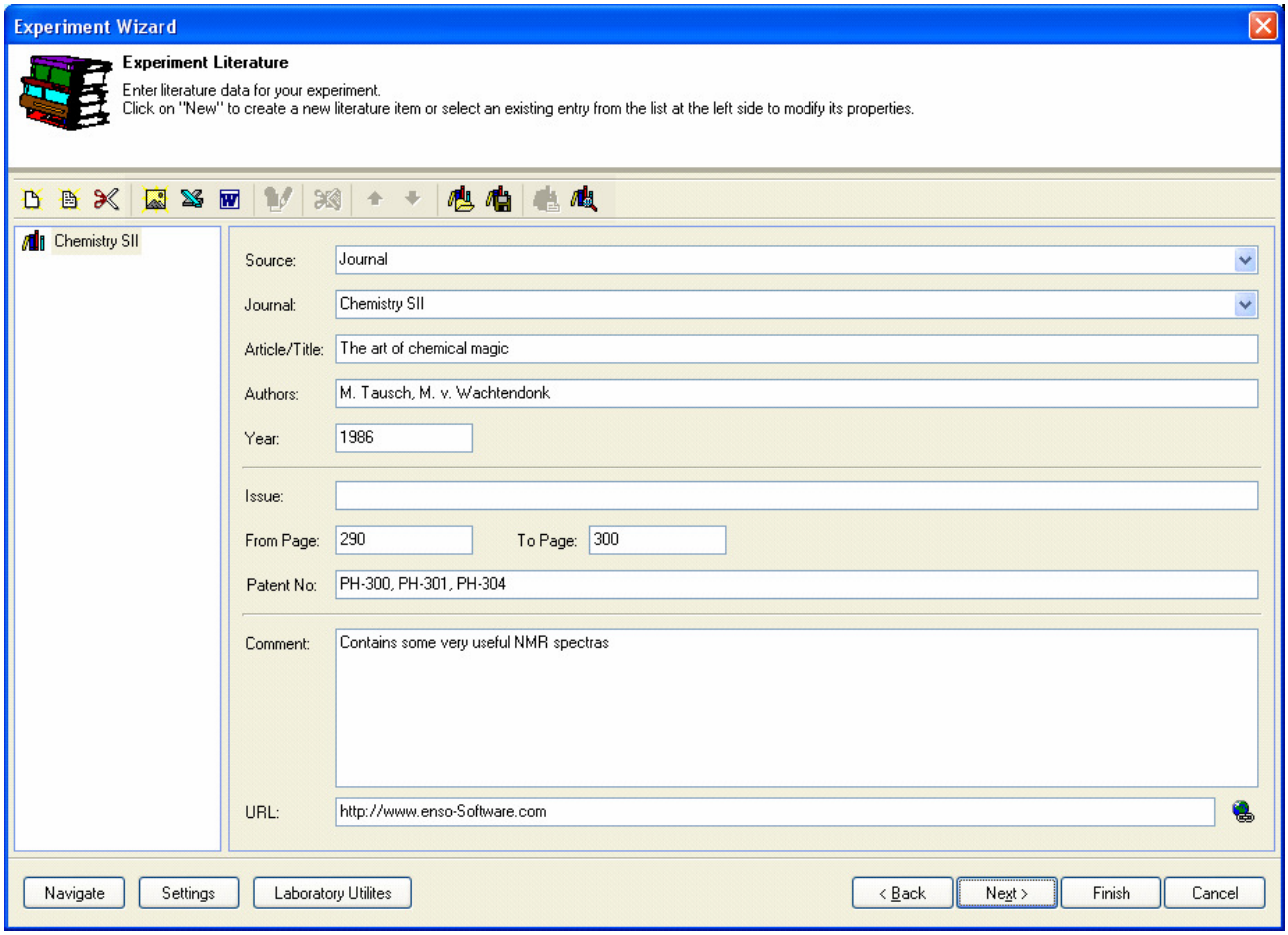
Every reaction parameter must have a name at least. If you enter a reaction parameter without a name, you’ll get an error message when trying to save the experiment.



The functions for editing the data are the same as those for the tabular description. You may also add an arbitrary number of records to your description and binaries (attachments) are not possible either.

Click on “Next“ to proceed with the assistant.

3.6. Literature



Now you can enter the literature you have used. Click on “New literature” ( ) to create a new literature entry. Then enter your data on the details pane at the right side of the window.
With the „Test URL“ button ( ) you can comfortable open the URL you have entered within your web browser.

With the list on the left side, you can select the literature entries you have already created. An existing entry can be deleted after being selected by using the function “Delete literature” ( ). The button “Copy literature” ( ) creates a copy of an existing entry. This is useful if you want to enter two different articles in the same journal or book where only the pages are different. Now, you do not need to enter the whole other data again.

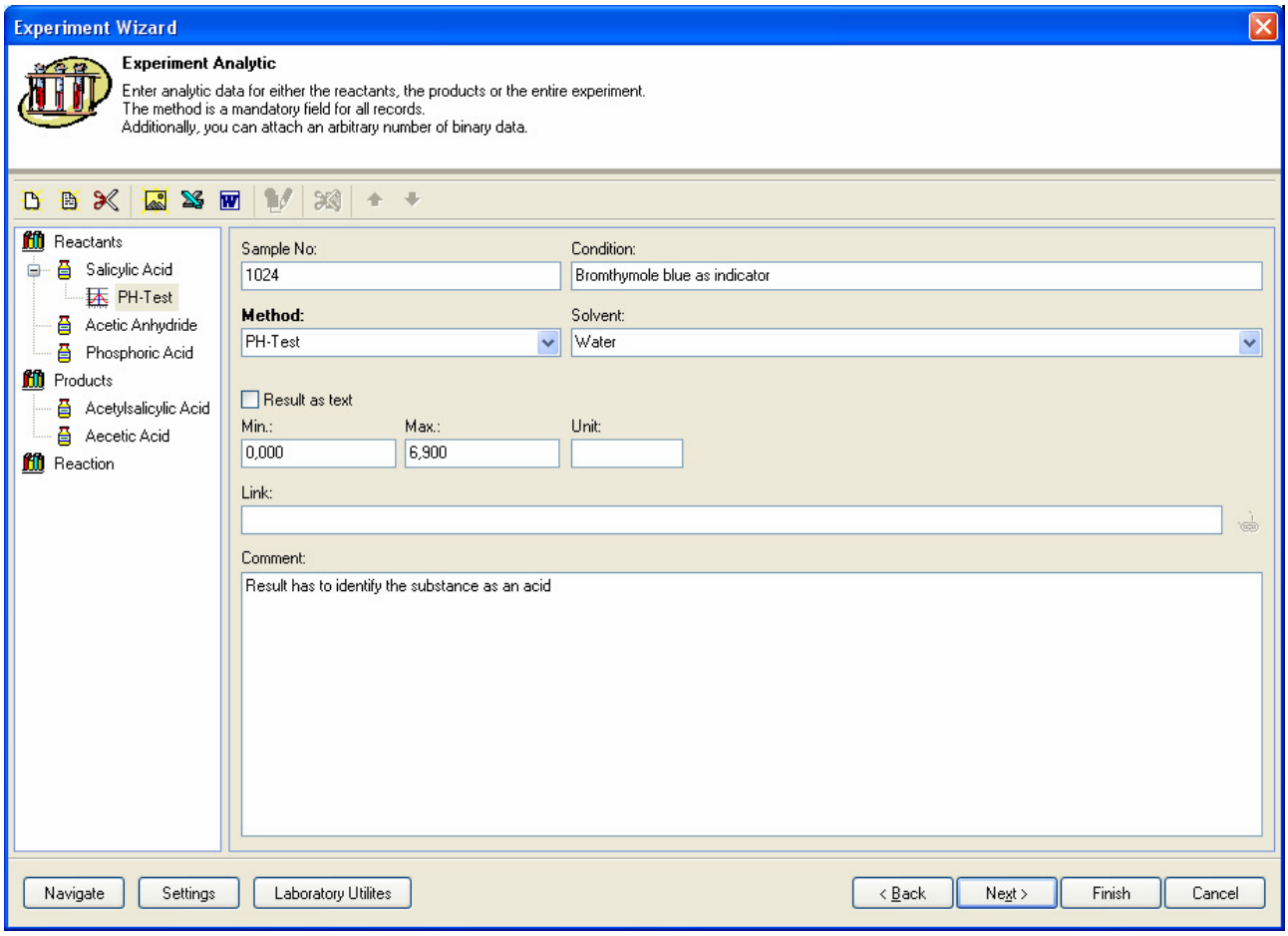
Using the green arrows ( ), you can change the order of your literature entries. This makes it possible to move your most important literature to the top of the list, for example.

It's also possible to import literature references from file ( ) or other experiments ( ). ensochemLab provides in addition to that an internal clipboard allowing you to paste data ( ) previously copied to that list. Last but not least you can export the selected literature to a file ( ). Files are expected and written respectively using the RIS format.

Just as you know it from the experiment description, you can add one or more binary attachments to your literature records. Please select a record and then use the “New binary” button () to add an attachment to it. Simply select the file you want to import and add additional information as an option.
If you want to delete an existing binary record, click on the “Delete binary” button ().

3.7. Analytics

Click on “Next“ to proceed to the analytics page.



On this page, you can enter the analytic procedures you have performed with the reactants, products or the whole reaction in your experiment.

Click on a reactant, a product or the whole reaction in the list at the left side of the window. Then select the “New” button ( ) to create a new analytics record or select an existing sub ordinary node to modify its data. The data is displayed in the details pane at the right side of the window where it can also be modified. You can have an unlimited number of analytics record for every category.
By clicking on the “Delete” button ( ), you can delete an existing analytics record. To duplicate an entry, just click on the “Copy” button ( ). These functions are only available when selecting an analytics entry, not a whole category or reactant / product.

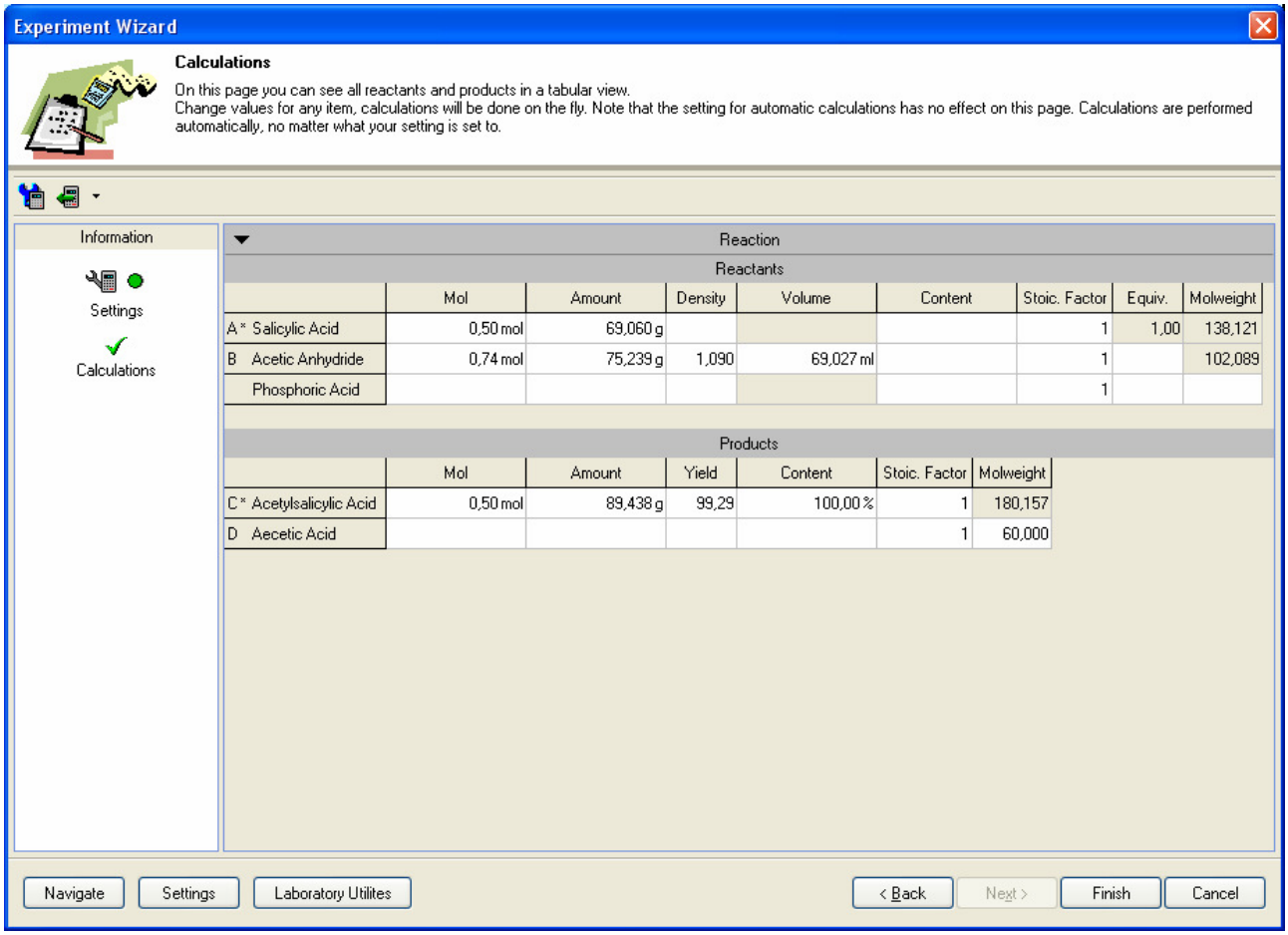
You have to enter a method for every record. You may either enter a free text value or select it from a list of analytic methods predefined by the administrator. If you enter a new value, it will be available for all other analytic records within this experiment. However, your value will not be added to the global list, and therefore, is not available when creating more experiments. Please contact your administrator if you want to enter a method for all experiments.
The list of solvents works exactly the same way.

The analytic result can either be a text or two numerical values: A minimal and a maximal value. You can define which mode you want to use by selecting the checkbox “Result as text”. ensochemLab will then modify the input fields accordingly. The “Comment” field is independent from your result type.

Just as you know it from the experiment description, you can add one or more binary attachments to your analytic records. Please select an analytic record and then use the “New binary” button ( ) to add an attachment to it. Unlike the description, you cannot enter other data concerning the binary (no descriptions …). It is completely sufficient to select the file you want to import.
If you want to delete an existing binary record, click on the “Delete binary” button ( ).

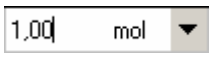
3.8. Calculations Page

Using the assistant’s “Next” button, you can proceed to the calculations page:



This page show all reactant and product data that can be calculated by ensochemLab in a summary table. The first table is for the reactants, the second one for the products. In addition to the fields known from the reactants and products pages within this assistant, there is also a “Volume” field which is only available if you have entered a density and the amount is specified as a mass. You can then work with mass and volume parallel.

Click into one of the cells to modify its content. As an example, we simple use the double reactant amounts for our experiments. Thus, please click into the “Mol” field in the “salicylic acid” row and enter a value of 1.00:



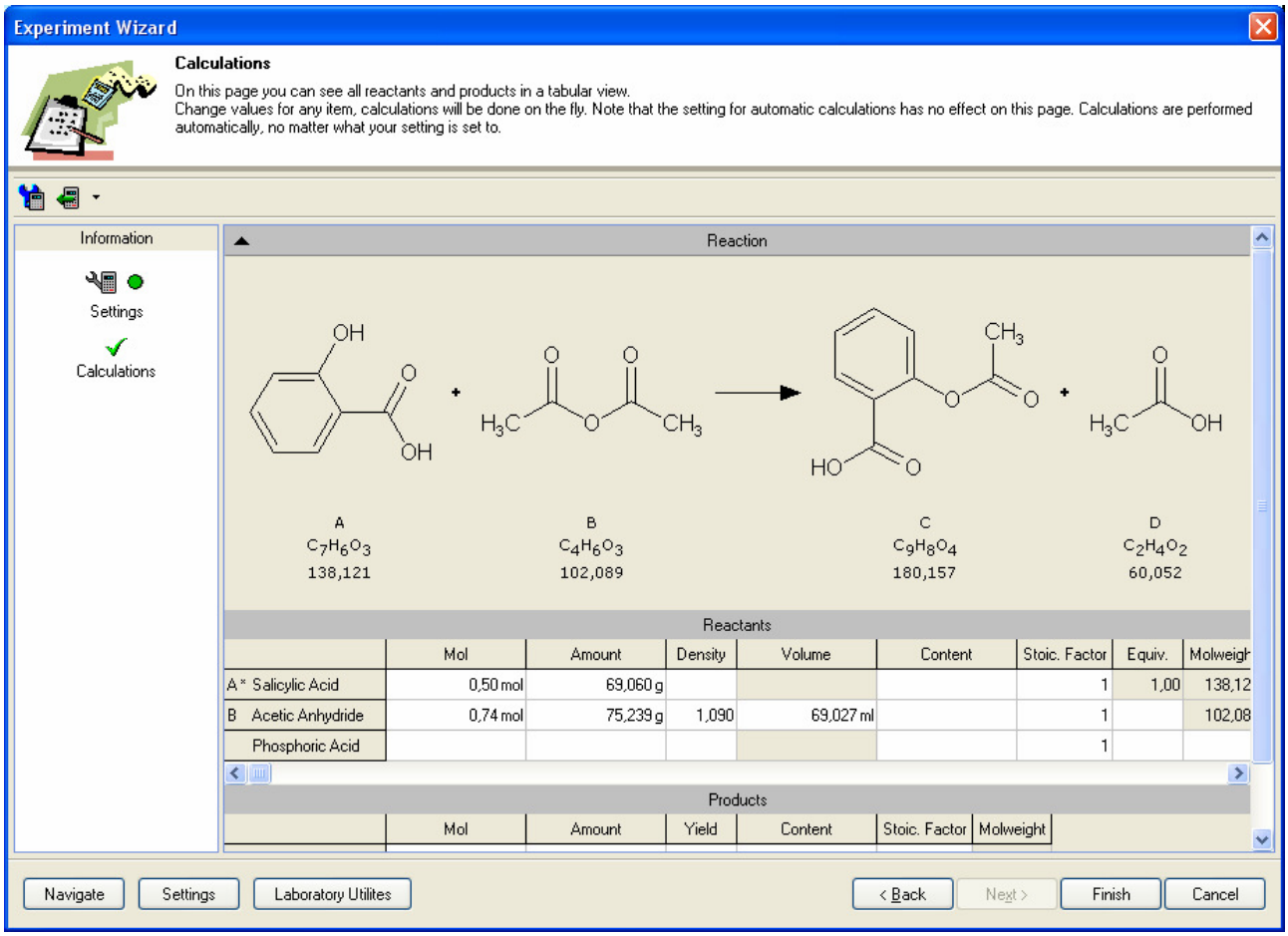
As soon as you exit the data field, ensochemLab will automatically recalculate all dependent values within the two tables. That means, that we are now also using 1,00 mol of acetic anhydride since both reactants are configured to have an equivalent of 1. The quantities have been doubled, too.

With the products, the yield has been decreased to 49,99 percent. That is almost the half minus a small value for rounding differences. The resulting amount is still a constant.
As we did not change the progress of our reaction, but have only used to double amount for each reactant, please enter the value of “100.00” as yield for both products.

With the products, the yield sank from 100%down to 49.99% which is about half as much minus a small rounding error. The resulting amount, however, has been kept as a constant.

Independent from whether the automatic recalculation of reactants and products is enabled in your personal settings or not, calculations are always automatically performed on this page. The calculation process (which value is calculated from which one?), however, is derived from your settings. The topic “Calculations” will be covered in detail by a dedicated chapter within this manual.

Using the arrow button in the reaction row, you can show the reaction. Due to its large size, it is normally not shown by default. You can hide it again by clicking on the button a second time.

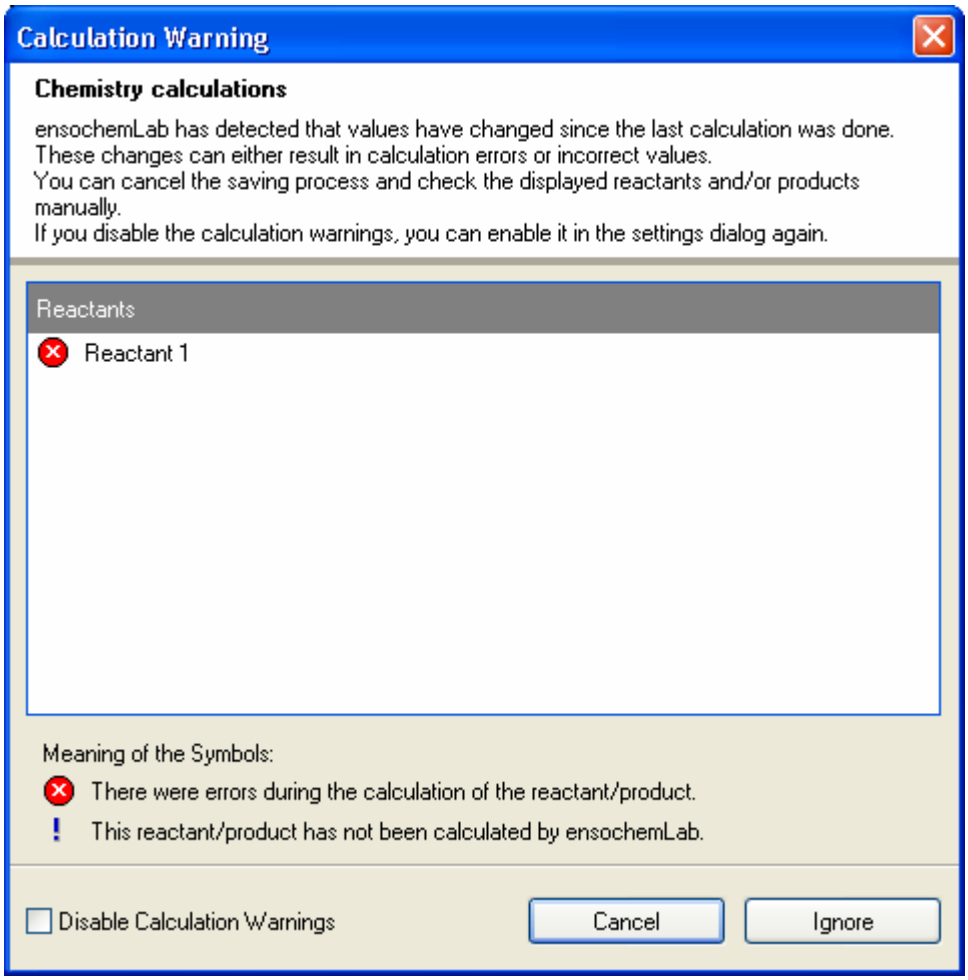


You have now entered all the data for your new experiment, so please click on “Finish”.

3.9. Saving Experiments

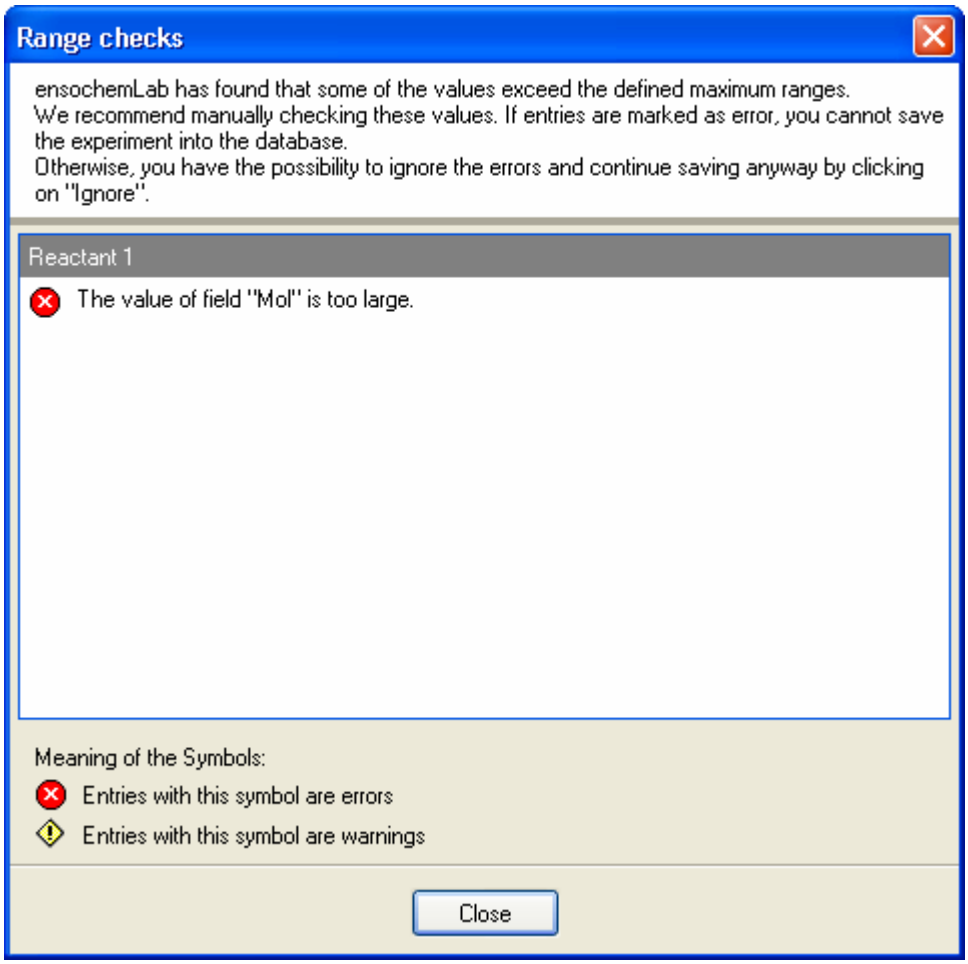
Before an experiment is actually saved, ensochemLab performs a number of checks regarding the data you have entered. For example, you are prompted to enter the mandatory data if it is still missing.

Additionally, ensochemLab recalculates your reactants and products in order to detect inconsistencies. During this process, the application also detects whether values needed for calculation have been omitted. The checks are performed regardless whether you have activated the automatic calculations or not. If errors are found, they are not automatically corrected, but displayed in a dialog for your information:



You can display the single error (⊗) or information (!) messages by moving your mouse cursor over the respective symbol in the list. There can be an arbitrary number of hints or alert for every reactant or product. With a click on “Cancel”, you can return to the experiment wizard for correcting your values or launching a manual recalculation. For ignoring the messages and continuing with the save process, please click on “Ignore”. With the “Disable calculation warnings” checkbox, you can select that messages of this kind shall not be displayed any more. However, please note that this is a global setting which means that it affects all current and future experiments. For later changing it again, please use the settings dialog (see chapter “Customizing your settings”).

Another important check is the number range verification. As this is just a check and not a calculation, the “Check calculation result ranges” setting is not applied either. If any errors or warnings are detected, the following dialog will be displayed:



The list shows all errors () and warnings () that have occurred grouped by the respective reactants and products.

Please that a value can never be saved into the database in the case of an error. That is why, in contrast to the calculation hint dialog described above, you can only ignore warnings, but not errors. Due to the errors, there is only a “Close” button in the dialog displayed above (see picture) which will take you back to the experiment wizard for changing your values.

If values are too large, you have to decrease the number of digits in front of the comma. The simplest way of doing so is changing to a larger unit. If there are not units that are large enough for your value, please contact your administrator.

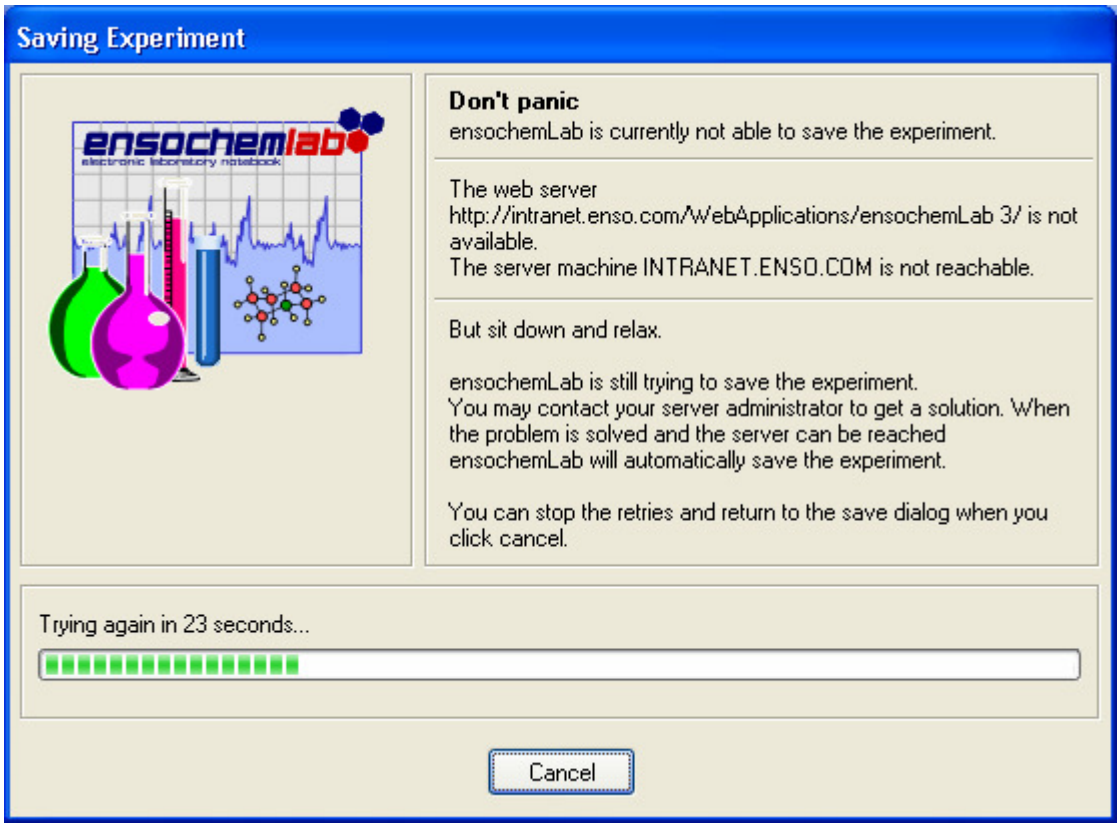
The following criteria are checked:

Type	Data field	Error criteria
Warning	Content	Value greater than 100
Warning	Yield	Value greater than 100
Error	Mol percent	More than 6 digits in front of the comma
Error	Equivalents	More than 4 digits in front of the comma

Error	Density	More than 2 digits in front of the comma
Error	Content	More than 3 digits in front of the comma
Error	Yield	More than 3 digits in front of the comma
Error	all data fields	The full value including digits in front and after the comma has a length of more than 18 characters.

ensochemLab will now save your experiment in the database. This may take some time, especially when you have added greater amounts of binary attachments.
As long as the saving progress is running, the program displays a black information window.

If the process cannot be completed (because of technical problems on your network for example), ensochemLab makes sure that your data is not lost. It will be stored in your computer's memory safely. Then the program waits until the server is accessible again and tries to save your experiment every 30 seconds. An information dialog shows whether your server machine is unreachable or whether there is a problem concerning only the ensochemLab server installation. You can forward these pieces of information to your system administrator if you like.



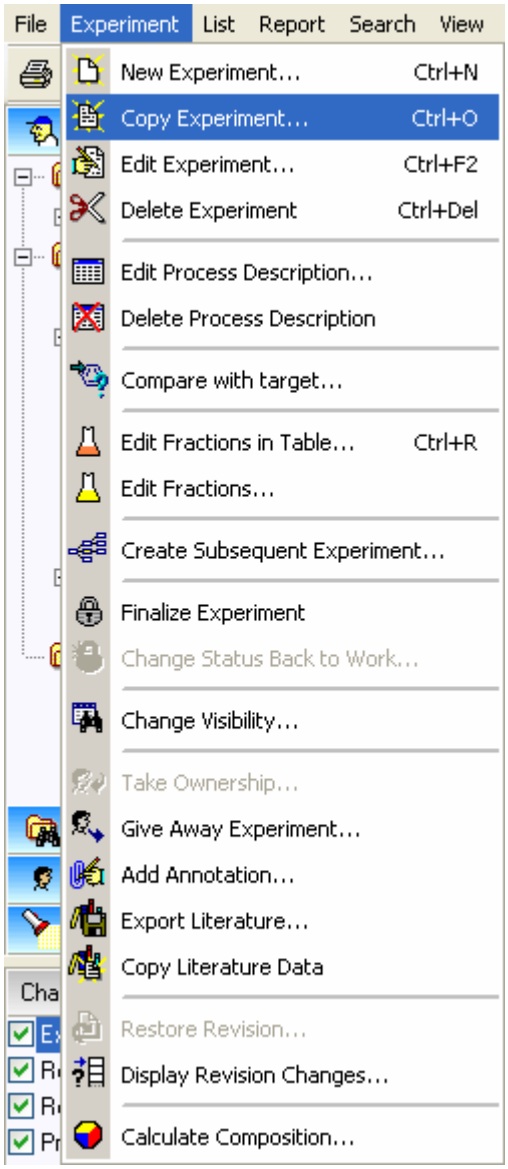
After ensochemLab has succeeded in saving your experiment, it will show an information dialog to notify you about this. If the experiment can be saved without any interruptions or errors, no message is displayed.

Summary:	The assistant can be used to create new experiment. It guides you step by step through the process. At its upper side, you can always find short help texts explaining what to do on the specific page.

3.10. Copying Experiments

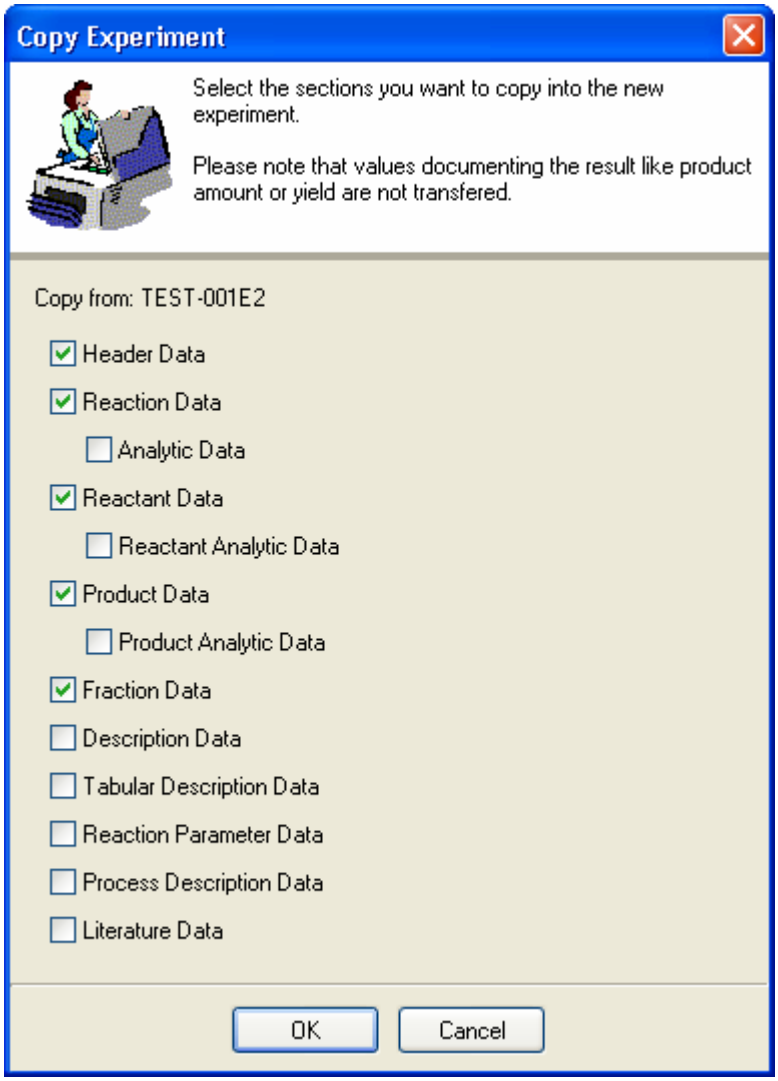
Before we proceed to the next “big” chapter in this manual, there is still another function in the context of creating new experiments that ought to be discussed. If you want to use an existing experiment as a template for creating new ones, and for example, change only the amount of reactant substances used, you can create a copy without having to manually reenter all the data. Furthermore, you can use this function to create slightly modified copies of other users’ experiments as you can copy every experiment you are allowed to view.

The respective function can be found in the main menu at “Experiment \ Copy Experiment”:



Alternatively, you can also use the associated toolbar button ().

A window will appear where you can select the data blocks you whish to copy:



Please select the entries for all data blocks to be copied and then click on “OK”. The experiment wizard will now open containing a copy of the original experiment, for which you will in best cases only have to enter a new experiment number. All data blocks that haven’t been copied remain empty.

Please note that result data like product yields is not copied as this data is regarded to be too dynamic for being the same for two experiments and that you will have to reenter it in any case.

The work with the experiment is exactly the same as it is when creating a completely new experiment which has already been explained in the upper parts of this chapter.

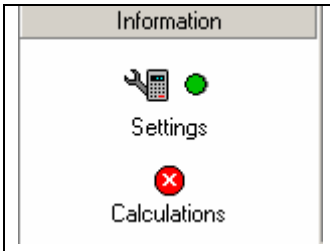
Summary:	With the “Copy Experiment” function, you can create a (modified) copy of an existing experiment without having to manually reenter all the data.

4. Automatic calculations

You have created your first experiment a few minutes ago and thereby used a number of simple, basic calculation functions. This chapter shall now explain the automatic calculation functions built into ensochemLab along with their configurable settings.
As there is a great deal of configuration settings, understanding of all the impacts of this function can be rather complex. Because of that, we have added some practical examples at the end of this chapter which shall ease your start with automatic calculations. Additionally, we recommend testing the function in order to get an own overview of the possibilities discussed herein. You can do so using the sample experiment we have just created, for example.

4.1. General settings

The automatic calculation functions can be widely configured in order to meet the current user's specific needs. You always have a quick overview over them because the following information box is displayed on every page where you can perform calculations:



Settings:

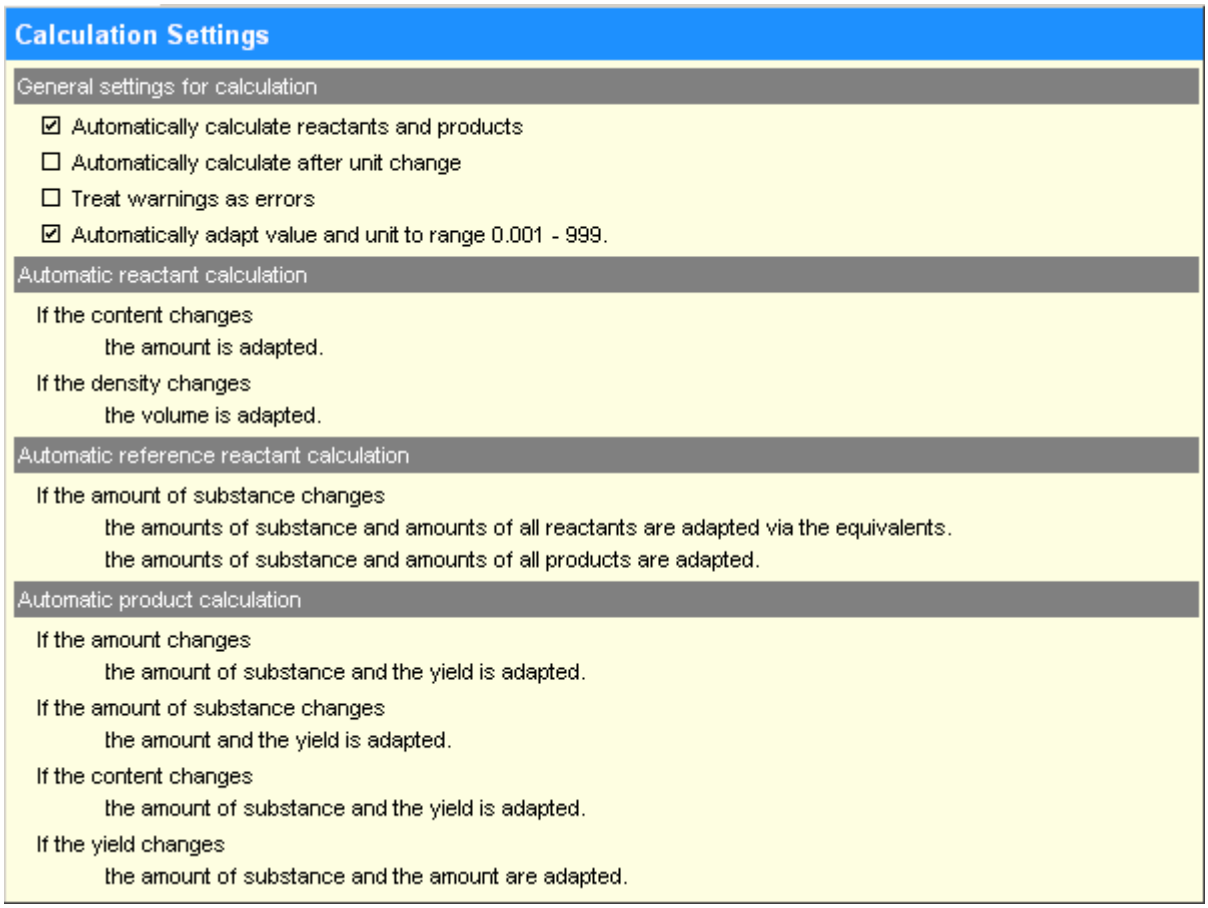
- Automatic calculation is enabled.
- Automatic calculation is normally activated, but has been temporarily disabled.
- Automatic calculation is disabled.
- Automatic calculation is normally disabled, but has been temporarily activated.

Calculations:

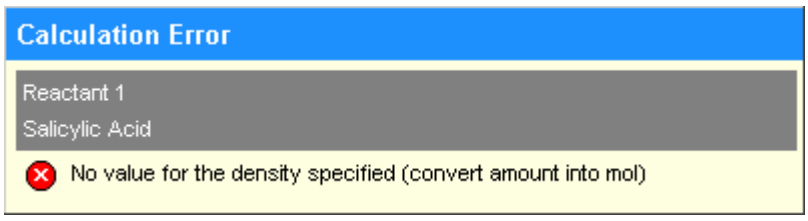
- There have been errors while calculating.
- The calculations have been performed without errors
- There are hints for this calculation.
- There are inconsistencies among the values. You should recalculate them

In order to get additional information concerning the calculations, please move your mouse cursor over the respective symbol.

If you move your mouse cursor over the symbol, the current calculation settings are displayed in the following hint window:



The ⊗ symbol indicates one or more errors in the calculations that have been performed. When you point over it with your mouse, these errors are displayed. For example, if you enter the amount as a volume and do not specify a density, you will get the following error message when leaving the data field for the amount:



Warnings and hints are displayed in the same way.

In addition to enabling automatic calculations, you can also specify that ensochemLab should adapt the calculation value (amount, mol, content) when you modify the corresponding unit so that it reflects the new unit. This means that 100 [ml] will become 0.1 [l] when the unit is changed to [l].
Please note that automatic calculations are always activated on the “Calculations” page within the experiment wizard.

Furthermore, ensochemLab is also able to adapt values to a range between 0.001 and 999. If a value falls out of this range, it is mapped to the respective bigger unit. For example, if a calculation yields in 1200 [ml], it becomes 1.2 [l]. Please note that this setting only affects calculation results.

The “Treat warnings as errors” option controls the behavior of the software when closing the wizard. If calculation errors occur, they are displayed before the experiment is saved. Normally warnings are not displayed. If this option is activated, ensochemLab will also show a dialog if there are only warnings.

4.2. Settings for automatic calculations

The options for the automatic calculations can be changed in the general settings dialog. Click on “Options” / “Settings” in the main menu and switch to the “Calculations” tab sheet. Within the experiment wizard, you can directly change these settings by clicking on the  button. Within the input sheet, they are additionally also available via the context menu.

If the automatic calculation functions are enabled, ensochemLab recalculates all dependent values when leaving a data field.

The way a recalculation has to be done greatly differs depending upon the respective situation (synthesis planning, correction of a value, newly entering a value and others). This is why there are special settings for every possible kind of calculation scenario:

Automatic reactant calculation

- If the content changes
  - the amopunt is adapted.
  - the amount of substance is adapted.
- If the density changes
  - the volume is adapted.
  - the mass is adapted.

Automatic reference reactant calculation

- If the amount of substance changes
  - the amounts of substance and amounts of all reactants are adapted via the equivalents.
  - the amounts of substance and amounts of all reactants are adapted with the factor (“old amount of substance” / “new amount of substance”)
- If the amount of substance changes
  - the amounts of substance and amounts of all products are adapted.
  - the product yields are adapted.
  - The amounts of substance and amounts of all products are adapted with the factor (“old amount of substance” / “new amount of substance”)

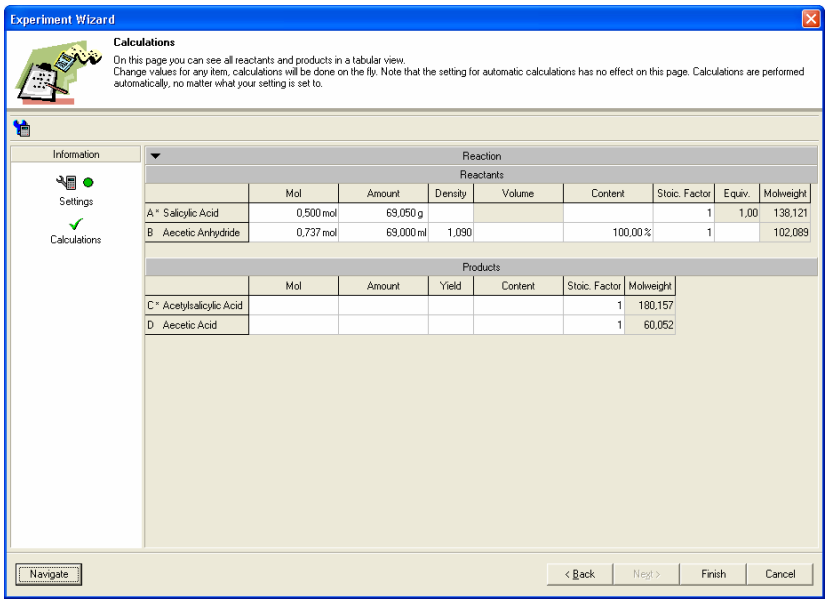
Automatic product calculation

- If the amount changes
  - the amount of substance and the yield is adapted.
  - the amount of substance of the product and the reference reactant is adapted.
- If the amount of substance changes
  - the amount and the yield is adapted.
  - the amount of substance of the reference reactant is adapted.
- If the content changes
  - the amount of substance and the yield is adapted.

- the amount is adapted.
- The amount of substance of the product and the reference reactant is adapted.

- If the yield changes
  - the amount of substance and the amount are adapted.
  - the amount of substance of the reference reactant is adapted.

The automatic recalculation of dependent calculation values can be activated for the reactant and product pages in the experiment wizard as well as for the editing of experiments “in display mode”. On the “calculations” page in the wizard, the function is always enabled:



In general, the aim of the automatic calculations feature is to calculate the amount of substance from amounts like mass or volume or vice versa. However, as these calculations depend on other values, changing them also has to trigger a recalculation.

Changes of the following values cause a recalculation:

1. Amount (mass, volume)
   - If the amount is changed, the amount of substance has to be changed, too, of course. When dealing with reactants, adapting the amount of substance also changes the equivalents. With products which have the additional yield value by definition, there are two additional calculation alternatives that can be configured in the user settings. Either the yield of the product or the amount of substance of the reference reactant is adapted. Changing the amount of substance of the reference reactant itself causes a great number of recalculations among reactants and products.
2. Amount of substance
   - Changing the amount of substance impacts the mass (or the volume respectively if a density is specified) in any case.
   - If the amount of substance of the reference reactant is changed, this impacts all reactants and products. For all reactants, the amounts of substance are recalculated either via the

equivalents or (if configured) via the factor “old amount of substance” / “new amount of substance”. This of course also changes the amounts of all reactants.

3. Content
    - Changing the content can either cause a recalculation of the amount of substance or of the amount. The direction in which ensochemLab shall calculate – amount of substance or amount – can be configured in the user settings.
4. Density
    - If the density is changed, the application can recalculate either the mass or the volume. The desired operation can be configured in the settings.
    - The density field is available only for reactants.
    - The volume can only be directly specified on the “Calculations” page in the experiment wizard or when editing experiments “in display mode”, if a density is available.
5. Molar Mass / Molweight
    - Changing the molweight (molar mass) is treated like changing the content.
6. Yield
    - Recalculations after changing the yield can impact either the amount of substance or amount of the respective product or on the amount of substance of the reference reactant. The latter will, of course, lead to a recalculation of all reactants and products.
7. Equivalent / Mol percent
    - If the equivalents are changed, the amount of substance and the amount of the reactant are adapted.
    - When changing the equivalent of the reference reactant, the amounts of substance of all other reactants are adapted regarding the new equivalents. When calculating vice versa, the equivalents are adapted when the user changes the amount of substance of a reactant.
8. Load / Charge
    - The charge [mmol/g] can be used independently of the content.
    - The calculation corresponds to the one of the content by regarding the unit [Mol/Mass].
    - In addition to using the content with the [Mol/Mass] unit, there is the possibility to specify a carrier substance along with the charge.
    - The [mmol/g] unit is built into the application and cannot be changed.
    - The behavior when changing the charge corresponds to the one when changing the content.

4.3. Examples on the impacts of automatic calculation settings

4.3.1 General

The complex impacts of some settings can be reviewed and more sophistically understood using the following examples:

Initial situation

	Mol	Amount	Density	Volume	Content	Equivalent	M
Reference Reactant	0,08 mol	16,660 g	1,100	15,146 ml		1,00	208,254
Reactant 2	0,46 mol	67,000 g			98,5 %	5,81	141,940
	Mol	Amount			Content	Yield	M
Product	17,35 mmol	3,3 g				21,68	190,238

In all sample cases, one value is always changed. This manually changed value is displayed in blue whereas the recalculated values are displayed in red.

4.3.2 Changing the amount of substance of the reference reactant

Settings "The amounts of substance and amounts of all reactants are adapted" and "The product yields are adapted"

You have planned to use 16.6 of the reference reactant. In reality, you have used 17g.

	Mol	Amount	Density	Volume	Content	Equivalent	M
Reference reactant	0,08 mol	**17,000** g	1,100	15,455 ml		1,00	208,254
Reactant 2	0,47 mol	68,366 g			98,5 %	5,81	141,940
	Mol	Amount			Content	Yield	M
Product	17,35 mmol	3,3 g				21,25	190,238

Setting "The amounts of substance and amounts of all products are adapted"

Which product amount do you get when use 17g of the reference reactant instead of 16.6g?

	Mol	Amount	Density	Volume	Content	Equivalent	M
Reference reactant	0,08 mol	**17,000** g	1,100	15,455 ml		1,00	208,254
Reactant 2	0,47 mol	68,366 g			98,5 %	5,81	141,940
	Mol	Amount			Content	Yield	M
Product	17,76 mol	3,367 g				21,68	190,238

4.3.3 Changing the amount of the product

The product's amount is corrected from 3.3g to 4g.

Setting "The amount of substance and the yield is adapted"

If the weighing out of the product is to be corrected, this setting is the right one.

	Mol	Amount	Density	Volume	Content	Equivalent	M
Reference reactant	0,08 mol	16,660 g	1,000	15,146 ml		1,00	208,254
Reactant 2	0,46 mol	67,000 g			98,5 %	5,81	141,940
	Mol	Amount			Content	Yield	M
Product	21,03 mmol	**4** g				21,68	190,238

Setting "The amount of substance of the product and the reference reactant is adapted"

You plan to create 4g of the product. With this setting, you calculate the weighing in amounts of the reactants.

	Mol	Amount	Density	Volume	Content	Equivalent	M
Reference reactant	0,10 mol	20,194 g	1,000	18,358 ml		1,00	208,254
Reactant 2	0,58 mol	83,579 g			98,5 %	5,81	141,940
	Mol	Amount			Content	Yield	M
Product	21,03 mmol	4 g				21,68	190,238

4.3.4 Changing the yield

The yield of the product is changed from 21.68% to 30.00%.

Setting "The amount of substance of the reference reactant is adapted"

	Mol	Amount	Density	Volume	Content	Equivalent	M
Reference reactant	0,06 mol	12,042 g	1,100	10,947 ml		1,00	208,254
Reactant 2	0,34 mol	48,995 g			98,5 %	5,81	141,940
	Mol	Amount			Content	Yield	M
Product	17,35 mmol	3,3 g				**30,00**	190,238

4.3.5 Changing the content

The content of the second reactant is decreased from 98.5% to 88.5%.

Setting "The amount is adapted"

	Mol	Amount	Density	Volume	Content	Equivalent	M
Reactant 2	0,46 mol	74,571 g			**88,5** %	5,81	141,940

Setting "The amount of substance is adapted"

	Mol	Amount	Density	Volume	Content	Equivalent	M
Reactant 2	0,42 mol	67,000 g			**88,5** %	5,22	141,940

4.4. Special content units

4.4.1 Mol percent

Mol percent values are only used when dealing with fractions for calculating the portion of the total amount of substance that is split upon a special product. The calculated values can be transferred to the products from that location. After applying the values from the fraction, you cannot continue working with mol percents.

4.4.2 Volume / Volume

As the density of the pure substance is unknown, it is not possible to perform calculations via volume / volume units. The application displays a hint in such a case and calculates an approximate value using the mass / volume unit.

4.4.3 Area percentages

Area percentages are approximately regarded as mass or volume percentages depending upon the amount unit. The specification of area percentages is for information purposes only.

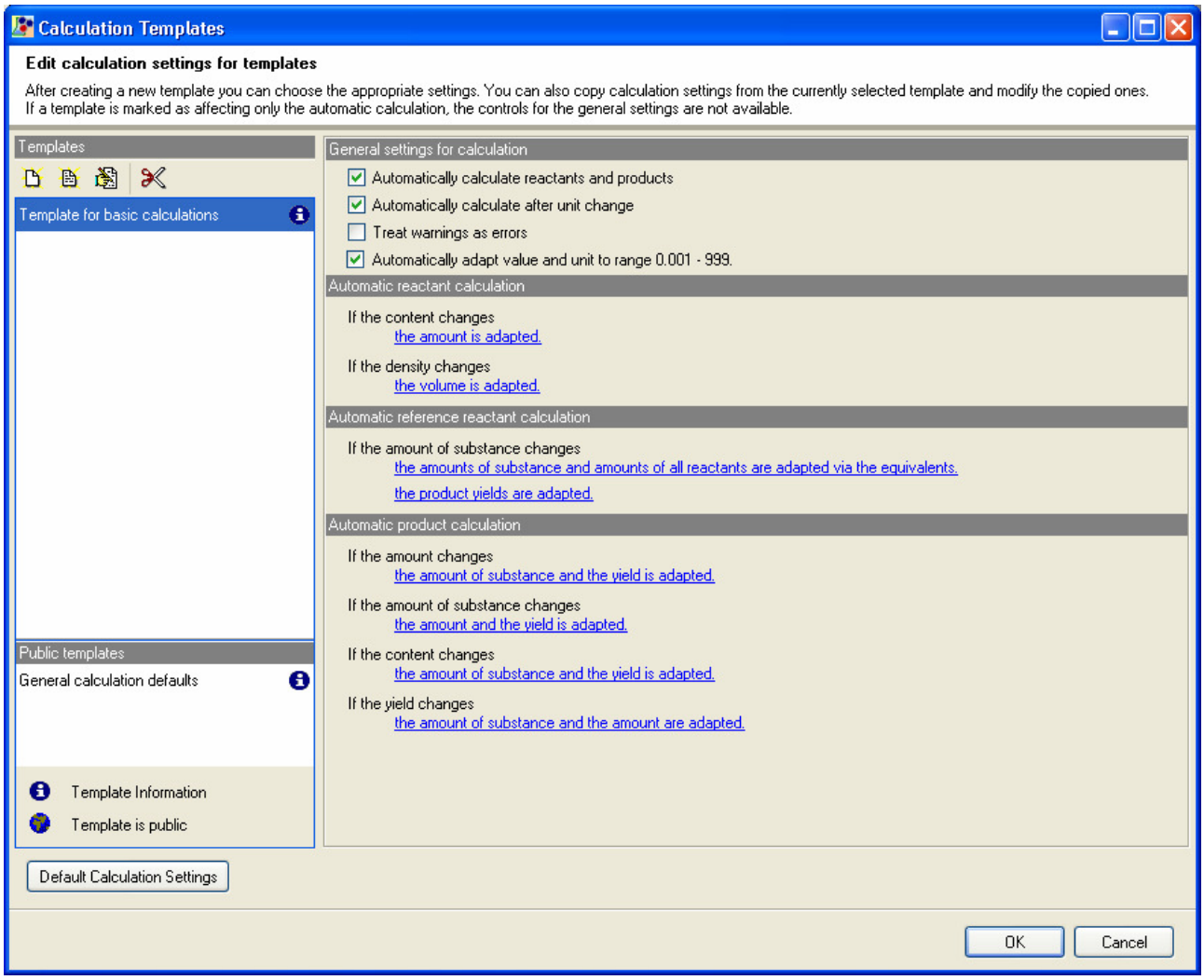
4.4.4 Fractions

From ensochemLab version 3 on, you can also use mol percentages instead of mass and area percentages. You can also apply this unit to the products along with the other data. The mol percentages are only used for calculations within the fractions module.

4.5. Calculation Templates

You can combine a set of calculation settings and save it as a template. This enables you to quickly switch between two or more sets of settings without having to reconfigure everything.

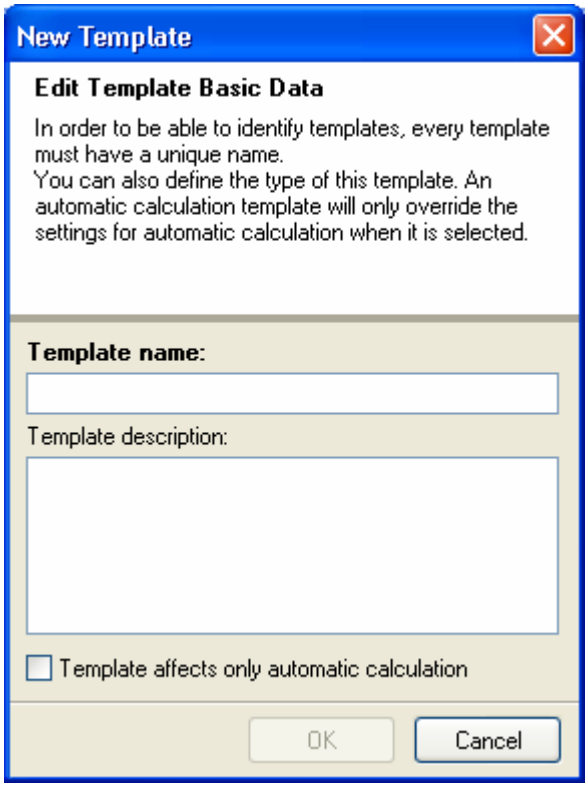
In order to create a calculation template, please click on the “Edit Calculation Templates” entry in the “Options” menu. The following dialog will appear:



In the upper left list, you can see your existing calculation templates (if any). In the lower left list, there are the public calculation templates your administrator has predefined for you.

A globe icon generally indicates that the respective template is public. If you move your mouse cursor over the information symbol, a hint containing the corresponding template’s owner and the comment he has entered is displayed. If the template does not have a comment, a respective hint is displayed.

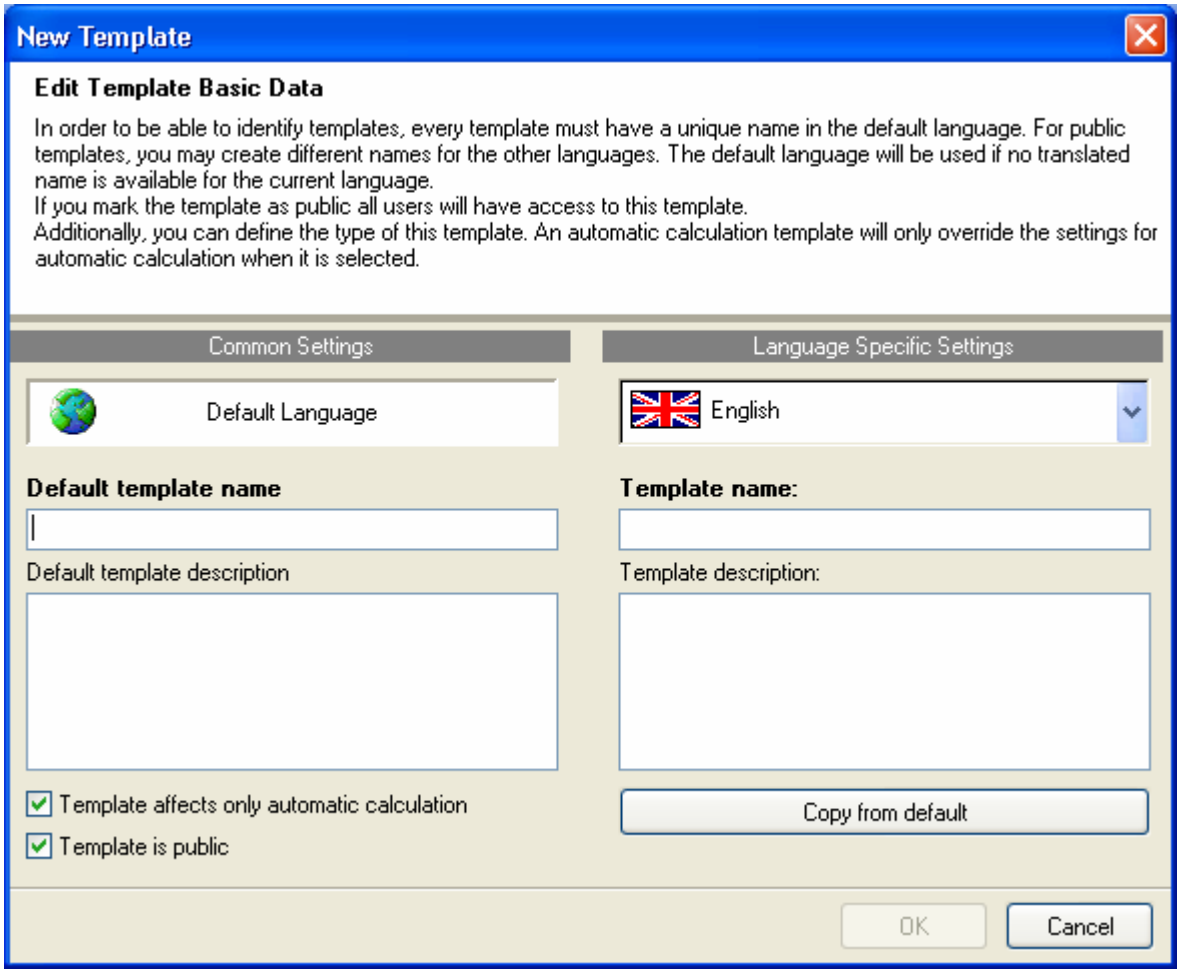
For creating a new private calculation template, please click on the “New” button ( ) in your toolbar. A dialog appears in which you can enter a name and a description (comment) for your new template:



With the checkbox “Template affects only automatic calculation”, you can define that all settings which do not apply to automatic calculation shall be removed from your calculation template.

After you have entered your data, please click on “OK”. The dialog will be closed and your new calculation template will be added the upper left list.

If your administrator has activated the function of creating public calculation templates for normal users, an extended description dialog is displayed instead of normal one visible on the last page. The data fields for name and description that have already been discussed correspond to those on the left, language-independent (common) side.
There, you can also specify whether you want to mark your calculation template as public in order to make it available to all ensochemLab users.



If you publish your calculation template, you can use the controls on the right side for entering optional translated description data that will be displayed to users who have started ensochemLab in a different language. For doing so, please first select the desired language and then enter the respective description data in the controls below. After entering a name and a description, you can switch to a different language and enter the data for it. For modifying the previous language's data, just switch back to it.
By clicking on "Copy from default", you can copy the language-independent data into the current language. However, please note that this only creates a copy which means that if you modify your language-independent data later, the change will not be applied to the localized copy.

You can modify an existing template's description data by first selecting it in the list and then clicking on . With the button, you can delete the current template. However, please note that these functions are only available for own templates, not for those predefined by the administrator.

If your administrator has allowed you to create own public calculation templates, a different, extended dialog will be displayed when you click on the "Next" or "Edit" button in the toolbar. This dialog is explained in detail within the administrator's guide. It does not only contain the option to mark the current template as public but also allows you to enter a translated title and description for every language supported by ensochemLab. You can do so on the right side of the dialog where you can use the drop-down menu to first select the desired language and then enter your data into the fields below.

The configuration of the calculation settings contained in your template is done in the main dialog (see the screenshot on the previous page). After you have selected a template, the right side of the window contains a settings panel as described earlier in this chapter. Just do your settings changes to an arbitrary number of templates and then close the dialog by clicking on "OK". With a click on "Cancel" you can return to ensochemLab by restoring all original settings and templates.

If you just want to slightly modify a template and then save it under a new name, please select the original template and then click on the "Copy" button ( ) in the toolbar. The same dialog as above will be opened in which you can enter a title and a description for the copy. After you have clicked on "OK", the copy will be added to the list as a normal template.

4.6. Calculation Functions

At the places within the application where calculations are performed, you can manipulate the calculation behavior via a number of buttons that are described in this sub-chapter. However, please note that there may not necessarily be all functions at all places.

With the "Calculation Settings" button ( ), you can open the settings dialog for modifying your own personal calculation configuration.
If you have normally activated the automatic calculation features, you can temporarily disable them just for the current editing session by just clicking on the respective button ( ). If the button is pressed, automatic calculation is disabled for the moment. For enabling it once again, please click the button again.

Of course, this process also works vice versa: If you have disabled the automatism in your personal settings, the button just looks slightly different ( ). Accordingly, a click on it enables the functions.

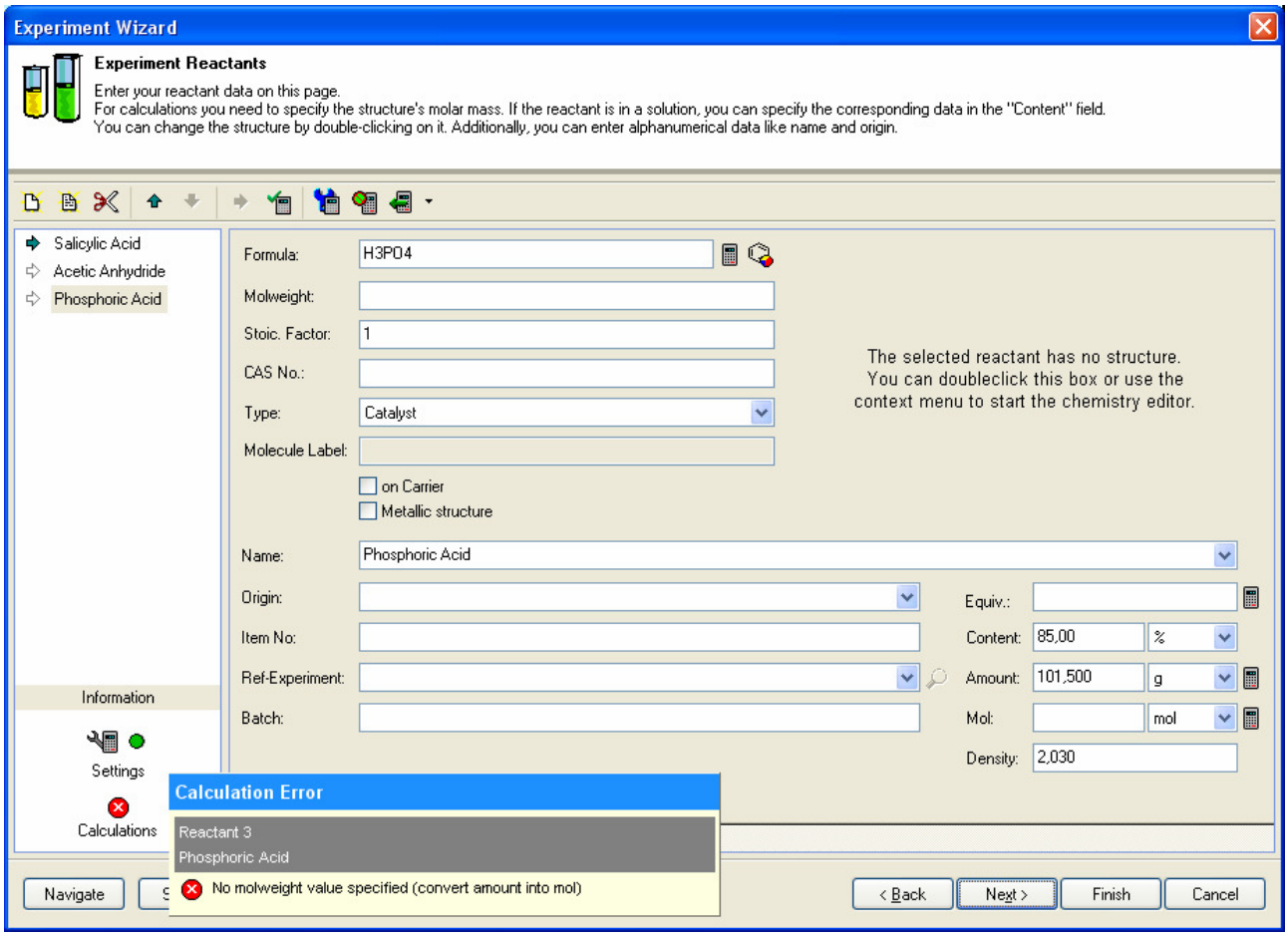
Please note that these options affect the whole current window or assistant page. It is not possible to for example distinguish between two places on the same page within the experiment wizard.

After leaving the current editing mode, the temporary settings become invalid are thus reset.

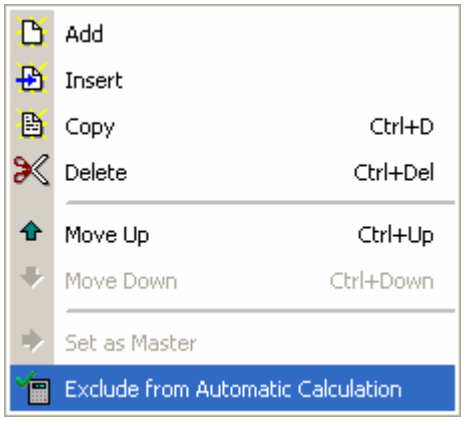
You can also permanently override your personal calculation settings with the values of a template by using the template button's ( ) pull-down menu.

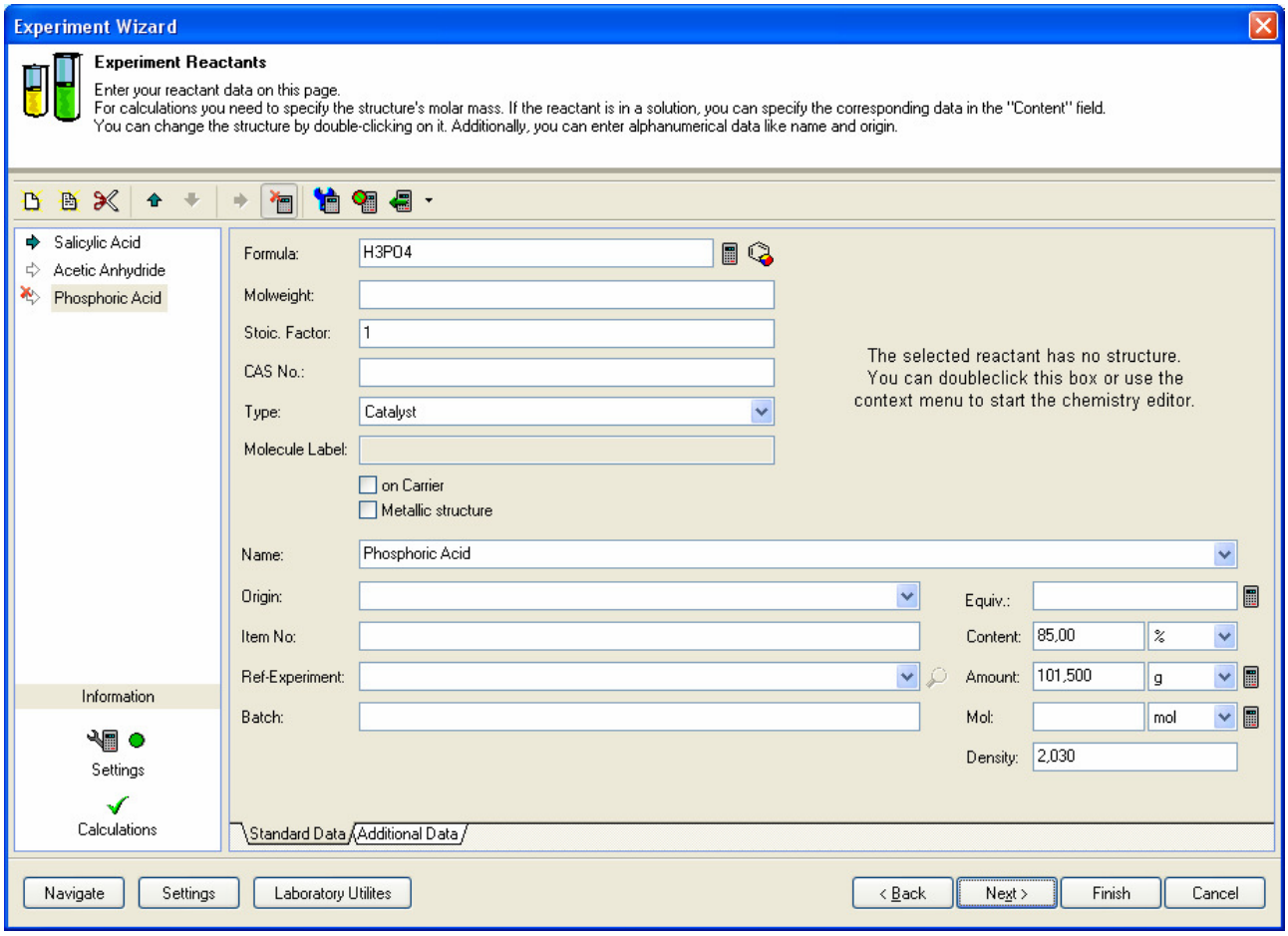
4.7. Exclude Reactants from Automatic Calculation

Under certain conditions it's helpful or necessary respectively to exclude dedicated reactants from automated calculation. Such a flag will be stored with the data of a reactant. That way it's persistent for later adjustments and permanently documented.

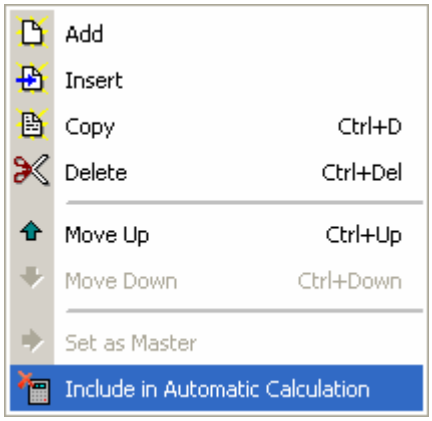


You can control the behavior by either choosing the button ( ) or using the context menu.





A currently excluded reactant can be added back to automatic calculation later. Simply use the appropriate button ( ) or the context menu.

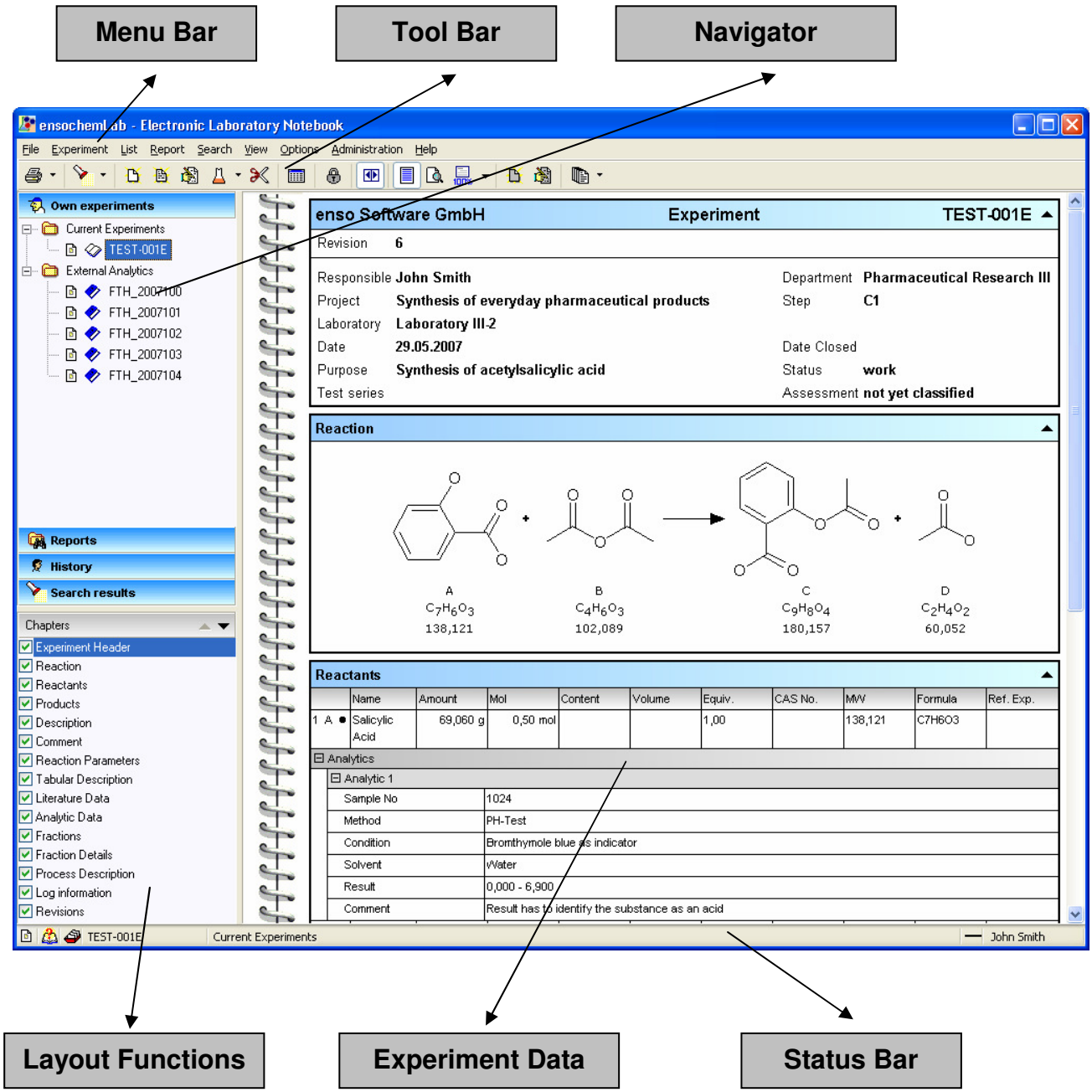


Summary:	Automatic calculations are a versatile feature to see the impacts of changing the amount, equivalents and other values of one molecule on other molecules within the reactions. However, this requires a configuration that meets your desired work flow and calculation scheme.

5. The main window

Having just saved our first experiment to the database, it is a good time to take a closer look at the main window. The main window is the place where experiments are displayed and managed.

You get there right after your login or when returning from the assistant. If you create or modify an experiment, ensochemLab will automatically display it when you return:



5.1. The navigator

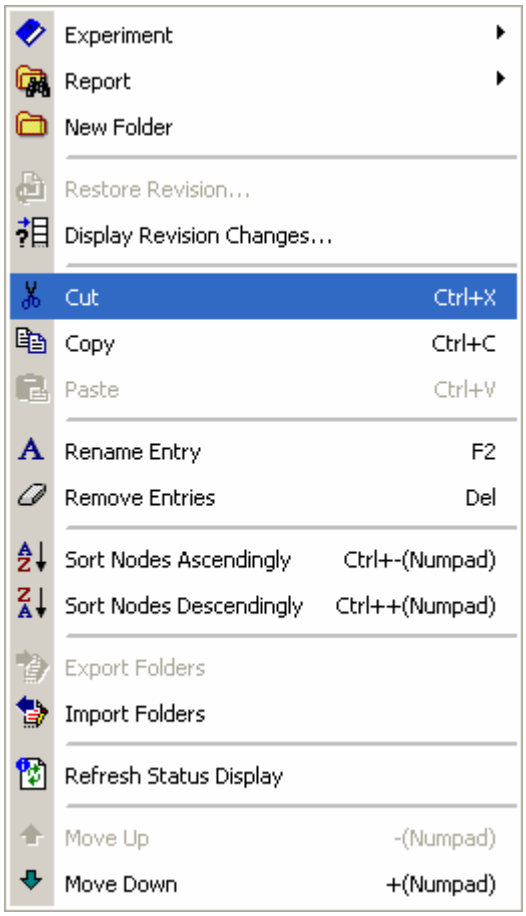
The experiment we have just created can be found in the navigation pane at the left side of the window where it is located in the category “History”. There are four different categories for experiments:

Own experiments	This is a category where you can manage your own hierarchical list of experiments – your “personal folder”
Reports	You can use this category to separately store, organize and manage your reports independently from your experiments.
History	The history folder contains all experiment you have created or edited during this session. That’s why our sample experiment is located here.
Search results	This folder is used to store all search results in. Searching experiments will be discussed later in this manual.

All categories can be opened by clicking on the respective header in the navigation pane at the left side of the main window.

The folders “Own experiments“, “Reports” and “History” are saved when terminating ensochemLab and, thus, are available in your next session, no matter which computer you use to access the program. The “Search results” folder will be deleted when logging out.

There are multiple possible ways to move an experiment from one of the other folders to the “New experiment” section. For the first example, please select it in the navigator and then open the context menu by right-clicking on it. Now choose the “Cut” option:

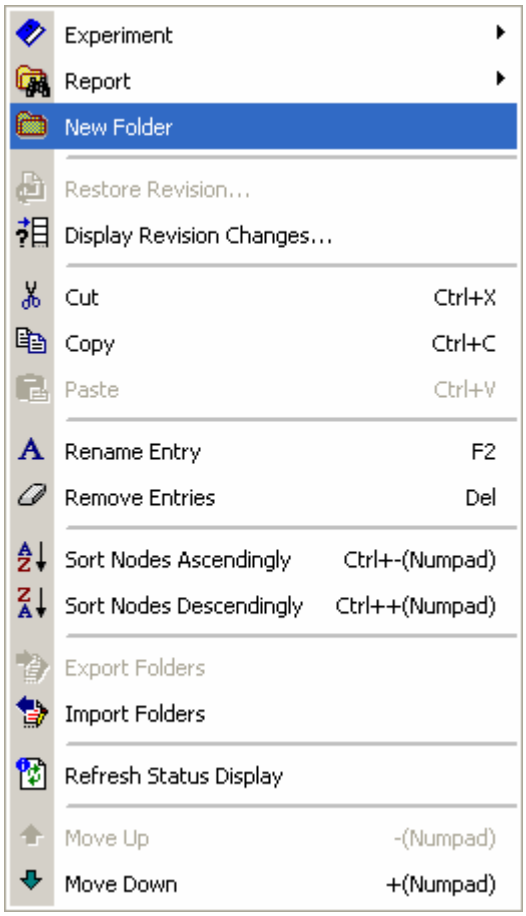


If you want to copy the experiment link without removing it from the “History”, please select the “Copy” option instead.

Now change to the “Own experiments” section where you can open the same context menu at any position (also in the free space). Now we only have to “Paste” function and the experiment is moved into your personal folder.

Of course, this can also be done much more quickly: Just move the entry into the desired target folder via drag & drop. If you want to move it into another category, please hold down the left mouse button over the category entry in the navigator for a short time while moving and ensochemLab will open it for you.

As already said, this folder can have any kind of hierarchy. To create subfolders, please click on “New Folder”:



ensochemLab creates a new, empty folder for you and entitles it “New folder”. At first, you should enter a name for it. To move an experiment into this new folder, you can use the same functions as described above.

Remarks:	Folders are always created as subfolders of the currently active folder. This can be a root node (category) or any other folder created by you.

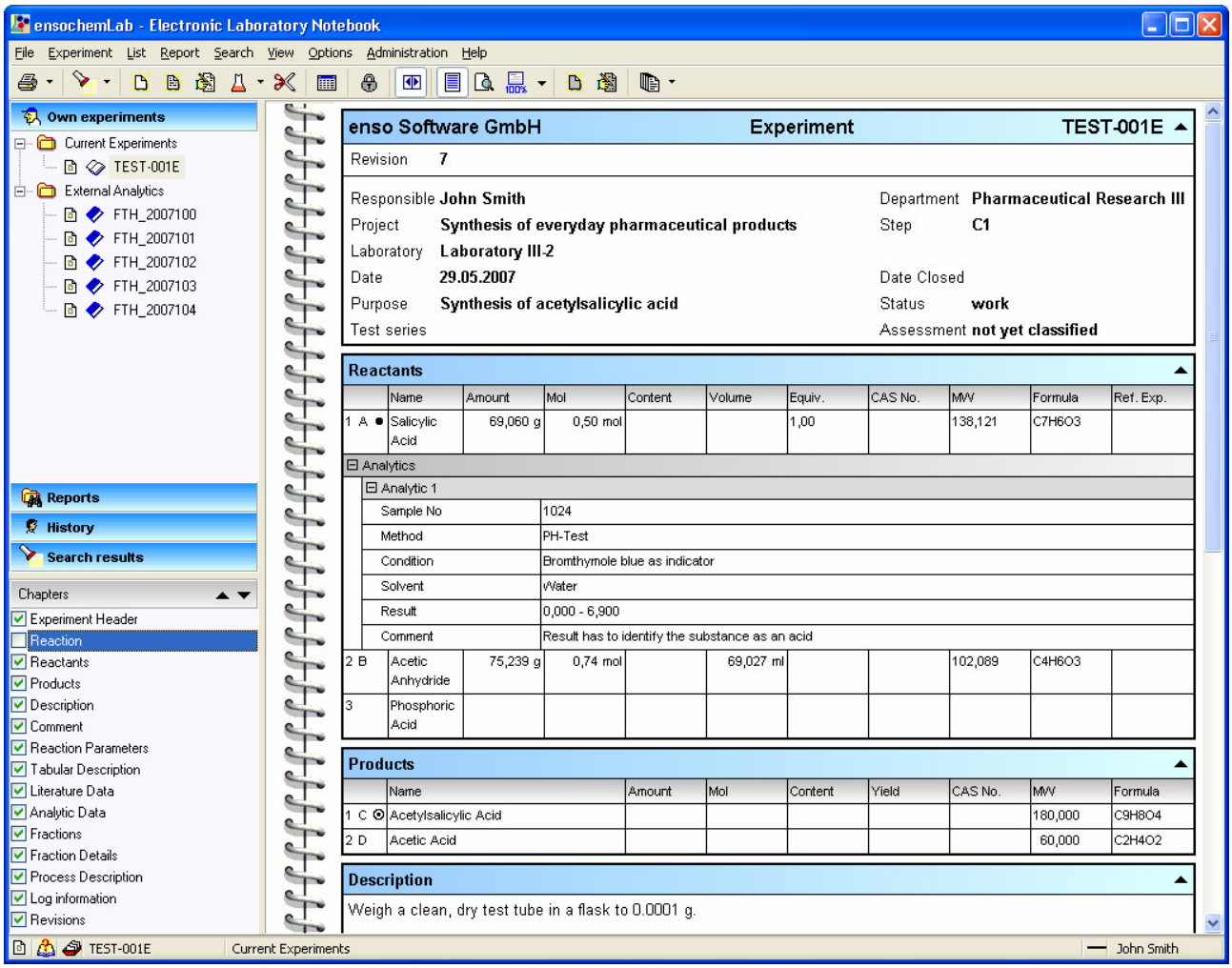
Later, you will have more than one experiment in your folder. Then you can use the “Move up” and “Move down” functions to change the experiment order within your folder. With the “Rename” function, you can assign a new name to existing folders.

Remarks:	ensochemLab does not actually save the whole experiment in your folder. The program only creates a link and that’s why the rename

	function, for example, cannot actually change the name of your experiment – it just changes the link to match another experiment. Furthermore, the “New” function cannot create a new experiment – it also creates just a link to an existing experiment. When using this function, you have to enter the name of a valid and already existing experiment.

5.2. The experiment display

Your experiment data can be found at the right side of the main window. If you do not want to see all the data, you can hide specific blocks of the display by deselecting them in the chapter box at the lower left side of the main window. As an example, please uncheck the box beside the “Reaction” entry and see what happens:

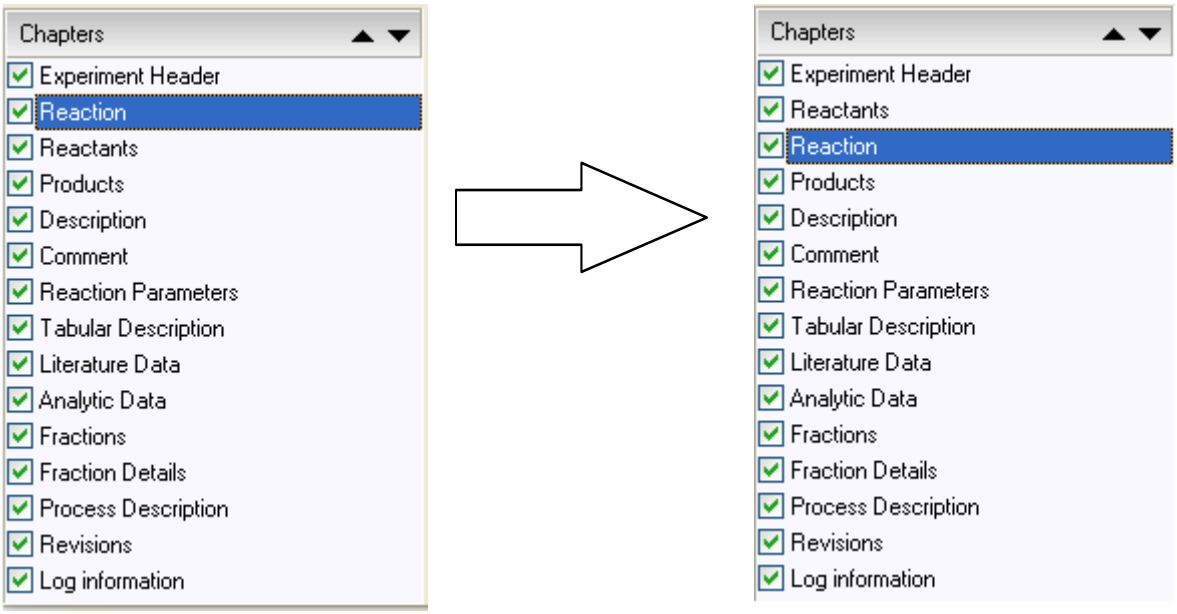


The reaction has been removed from the experiment display frame. You can insert it again by selecting the checkbox beside “Reaction” once more.

Remarks:	When hiding a block from the experiment display, your data is not deleted of course. It is only invisible, but still there, even if you terminate the program in the meantime.

The list of chapters may look different on your system because the administrator can configure the availability for some of the chapters

You can also move certain chapters by changing their titles’ orders in the list you have just used to hide the reaction block. For doing so, click on the arrow buttons (▲ ▼) in the headline of the chapter box.

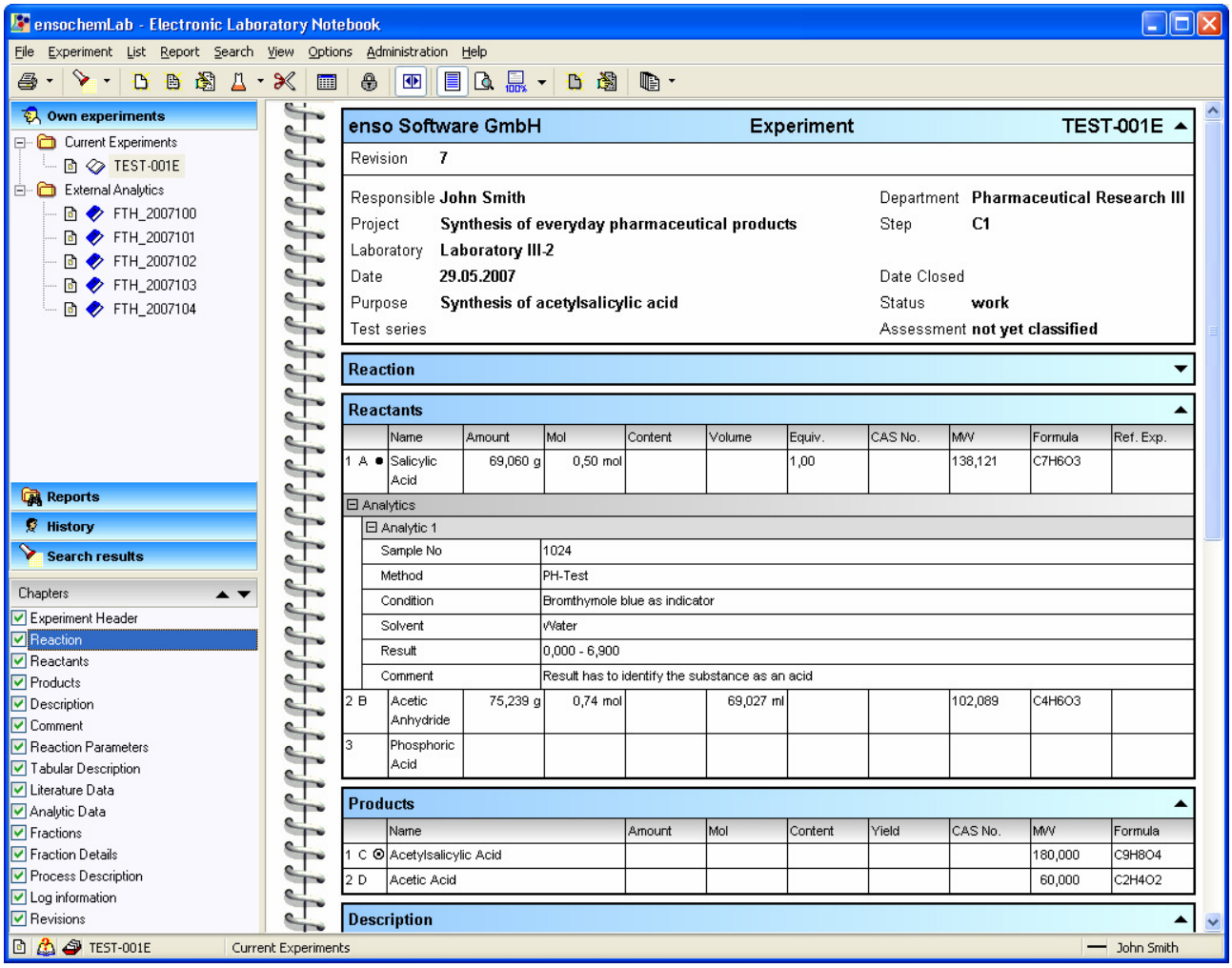


For this example, we return to the original display order and take a look at another possibility to show or hide chapters. Please click on the small in arrow in the headline of the specific chapter to demonstrate this function:

As we have seen, the arrow has changed its direction: If the data block is open, the arrow points to the top and closes the chapter when you click on it. If the chapter is already closed, the arrow points to the button enabling you to open the chapter again by clicking on it.

If you close a chapter this way its headline remains visible, but without the respective data. Please note that this also includes other display modes and even printouts. We will discuss further details of this aspect in another chapter of this manual (see chapter “Printouts”).

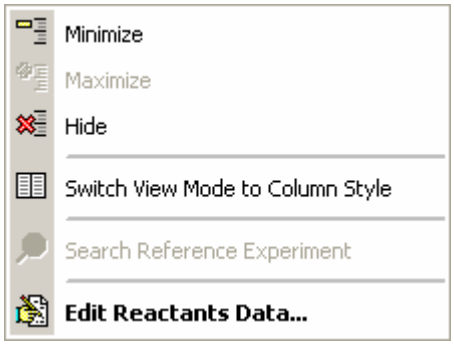
The main window with closed reaction block:



Depending on your current ensochemLab settings, the reaction will be displayed differently. There is the possibility to highlight reagents, target molecules and solvents with colors in a number of different ways if demanded. More information about this topic can be found in the “Customizing your settings” chapter.

In the “normal” experiment view (which means not in one of the print preview modes), you can double-click on a field in order to open the experiment wizard which will then automatically navigate to the correct page and place the input focus upon the selected field. With this method, you can directly change a value. Of course, you can also use all other assistant functions.

The reactants and products can be displayed in two different ways: in row style and in column style. To change the view style, open the context menu by right-clicking at an arbitrary position of the experiment display. However, the context menu changes its contents depending on the current data block you are pointing at. It only shows the commands that are possible for that kind of data, so please click directly on the reactant or product display:



The entry “Switch view mode to row style” shows the products below the reactants. They are divided in two separate groups and, as we have seen, can be arranged as you like. If this view style is already active, the context menu contains the entry “Switch view mode to column style” that can be used to connect the two groups again. The condensed group will display its contents in two columns: One for the reactants and one for the products. This display function is special for the reactants and products block, but all other functions described here also apply to all the other blocks.

The functions for hiding / viewing chapters that we have already discussed can also be accessed through the context menu.

The function “Change view style” can change the current table towards table or tree style. The following image shows a reactant in table display type:

	Name	MW	Stoic.	Formula	Ref. E...	Amount	Mol	Mol %	Content	CAS No.
1 ●	Salicylic acid	138,120	1	C7H6O3		69,050 g	0,49 mol		%	69-72-7

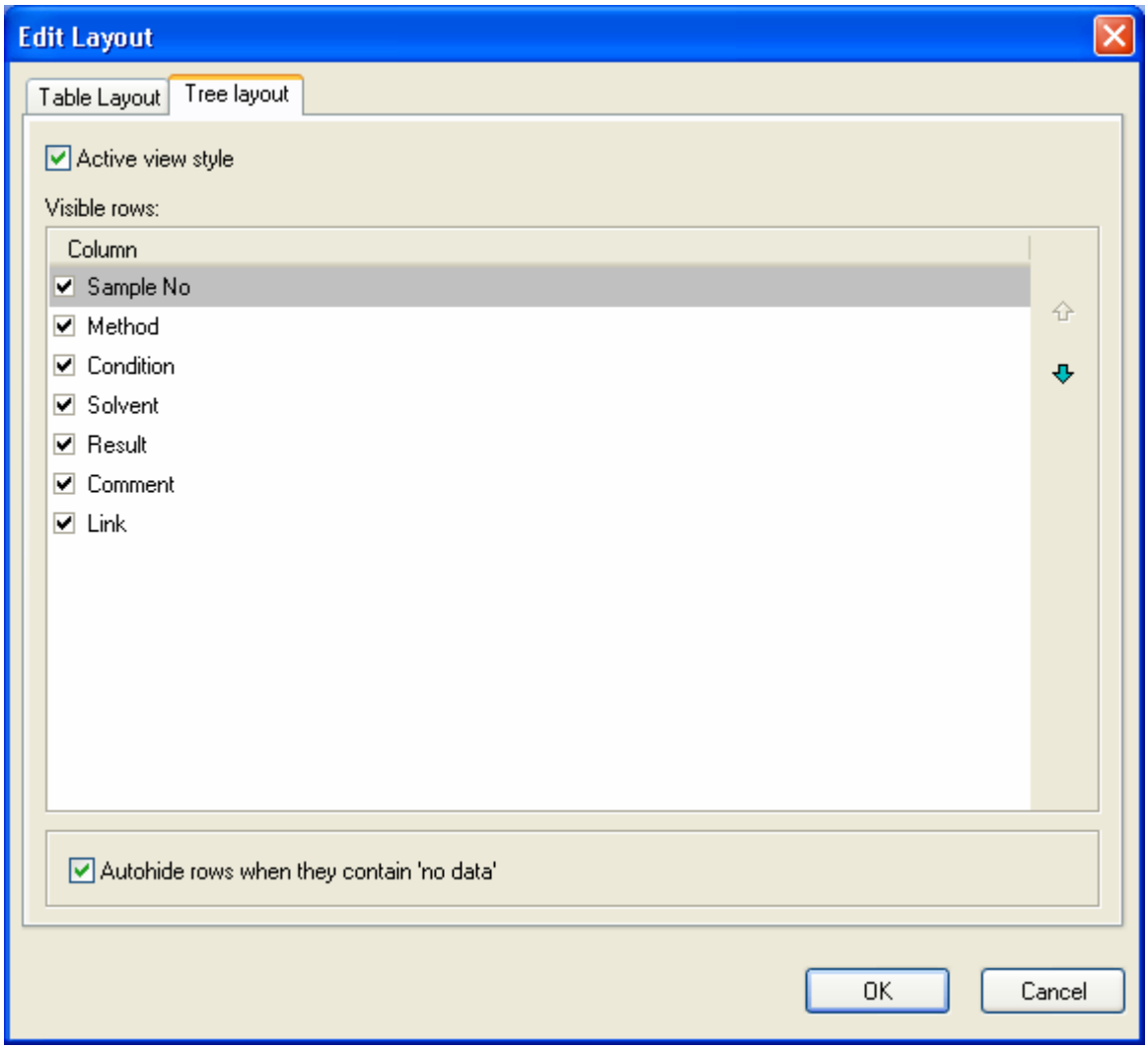
In comparison, this shows the tree view style:

⊟ Reactant 1	●
MW	138,120
Formula	C7H6O3
Stoic.	1
Item. No.	10023
Name	Salicylic acid
Origin	Supplier 1
Amount	69,050 g
Mol	0,49 mol
CAS No.	69-72-7

The various printout modes in ensochemLab will be handled in a separate chapter as they are quite powerful and contain many functions. Thus, we will not take a look at them now.

As you might have already noticed, there is a special mark at one of your reactants. In the tabular view, it is located in the first column, with the tree structure; you can find it on the very right side of the title bar: The black dot (see pictures above). It marks the respective reactant as the reference reactant.
Target molecules are marked quite similar in the products block: With a dot in a circle. If you move your mouse over this symbol, an information window containing the target molecule’s names and structure will appear.

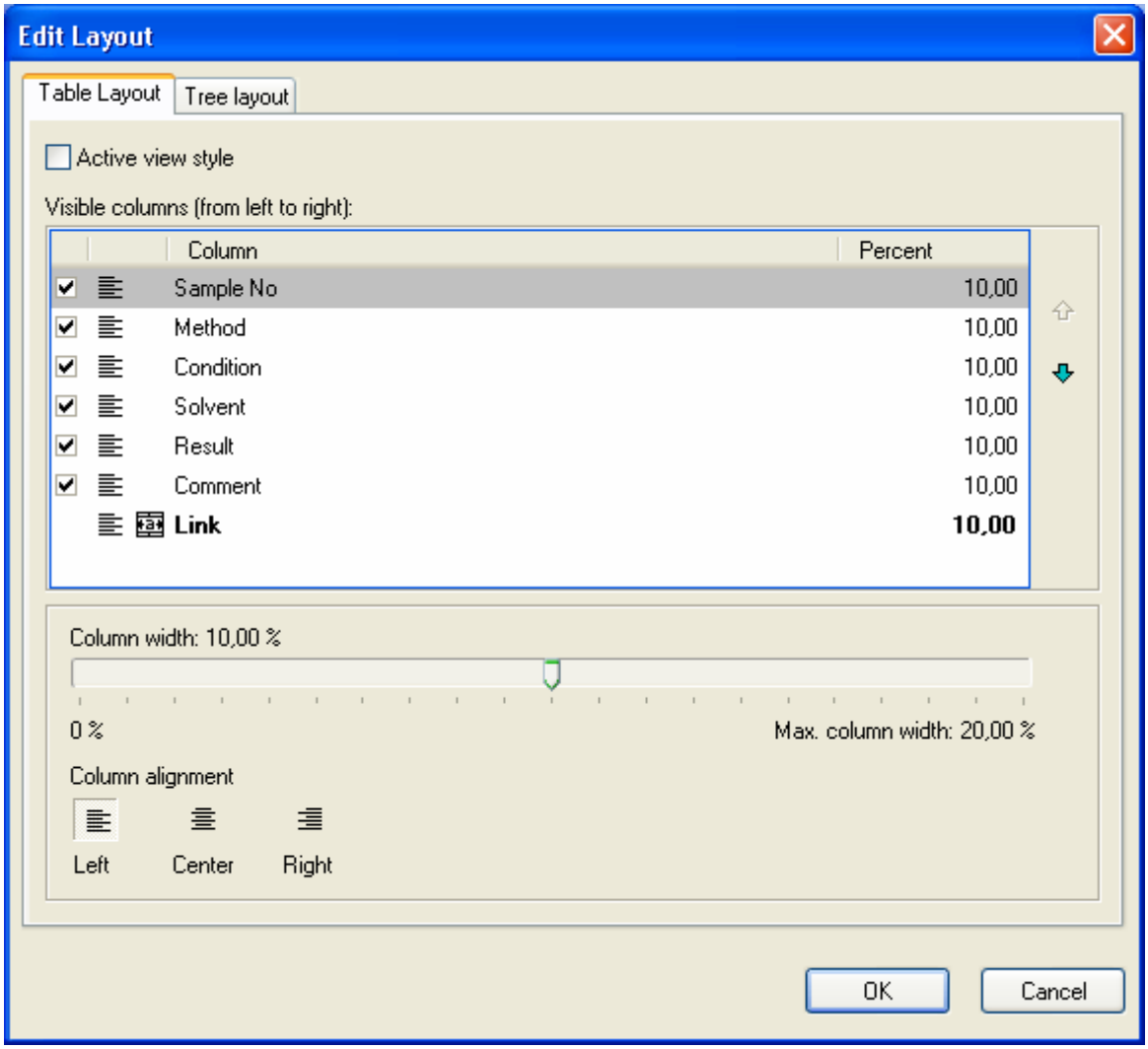
The context menu function “Edit layout” enables you to define more detailed properties of the display style and choose a view that is the most appropriate one for your work. After clicking on the entry, the following window appears:



Once again, this dialog offers you the possibility to change between table and tree layout. The active view style is chosen by selecting the checkbox “Active view style”. For each display type, you can change the column order by clicking on the green arrows at the right side of the window ( ).

If you deselect one of the data columns in the list, they will no longer be visible in the experiment display.

When using the table layout, you can also change the width of each column by first selecting it in the list and then moving the slider bar at the bottom of the window.
Additionally, you can also select the desired text alignment: Left justified ( ), centered ( ) and right justified ( ) are possible. Just click at the corresponding button!



Remarks:	You cannot change the width of main and static columns. The comment field within the analytic, for example, is used to consume the space left over by the other columns. Furthermore, you cannot change the width of invisible (e.g. deactivated) columns either.

However, there is also a much easier way to change the width of table column: Just move the corresponding right boundary lines a bit to the left or to right for making the column smaller or larger.

Another function in the context menu is the editing of the selected data block. It opens the assistant directly at the page that is used to modify the corresponding data. Beside that, you can reach the same aim by double-clicking on any position within the data block. The real data editing is done in the assistant that we have introduced in the “Create your first experiment” chapter.

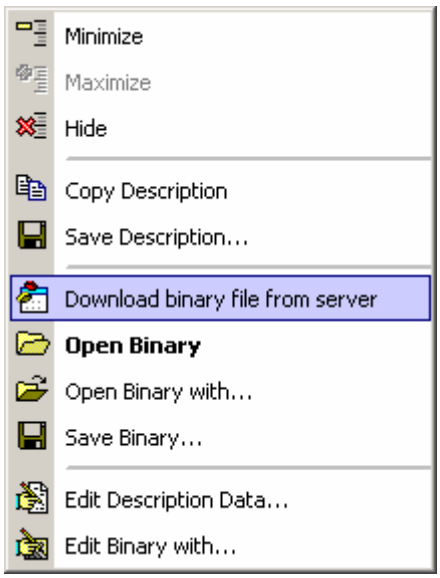
Now we should proceed to another topic: Let’s assume that you have created an experiment some weeks ago and do not need it regularly any more. Thus, you want to delete it from your “History” folder. To demonstrate this function, please right-click on the “Test_0001E” experiment and then click on “Delete” in the context menu. Please note that this **does not delete your experiment**. It just deletes the experiment reference that is stored in the list.

At the time of certain activities like taking over an experiment from a different user, ensochemLab creates a protocol entry for the respective experiment. If you are an administrator or if your administration has enabled the function for normal users you can display this information. For doing so, please move your mouse cursor over the “Protocol Information” symbol () in the application’s status bar.
If this symbol is normally displayed, but is missing for some experiments, this indicates that these experiments do not contain any protocol information.

5.3. Displaying and managing binary data

Normally, ensochemLab automatically displays binary data attached to an experiment like images or PDF documents. However, depending on your current settings, ensochemLab may also display just a placeholder instead of a binary attachment within the experiment display:

In this case, it is possible that the size of the binary file is larger than the maximum file size the automatic download. Please click on the placeholder with the right button on your mouse and select the “Download binary file from server” entry to manually download the attachment:



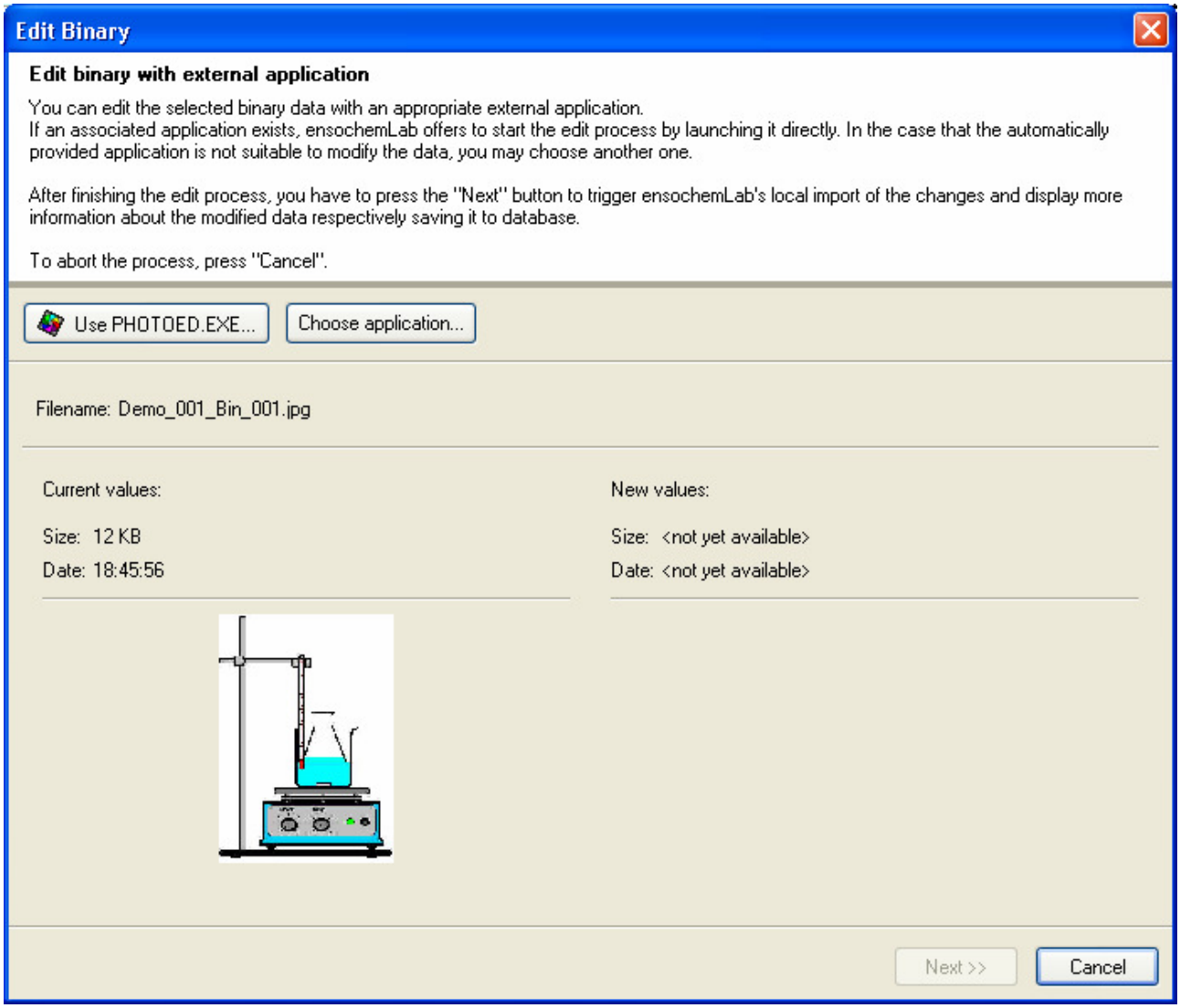
If possible, that is if the attachment is an image in one of the file formats supported by ensochemLab, a preview image will be shown where the placeholder was. This function of delayed loading enables you to load only those attachments from the server that you really need which can be especially useful when you are connected to your ensochemLab server over a slow or dialup connection.

You can look up the current maximum size up to which binary files are automatically downloaded in your personal settings. If your administrator has enabled the respective function, you can also enter an own personal value or define that the automatic download shall always / ever occur.

However, please note that the manual download function can of course not be used for displaying image or other files with a format that ensochemLab does not support.

In order to modify a binary file attached to an experiment, you of course could start the experiment wizard, export the file, externally modify it and then re-import it to ensochemLab. However, there is a much more comfortable solution: Simply click on the “Edit Binary” entry () in the preview image’s or placeholder’s context menu.

A special dialog in which you can control the editing process will be started:



In the column on the left beneath the “Current values” headline, you can see the current properties of your binary file containing the date when the file was last modified and its size on disk. If possible, a preview image is shown beneath this table.

ensochemLab automatically detects the program that is assigned to the file type of the binary record you are going to edit on the local computer. With a click on “Use …”, you can take this default selection and proceed directly. If you want to use a different program, please click on “Choose application”.

After that, the selected program will be started and you can use it just as you like.

Having finished working with the file please close your external application. If you are asked whether to save your changes or not, please choose “Yes” or a likewise option. However, please note that your changes will not be applied if you save your file under a new name or at a different location.

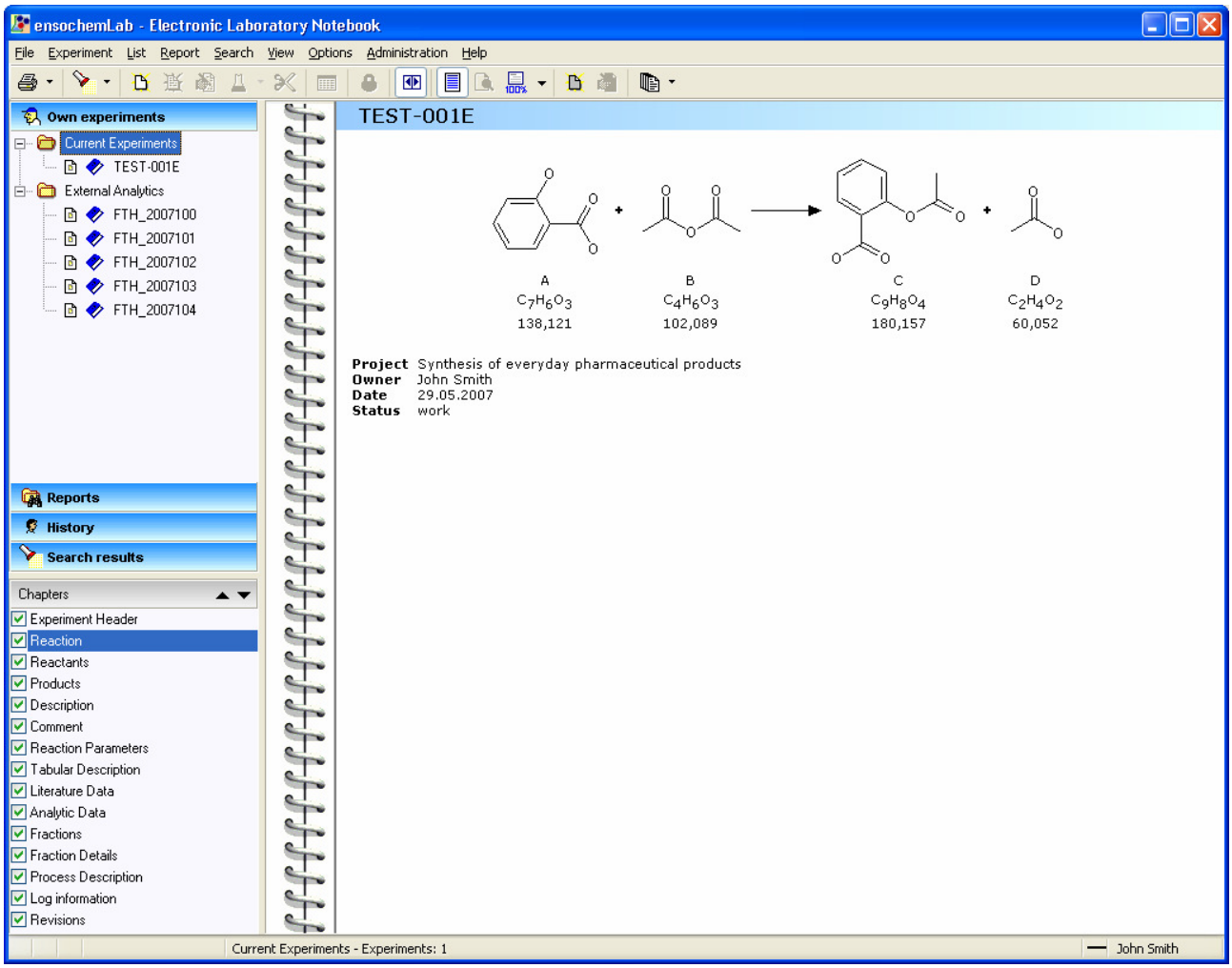
Back in ensochemLab, use the “Next” button to proceed to the next page within the assistant.

The application now applies the new file information to the table at the right side of the window. This enables you to directly compare these values before and after changing the file. With a click on “OK”, you can save the record; with the ”Cancel” button, you return to the ensochemLab main window and keep your old binary record.

If you only want to save your binary file to your local hard disk, you do not need this dialog. The preview image’s context menu in the experiment display offers you the “Save Binary” () function for such an action. For opening the binary file with the local default application associated with the respective file type, you can either double-click on the preview image or use the entry “Open Binary” () which is also located in the context menu. If you want top use a different application than the default one, please choose “Open Binary File with” (). A dialog in which you can select the application to be used will appear.
However, please note that you can only use these methods for read-only (display) operations as no changes will be applied to the database.

5.4. The folder overview

A completely different view style can be found by selecting a folder in the navigator at the right side of the window instead of an experiment. In this case, ensochemLab shows an overview over all experiments in the selected folder:



For displaying one of the experiments in the overview list, please either double-click on it or use the “Select Experiment in Navigator” ( ) command from the context menu.

It is also possible that a company uses a customized folder overview module. In this case, your display will look different than the one of the standard edition depicted here.

5.5. The versioning module

The functions described in this subchapter are only available if the optional revision management module is installed on your ensochemLab server. If you are in doubt, please contact your system administrator or supervisor.

Depending on its configuration, ensochemLab automatically creates a new version of an experiment at certain times. A version is regarded as a snapshot of your experiment at this precise moment in time including all its data. Such a snapshot is "freeze" which means that one cannot perform any changes to it. You can always only change the current (working) version of an experiment.
Therefore, it is not possible to delete one or all old versions of an experiment either.

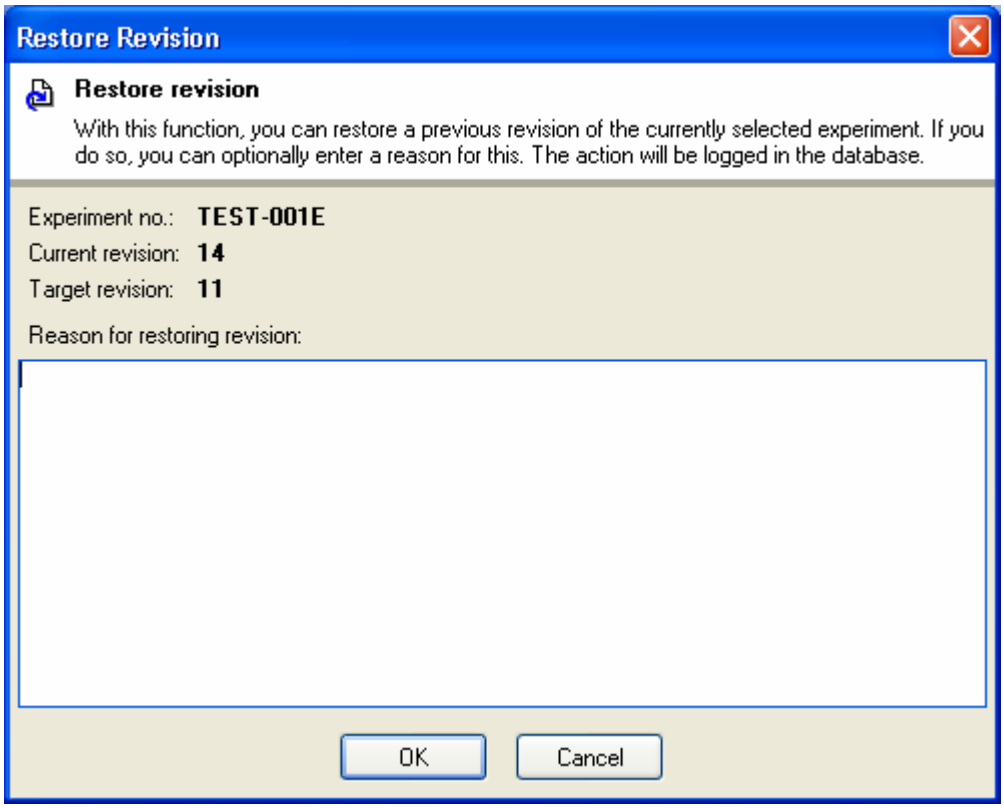
Your administrator has enabled one of the following options for defining when archived versions shall be created. Please note that some of the values can also be combined.

Never	The software never creates new experiment versions – revision management is disabled
When Finished	A new version is created with every change to the experiment given that it has already been in the "closed" state at least once.
At Owner Change	A new version is created whenever the experiment owner changes.
Always	A new version is created whenever the experiment is changed or the ownership is transferred to another user.

The ensochemLab main window allows you to access old, archived experiment versions.

If you have enabled the corresponding option in your personal settings, all versions are displayed as sub-ordinary nodes to the respective experiment node in the navigator.
Independently of the configuration, ensochemLab also displays a small icon in the status bar () whenever older versions exist for an experiment. For displaying a different version, please click on the symbol and choose the desired entry from the popup menu.
However, this list only displays the ten most recent experiment revisions. If you want to display an older revision, please click on the "Older Revisions" entry. A dialog containing a list of all available experiment revisions will appear. For every entry, the list shows you the version number, the user who triggered the version creation and the corresponding creation date. For displaying a revision, please select it in the list and then click on "OK".
For returning to the current work revision, there is an entry called "Current Revision" in the versioning symbol's context menu.

You can also restore older versions. This means that you declare an older experiment revision as the current working version. The existing working version will then be archived as the second newest version.
For doing so, please just select the version you want to restore and then click on “Restore Revision” (). The following dialog is displayed:



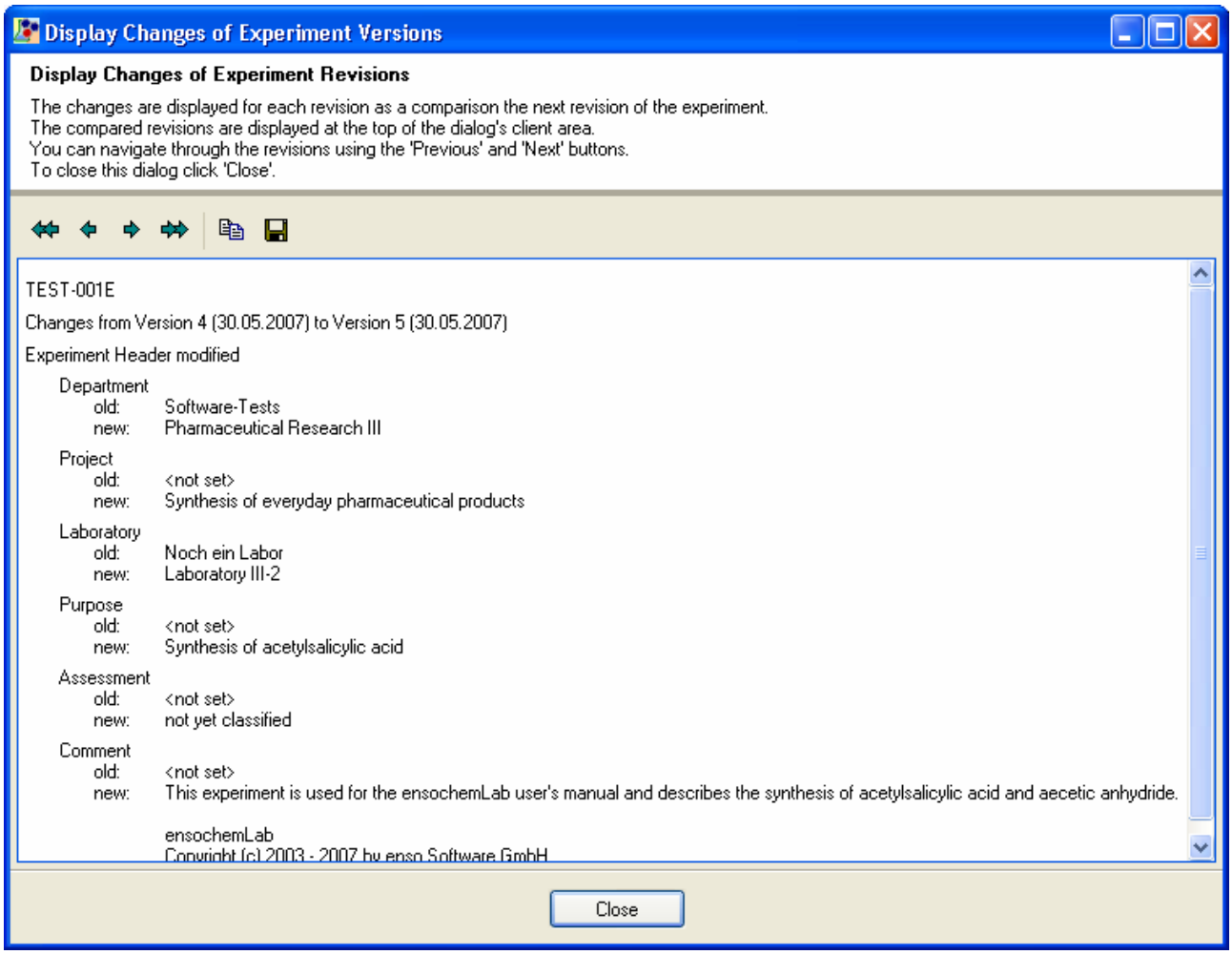
ensochemLab always creates an entry in the experiment protocol table when an old revision is restored. If you enter an optional reason in the dialog, it will be appended to the protocol entry.

Additionally, you can find the current experiment number in the upper pane, together with the revision number you are about to restore and the revision that is currently being used.

A special chapter in the experiment display lists all archived versions of an experiment together with their respective creation dates and the name of the user that has caused the creation. Via the context menu, you can also access revision functions from here instead as an alternative to using the main menu.
This list can also be copied into your clipboard or be saved to disk as a text file.

With the “Display Revision Changes” command ( ) that is located in the main menu beneath “Experiment” as well as in the version display chapter’s context menu, you can systematically compare one experiment version to the following one. Comparing to versions not following each other is not possible.

The change description dialog looks like this:



In the first row, you can see the experiment number. The second row describes the versions which are currently being compared by showing their version numbers and creation dates. In the following text, you can then see all changes between the two versions in a hierarchical structure.

With the buttons in the toolbar, you can switch the versions whose changes are currently in display. This means, if you compare version 4 to version 5 just as in the example above, you can switch to the comparison of version 3 with version 5 by clicking on the “Display Previous Changes” button ( ). By clicking on the “Display Next Changes” button ( ), you can return to the previous setup (versions 4 and 5).

With the “Display First Changes” button ( ), you can compare the first two, with the “Display Last Changes” button ( ) the last two experiment versions.

Additionally, you can copy the text containing the revision changes into your clipboard by using the “Copy changes to clipboard” button (). With “Export changes to file” (), you can save the description text into a text file on your hard disk.

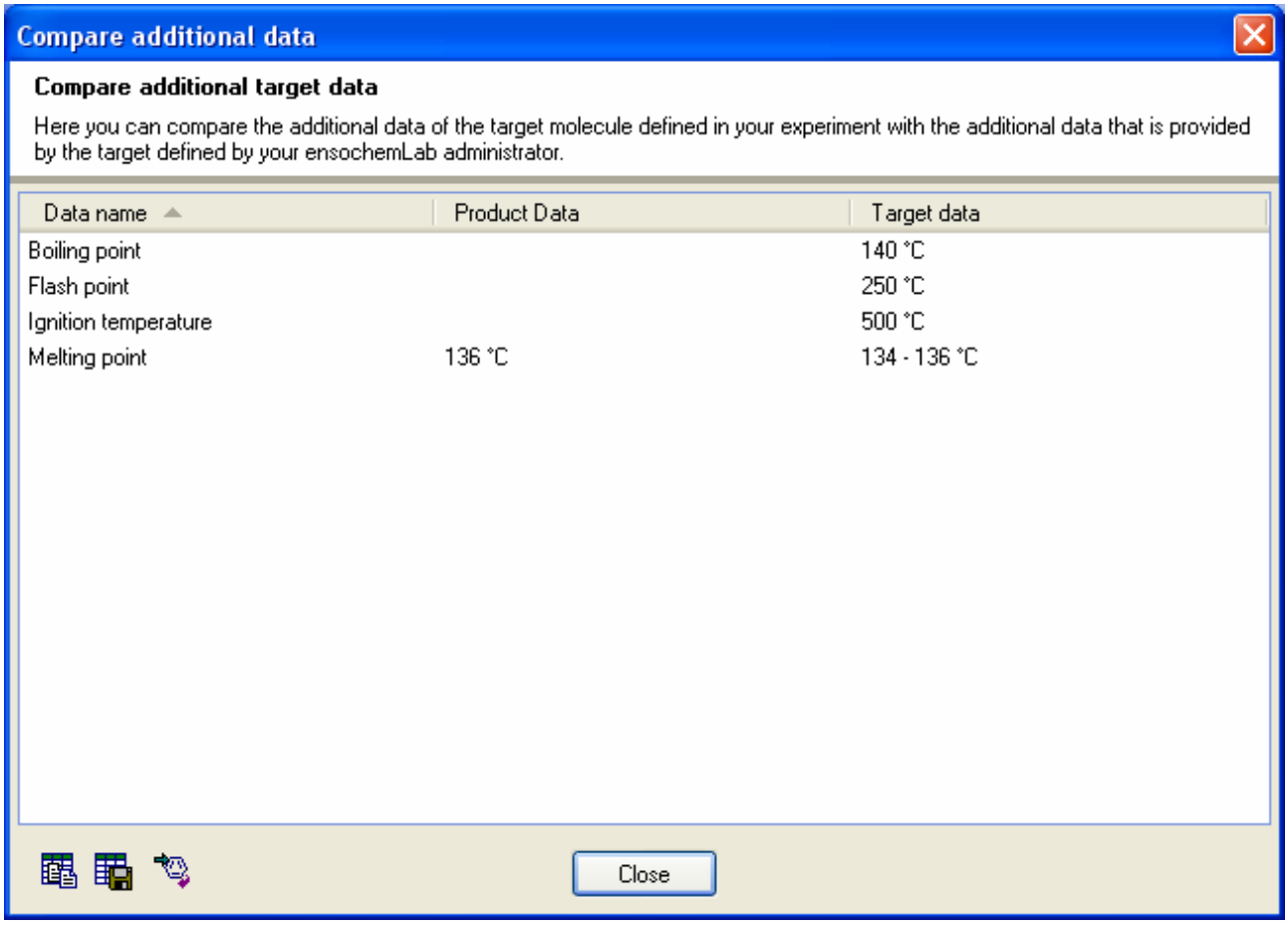
5.6. Additional functions

Via the main window, you can start a couple of additional functions. A full reference of toolbar and menu can be found in two of the following chapters. This chapter shall explain some of the features in detail.

5.6.1. Compare product data with target molecule

You have already seen that you can register a product as a target molecule and you can copy the target molecule's additional data defined by the administrator into your product during this process. This data, however, is only a copy, so if the administrator changes the target molecule, your product will not be affected in any case. This enables you to for example enter the theoretical desired value for the target molecule and the measured actual value for the product.

If you now want to compare your product's data to that of the target molecule, please select the respective experiment in the navigator and then click on "Experiment" / "Compare with target" ( ) in the main menu. A dialog containing a tabular overview of all the differences will appear:



This dialog only provides you with a display; it does not contain any functions for changing single values. For this purpose, you can use the experiment wizard that has already been explained in a previous chapter.

In order to sort the table according to a specific column, please just click on the corresponding headline. With another click, you can change the sorting direction (ascending / descending). If you are using the Windows 2000 operating system, a small arrow indicates the current direction.

With the “Copy to clipboard” button (), you can copy the displayed data into your clipboard for further processing it in an external application. With the “Export” function (), you can save the table contents into a CSV file on your hard disk.

If you are allowed to modify current experiment's data, in case of differences between product and target data you can launch a dialog with the "Apply additional data" button (). This enables you selecting the target data to be copied to the product of the selected experiment. Changes are immediately written to the database.

Please click on “Close” to return to the main window.

5.7. Command overview (toolbar)

The following list gives an overview over the functions available in the toolbar:

 Print current display	Prints the current display page. The dropdown menu allows you manually select whether you want to print the experiment or the containing list. See chapter “Printouts”.
 Search Experiments	Searches for all own experiments. The dropdown menu enables you to select another search mode.
 New Experiment	Creates a new experiment See chapter “Create your first experiment”
 Copy Experiment	Opens a dialog for copying the current experiment
 Edit Experiment	Opens the wizard for editing an existing experiment. The functions are analogical to a new experiment.
 Edit Fractions	Open the fractions dialog allowing you to edit the experiment fractions (see chapter “Working with fractions”)
 Delete Experiment	Deletes the current experiment from the database
 Edit Process Description	Creates or edits the current experiment’s process description
 Finalize Experiment	Sets the current experiment’s status to “finalized” and prevents all further changes
 Show / hide navigator	Switches the visibility of the navigator pane
 Normal display mode	Sets the normal experiment display mode (no print preview). See chapter “Printouts”.
 Normal display on page width	Sets the normal display mode on page width as current display mode. See chapter “Printouts”.
 Scale to page width	Scales the current experiment’s print preview to fit the display page width.
 Scale to window size	Scales the current experiment’s print preview to fit one whole page per screen page.
 Scale as full page width	Scales the current experiment’s print preview to use the actual printing page width.
 New Experiment in Display Mode	Creates a new, empty experiment and opens it for editing in display mode.
 Edit Experiment in Display Mode	Opens the current experiment for editing in display mode.
 Choose Display Layout	Opens a dialog to select and apply one of your display layouts. See chapter “Managing display layouts”.
 Choose Display Layout	Opens a dialog to select and apply one of your display layouts.
 Edit Display Layouts	Edits the properties of the already defined display layouts.
 Save Current Layout	Saves the current display layout under a new name.
 Set Current Layout as Default	Sets the currently active display layout as your default layout.

5.8. Command reference (main menu)

The main menu offers a lot of other functions. We have already spoken about some of them; others will follow in the next chapters of this manual. This list shows an overview including the function symbols, names and their descriptions.
Please note that all of the toolbar's functions are also available via the main menu.

File menu
Commands for printing and terminating the program.

 Login	Terminates your session and shows the login dialog so that another user can start his work with ensochemLab
 Page Setup	Opens the dialog for page setup See chapter "Printouts".
 Print Experiment	Prints the current experiment See chapter "Printouts".
 Print Overview of Experiment List	Prints an overview (a coversheet) for the currently selected list of experiments. See chapter "Printouts".
 Print Experiment List	Prints all experiments in the current folder See chapter "Printouts".
 Print Report	Prints the currently selected report. See chapter "Reports".
 Exit	Terminates the program

Experiment menu
Commands for editing experiments

 New Experiment	Creates a new experiment See chapter "Create your first experiment"
 Copy Experiment	Opens a dialog for copying the current experiment
 Edit Experiment	Opens the wizard for editing an existing experiment. The functions are analogical to a new experiment.
 Delete Experiment	Deletes the current experiment from the database
 Edit Process Description	Edit the current experiment's process description
 Delete Process Description	Delete the current experiment's process description
 Compare with target	Compares a product's additional data with one of the assigned target molecule. (See chapter ""Compare product data with target molecule")
 Edit Fractions in Table	Opens the tabular dialog for editing fractions. (See chapter "Working with fractions")
 Edit Fractions	Open the fractions dialog allowing you to edit the experiment fractions (see chapter "Working with fractions")
 Create subsequent experiment	Creates a subsequent experiment on the basis of the current experiment. This means that one of the current products is selected as a reactant for the new experiment.
 Finalize Experiment	Sets the current experiment's status to "finalized" and prevents all further changes

	Change status back to work	Changes the status of an experiment back to “in work“ and re-allows changes. In order to do so, you must enter a reason that is logged in the database. The function is only active when enabled by the administrator.
	Change Visibility	Changes the current experiment’s visibility settings and defines which users are allowed to display it.
	Take Ownership	Registers you as the new owner of the experiment. This allows you to make changes to the experiment. However, the function is only active when enabled by the administrator and you also have to enter a reason for doing so.
	Give away experiment	Gives the ownership of one of your experiments to another user.
	Add Annotation	Adds annotations with title, comment and an optional binary file attachment to experiments. This functionality exists regardless of the experiment's owner or status. However, the function is only active when enabled by the administrator.
	Export Literature	Export literature items of experiment to RIS file.
	Copy Literature	Copy literature items of experiment to internal clipboard.
	Restore Revision	Restores the currently selected revision of the experiment and saves it as the current one.
	Display Revision Changes	Displays the changes between two revisions of an experiment.

List menu
Commands for working with experiment lists. See chapters “List Operations”, “Working with experiment list”.

	Finalize Experiment List	Finalize all the experiments in the current folder. See chapter “Working with experiment lists”.
	Change visibility of experiment list	Changes the visibility of all experiments in the current folder. See chapter “Working with experiment lists”.
	Take over list of experiments	Takes over all the experiments in the current folder. See chapter “Working with experiment lists”.
	Give away list of experiments	Gives the ownership of all your experiments in the current folder to another user. See chapter “Working with experiment lists”.
	Export Experiments	Export reactant or product data from the experiments in the current folder into a CSV file. See chapter “CSV Data Exchange”.
	Import Experiments	Import reactant or product data from a CSV file into the respective experiments. See chapter “CSV Data Exchange”.
	List Handling	Opens a dialog for processing experiment lists. See chapter “List Operations”.

Report menu
Commands for creating and modifying reports. See chapter “Reports”.

	New Report	Opens the report wizard for creating a new report.
	Copy report	Opens the report wizard with a copy of the current report’s data.
	Edit Report	Opens the report wizard for editing the current report.
	Edit Report Information	Opens a dialog for modifying the current report’s description data.

	Delete Report	Deletes the current report / the current report reference. For further information, please refer to the “Reports” chapter.
	Show Report	Displays the current report’s data. The report query will be executed again for the report to include the newest result data.
	Show Report Information	Displays the current report’s description data.
	Reload Report	Reloads the current report from the database and updates the contained result data.
	Manage Reports	Opens a dialog for administrating reports and report references.
	Manage List & Label Reports	Opens a dialog for administrating the List & Label reports associated with the current ensochemLab report.
	Print List & Label Report	Opens a dialog for printing one of the List & Label reports associated with the current ensochemLab report.

Search menu
Commands for searching experiments. See chapter “Search functions”.

	Reactions or Molecules	Searches for structures / substructures within the experiment reaction.
	Experiments	Searches for experiment numbers.
	Test Series	Searches for test series
	Search Targets	Searches for experiments that include a specific target molecule
	Own Experiments	Searches for all own experiments
	Own Experiments in Status Work	Searches for all own experiments whose status is “in work“
	Query Builder	Creates a complex search query that logically combines multiple data fields.

View menu
Commands for variably displaying the current experiment

	Normal View Mode	Displays the experiment in the normal display mode
	Display as Single Page	Views the normal display mode on printer page width. See chapter “Printouts”
	Print Preview	Selects a print preview mode. See chapter “Printouts”

ACD menu
Commands for the ACD interface
This menu is only available if the ACD interface has been installed

	Search Structure	Searches for specters in ACD using one of the current experiment’s product or reactant structures
	Show Spectrum	Shows a spectrum for the current experiment in ACD

Extensions menu
Customer-specific extension modules
If your company uses customer-specific extension modules for ensochemLab, the respective functions can be launched from this menu. The menu is only available if at least one extension has been installed.

For further information on the features located herein, please refer to the respective documentation or contact your administrator or support personnel.

Options menu
Commands for editing settings and additional functions

Settings	Changes your personal settings for ensochemLab See chapter “Customize your settings”.
Version Info	Shows information and version data concerning the ensochemLab program modules on both client and server
Language	Opens a submenu where you can change the language for ensochemLab.
German	Changes the application language to German.
English	Changes the application language to English.
French	Changes the application language to French.
Clear Experiment Cache	Clears the integrated experiment cache. Please note that this function has nothing to do with the Windows clipboard.
Reload Experiment	Reloads the current experiment from the database to reflect newest changes.
Laboratory Utilities	Opens a submenu that can be used to start the laboratory utilities. See chapter “Laboratory Utilities”.
Unit Calculator	Opens the unit calculation tool
Mixing Ratio Tool	Opens a tool to calculate mixing ratios
Compositions	Opens a tool that calculates a formula’s composition
Edit Phrases	Edits public and private phrases. See chapter “User defined phrases “.
Templates for Process Description	Edits public and private process description templates. See chapter “Working with Process Descriptions“.
Display Layouts	Opens a submenu containing the commands for managing display layouts. See chapter “Managing display layouts”.
Choose Display Layout	Opens a dialog to select and apply one of your display layouts.
Edit Display Layouts	Edits the properties of the already defined display layouts.
Save Current Layout	Saves the current display layout under a new name.
Set Current Layout as Default	Sets the currently active display layout as your default layout.
Edit Calculation Templates	Modifies your personal templates for automatic and manual calculation settings.

Administration menu
Commands for changing general ensochemLab settings for all users.
This menu is available only for ensochemLab administrators.
Its contents are explained in a separate administrator’s guide.

Administration	Opens the administration dialog where you can change user-independent settings for ensochemLab. This function is only available

	when you are logged in as an administrator.
 User Administration	Opens the user administration dialog where you can manage users, laboratories, departments and sites. This function is only available when you are logged in as an administrator and the default user administration module is activated. *Not available in ensochemLab Personal Edition*
 Edit Catalog Compounds	Changes the entries of the compound catalog integrated into ensochemLab.
 Edit Additional Data Definitions	Changes the field definitions for additional (physical) data records in ensochemLab. You can add new properties here, for example.
 Manage Targets	Opens a dialog where you can manage all target molecules defined in ensochemLab along with their synonyms.
 Edit Predefined Phrases	Edits the list of predefined phrases for all ensochemLab users.
 Edit Calculation Templates	Modifies the common templates for automatic and manual calculation settings.
 Edit Process Description Templates	Modifies the common (administrative) process description templates.
 Edit Reports	Modifies the common predefined reports.
 Display Layouts	Opens a submenu containing the commands for managing predefined display layouts.
 Choose Display Layout	Opens a dialog allowing you select and apply one of the predefined display layouts.
 Edit Display Layouts	Edits the properties of the already existing predefined display layouts.
 Save Current Layout	Saves the current display layout as a predefined one under a new name.
 Change Visibility	Changes the visibility of all experiments of one specific user.
 Change Owner	Changes the owner of all experiments of one specific user.
 Manage User Objects	Opens the dialog for the administration of user-created objects. They can be deleted, taken over and given away in the dialog.

Help menu
Commands for displaying program information / sending help requests

 Send E-Mail to ensochemLab support	Send a support request to the ensochemLab service team in your corporation. This function is only available if it has been activated by the administrator.
 Administrators Guide	Opens the Administrators Guide containing a description of the application's administrative feature. This function is only available for administrators.
 Users Guide	Opens the user's guide.
 License Agreement	Opens the license agreement for ensochemLab.
 Release Notes	Opens the Release Notes (remarks and news for concerning the current ensochemLab version).
 Visit enso Homepage	Opens your web browser at the homepage of enso Software GmbH
 Info	Shows the copyright remarks for ensochemLab

The most common functions are also accessible through the toolbar. The symbols correspond to those in the main menu.

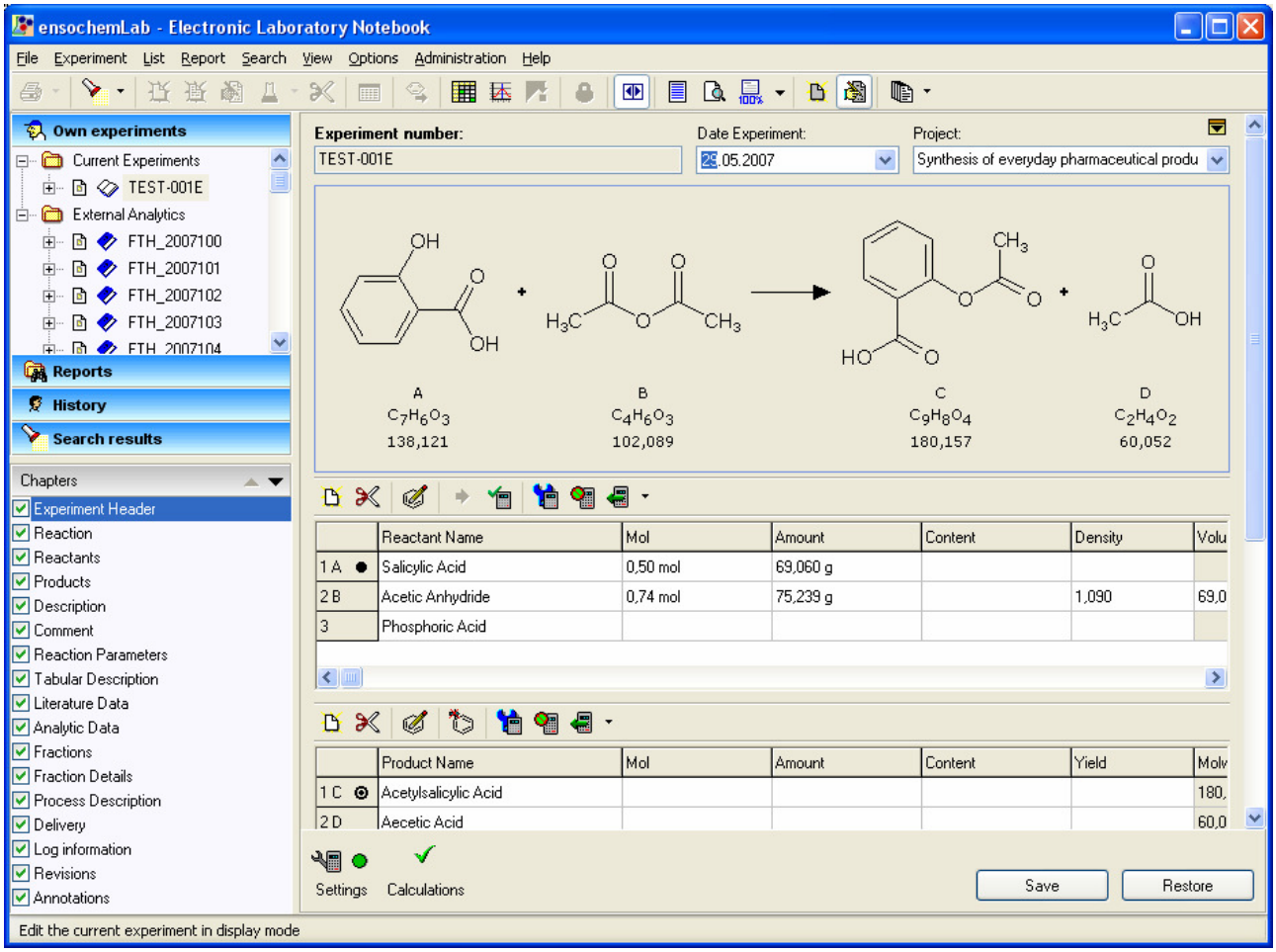
Summary:	The main window is the display and management place for experiments in ensochemLab. The search functions are also launched from here. The navigator offers an overview over your experiments. The actions you perform there do not affect the experiments themselves, but only references pointing at them.

6. The input sheet

In one of the former chapters you have learned how to use the experiment wizard to comfortably create new experiment records. In some cases, however, this great set of functions is not needed at all – for example if you just want to add the yield data for a batch of ten experiments. For such a scenario, there is a different module that gives you faster access to just the most important experiment data.

This module is called the “input sheet”. All data is displayed on a single page within the ensochemLab main window and can also be directly edited there. For creating a new experiment in the input sheet, please click on the “New Experiment in Display” button ( ) in the main window’s toolbar. If you want to use the input sheet for modifying the experiment that is currently selected in the navigator, please click on “Edit Experiment in Display” ( ).

In any case, the currently selected display mode at the right side of the window (experiment, report, print preview …) is exchanged with the editing mode:



As you can see, only the most important data fields are available for editing. Modifying the reaction is done the same way as within the experiment wizard.

The first real difference can be found with the reactants: They are displayed in a table without their respective structure. For changing a value, please just replace the corresponding cell's entry in the table. If you want to edit or display the structure please select the desired row and then click on the "Edit structure" button () in the toolbar. Your chemistry editor will then be launched containing the reactant's structure.

With the toolbar's "Add reactant" button (), you can create a new reactant in the list. The "Delete reactant" function () removes the currently selected reactant. However, please note that these toolbar buttons are disabled due to security reasons during the "real" editing process (e.g. when your cursor is located within a data cell).
For selecting a reactant as the reference reactant, please select it in the list and then click on the "Define as limiting reactant" button ().

The automatic calculations functions are of course not limited to the experiment wizard and are also available in the input sheet. Their exact impacts depend on your personal calculation settings. Additional information on this topic is available in a separate chapter of this user's manual.

The product table is completely likewise to the reactant table. Furthermore, it contains some more functionality for registering target molecules () or deleting the corresponding associations (). A click on one of these buttons launches the same functions that you already know from the experiment wizard including the assistant for registering target molecules.

In the lower section of the input sheet, there is the area for entering the experiment description. However, you cannot add, modify or delete attached binary inside the input sheet. The functions for text editing and formatting are described in detail in the chapter about the experiment wizard in this manual.
If you want to see a larger section of your description text without having to scroll you can enlarge the text area downwards by clicking on "Enlarge text field". With the "Minimize text field" button, you can undo this operation. Altogether, the text area can be enlarged up to eight times.
For inserting a predefined phrase, please click on the "Phrases" button. The well-known phrases window will appear from which you can insert text phrases by either double-clicking on the desired entry or selecting it and then clicking on the "Insert" button ().

Independently from you current scrolling position, there is always a bar containing two symbols and two buttons visible at the very lowest part of the frame.

When you move your mouse cursor over the symbol on the left side, a hint window containing a summary of your calculation settings will be displayed. On the right side of the iconic calculator, there is a symbol indicating the current state of the automatic calculation functions just as described in the "Automatic Calculations" chapter.
The symbol on the right side indicates whether the last calculation in the "document" as a whole was successful or not. For displaying additional information on errors, warnings and hints, please move your mouse cursor over the symbol.

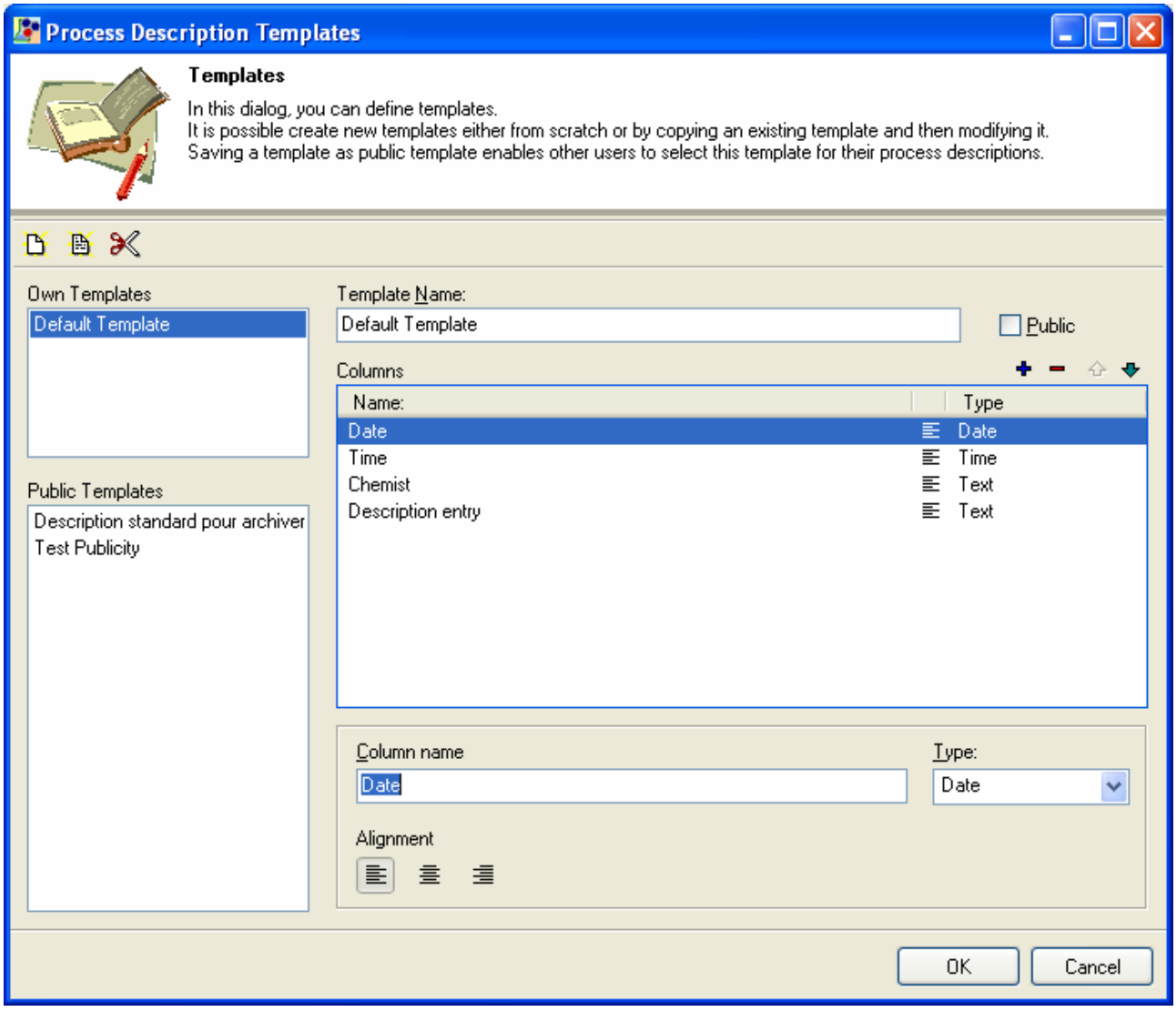
With the two buttons, you can either save or discard your changes. You always remain in editing mode, after a click on "Restore", however, the original data is displayed once again.

Summary:	The input sheet is an addition to the experiment wizard with which you can comfortably add results or addendums for large quantities of experiments. Furthermore, it can also be used for creating new experiments with a defined set of basic data.

7. Working with process descriptions

Now you have a sample experiment in your database and know the functions within the main menu. Thus, it is the time to complete our experiment with the last part still missing: The process description.
In contrast to the tabular experiment description, the process description offers flexible columns which means that you can an arbitrary number of columns with different data types and header names. However, this flexibility has the price that you cannot search for your process description data.

ensochemLab offers the possibility to create templates for process descriptions so that you don't have to enter the field descriptions and data types again every time. Therefore, this chapter will start with creating such a template. To do so, please open the main window and then click on the menu item "Options" there. Now, please select the "Templates for Process Description" function. The following window will appear:



In order to create a new template, please click on the "New" button ( ). Afterwards, you can enter a name for the template into the "Template Name" field. If possible, this name should be unique. If your administrator

has enabled the respective function, you can also mark your template as public so that it is available to all ensochemLab users. In this case, the name has to be unique.

To add columns to you template, please click on the “New column“ button (). Then you can use the “Column Name” field to specify a description title for its headline. The “Type” selection box allows you to choose which kind of data you want to store in the column. Possible types are:

Data type	Explanation
Text	A text field can contain arbitrary text. Letters, numbers and additional characters are possible.
Integer value	This field type supports only whole numbers. No other characters can be entered.
Floating point value	This field type supports only decimal numbers. No other characters can be entered.
Date	This field type allows you to enter a time
Time	This field type allows you to enter either a point in or a period of time.
Boolean	This field type represents a logical “Yes / No” value.
Multiline Text	This field type can contain text of any length which can also, in contrast to the normal text field, consist of multiple lines.
Formatted Text	This field type can contain of multiple lines and any length which can also, in contrast to the multiline text field, add text properties like font, size, bold, italic, underline and color..

However, it is not possible to define own data types.

Additionally, you can select how your data should be arranged in display mode. Three modes are supported: left-aligned (), centered () and right-aligned ().

The data type and the alignment are always configured for a whole column. It is not possible to use a different configuration for single rows. The only exception to this rule is that you can define a row completely as a comment row (for more information see below).

You can modify the column order by selecting one of the columns and then clicking on the up () or down () arrow to either move it one entry up or down in the list.

Using the “Delete” button (), you can delete an existing column from the template.
Furthermore, if your administrator has enabled the respective function, you can decide whether you want to mark your template as public and thereby make it accessible to the other ensochemLab users. In order to do so, please just check the “Public” checkbox.
Other users will be able to read and apply your template, but not to modify or delete it.

Already existing templates are displayed in the two lists at left side of the dialog. The upper list contains your own templates (both public and private ones). The lower list contains all public templates created by other users.
You can also start with a new template by copying another one. This can be done by first selecting the desired start template and then clicking on the “Copy” button ().

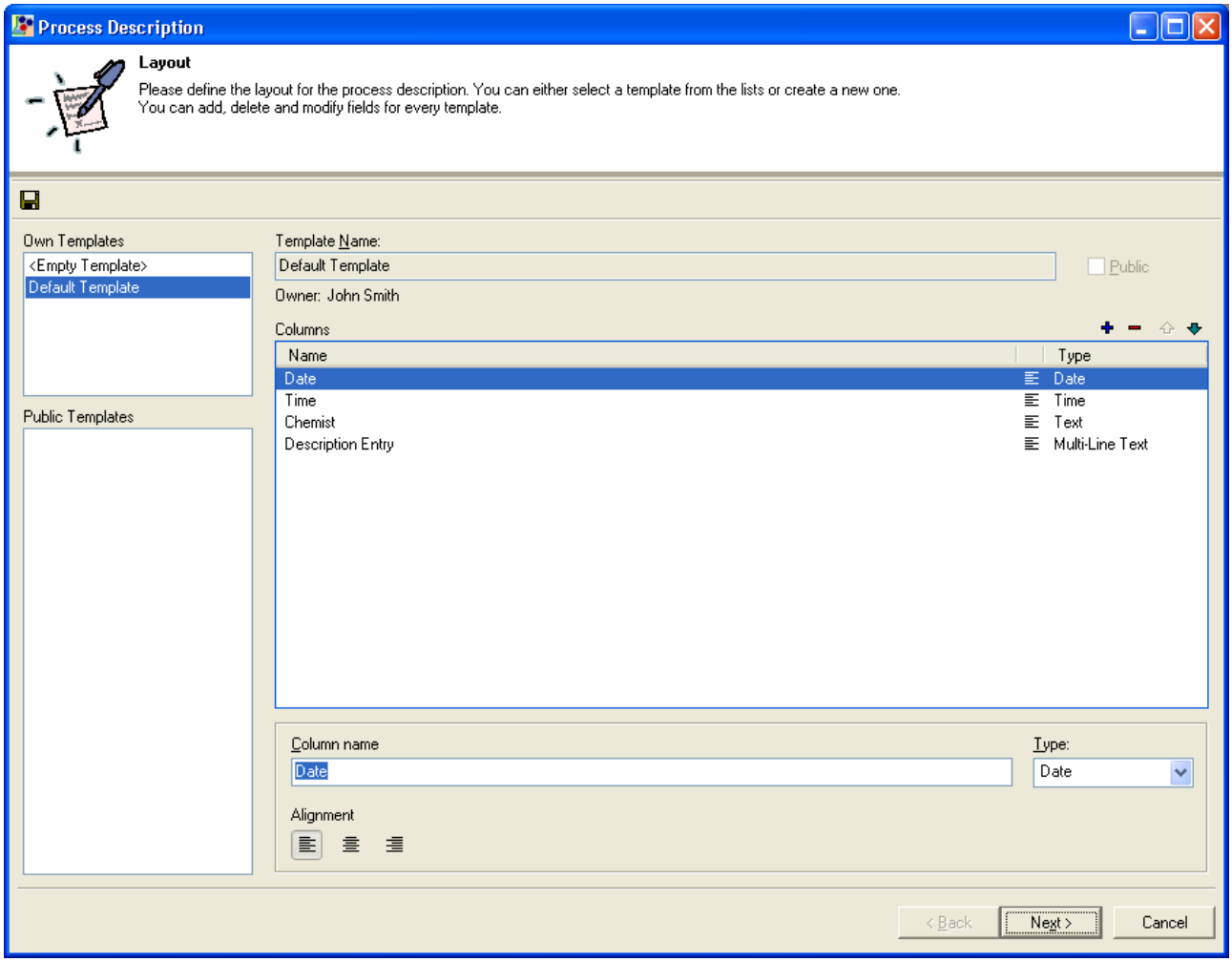
As already discussed earlier in this chapter, the “Delete“ button () to remove a template is only available for own templates. This restriction also applies to administrators.

In general, a template can contain an arbitrary number of columns. ensochemLab does not include any restrictions at this point.

For the example, please name the template “Process Description corresponding to A-13” and define the following columns:

Name	Type
Date	Date
Time	Time
Chemist	Text
Description entry	Multiline Text

As you now have a template for a process description, we can now continue with the process description itself. To proceed, please close the dialog with “OK” in order to save your data. Then please select the experiment you want to create a process description for in the main menu and click on the “Edit process description” button ( ) in the toolbar. The following assistant will appear:

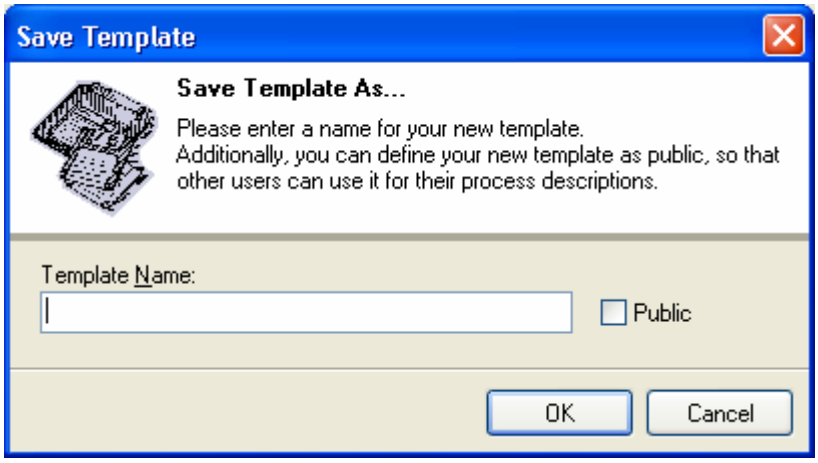


This dialog is used to select a template for the process description. If you are modifying an existing process description, the upper left table also contains an entry called <Existing Template> that represents your current data regardless whether the template has been modified in the meantime.

This dialog also offers you the possibility to create addition al templates. In order to create a completely new template, please click on the <Empty Template> entry in the list on the upper left side of the window. Then

enter your detail data for the template just as described earlier in this chapter. With the “Save” button (), you can save your template to the database.
You cannot modify existing templates in this dialog. To do so, you have to enter the separate administration dialog that we have discussed at the beginning. However, you can use an existing record as a base for creating a new, altered one by first selecting it in one of the list, modifying the desired data and then also clicking on “Save”.

The following dialog appears:

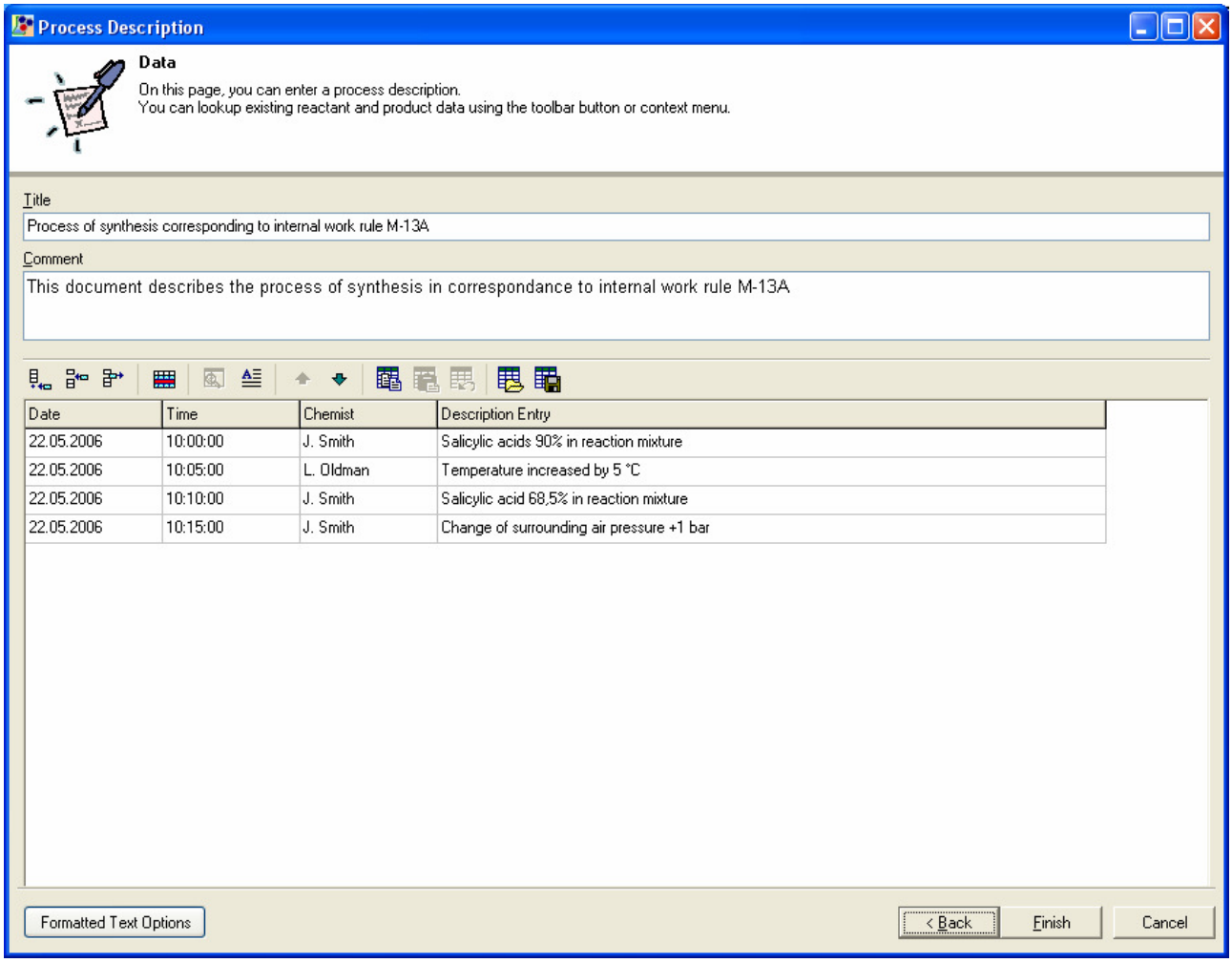


Please enter a name for the new template and decide whether you want to mark the template as a public one. Then doing so, there are the same remarks as when creating templates using the separate administration dialog. Afterwards, please click on “OK” to save your changes or click on “Cancel” to return to the assistant without sending your changes to the server.

Of course, it is also possible to use a temporary template only for this specific process description by just not saving your selection.
As we have already created a template for this example, please select it from the list and then click on “Next” in the assistant.

Now you get to the actual process description entry page. Here you can enter general information like title and comment as well as the data for the fields defined in the template you have just created. In case of entering comment data you'll have the same options as with formatted text.
You can create an arbitrary number of data rows. However, ensochemLab will only save those rows that contain data in at least one of the columns. All completely empty data rows are ignored.
The following example uses the template structure shown in one of the previous screenshots with the following data fields:

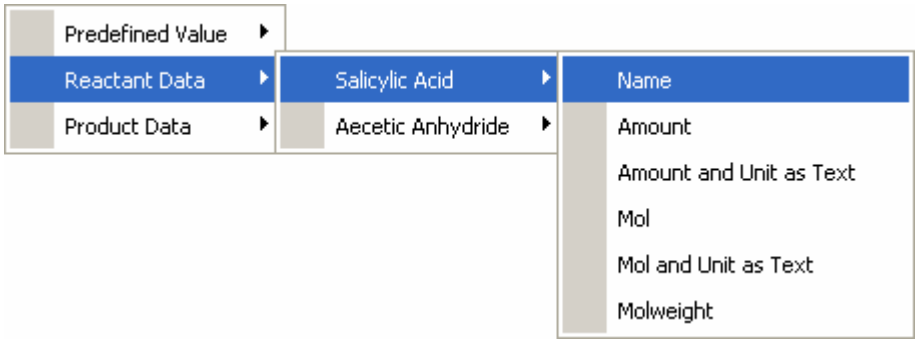
Data field	Data type
Date	Date
Time	Time
Chemist	Text
Description entry	Text



By default, the table already contains one empty entry for the first row. This entry cannot be deleted, too. When trying to do so, it will automatically be recreated with empty columns.

In order to enter or modify column data, please use your mouse to click into the respective cell or select the cell and then press <Return>. Please note that ensochemLab only allows you to enter the characters valid for the corresponding field type. This means that you are bound to the template definition created in the previous step.

When entering data, it is also possible to look up the most important reactant and product data within the experiment to automatically fill it into the current data cell. For using this function please click the “Lookup Reactant/Product Data” button (). ensochemLab now opens a selection menu where you can choose between reactants and products. On the next level, you will find the substance names and beneath that their data fields:



Of course, you can also directly right-click on a cell and enter one of these values from the context menu.

ensochemLab can also automatically fill the current date or time into a process description cell. These values are available from the “Predefined values” section.
However, regardless of the category, please note that the value to be inserted has to correspond to the column’s data type. The only exceptions from this rule are text columns that can hold all kinds of data.

For improved usability, you can also take the phrases window which you already know from the “Create your first experiment” chapter as an alternative for the drop-down selection list or the context menu. For opening it, please just click on “Show / hide phrases window” ( ). Despite its name, it only contains the states values, but no phrases.

Whenever you enter comment data or values into a cell with that type, the text options can be adjusted using a tool window. Please just click on the "Formatted Text Options" button (Formatted Text Options), to show / hide the appropriate helper form.

If you want to add another row, please click on the “Add Row” button ( ). The new data row will then be created at the end of the table. Sometimes, it can be useful to insert a row exactly above the currently selected one. For this purpose, ensochemLab offers the “Insert Row” function ( ). With the “Delete Row” button ( ), you can remove an existing data row.

In a process description, there are two kinds of rows: Up to now, we have only worked with data rows. Such a kind of row is defined through the field structure you have created in your layout. Additionally, there are also comment rows. They allow you to enter a free text comment covering a whole row without any regards to your data structure. You can switch both modes by clicking on the “Use entire row for comment” button ( ).

The process description enables you to use the same features which are also available in the tabular description you have entered in the experiment assistant. With the “Copy” button ( ), you can copy the complete contents of your table into the clipboard. A click on “Paste” ( ) afterwards re-imports them back into ensochemLab. If you have inserted data in error, you can undo the last paste operation by clicking on “Undo” ( ).

If your data table contains comment rows, they are assigned a “$$cmt$$” prefix when they are copied into the clipboard. This information is intended to enable an automatic processing by the target application if supported. The mark is also necessary to correctly identify the row as a comment when importing the data back into ensochemLab.

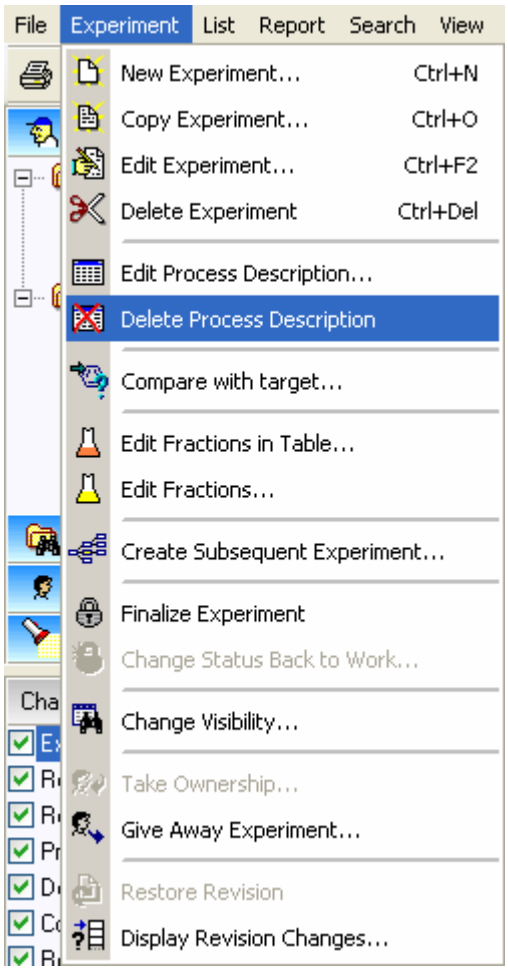
In this dialog, there are the same functions for exporting data into CSV files ( ) and importing it from there ( ). For further information on this subject, please refer to the separate “CSV Data Exchange” chapter in this manual.

In case you need to adapt date / time values, which are e.g. the result of using another experiment as a template, to meet the actual synthesis execution, a wizard is available (Adjust Date / Time…) via context menu to assist you in doing so. By providing a new date or time reference respectively the corresponding values are calculated automatically.

If you are modifying an existing process description, ensochemLab will automatically start the assistant at the last page.

To close the assistant and save your data into the experiment, please click on “Finish“

If you want to delete an existing process description from an experiment, you can start by first loading it in a display mode of your choice. Then open the “Experiment” entry in the main menu and click on “Delete Process Description”:



However, please note that your process description will irreversibly be deleted. The only way to restore it is to reactivate an older experiment revision using the optionally available revision management module.

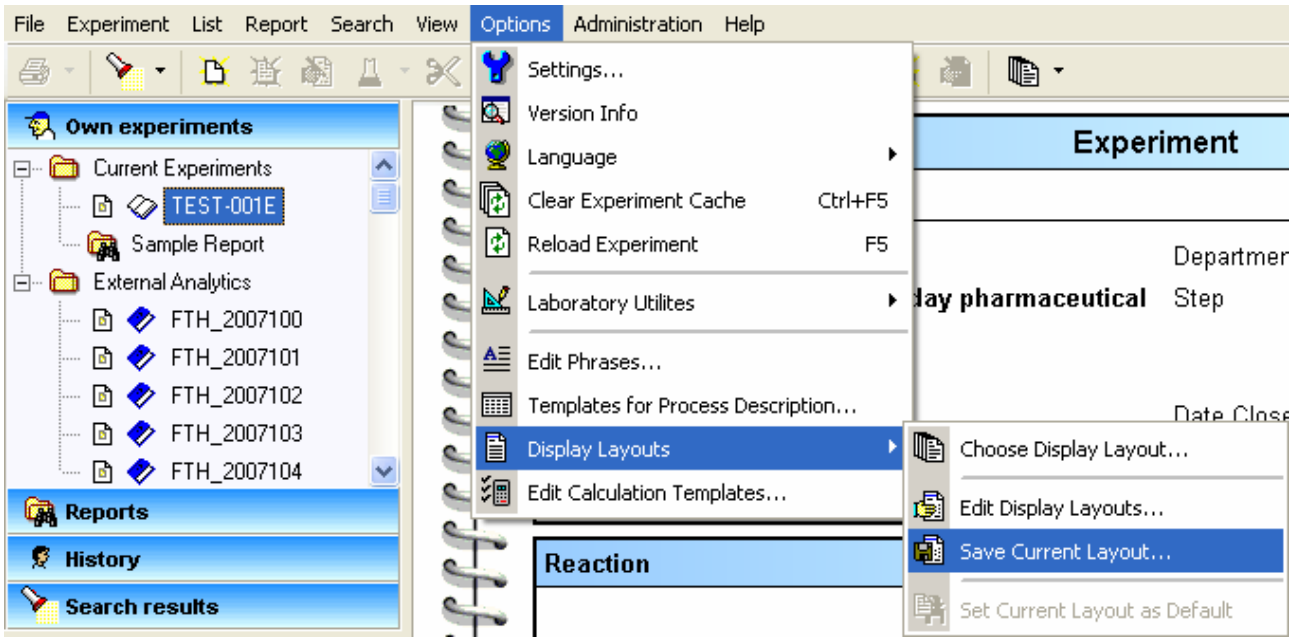
Summary:	You can optionally add a process description to your experiment in

	order to document your test. Templates enable you to save regularly used table structures. You can save company-wide documentation policies as public templates and make them accessible for all users.

8. Managing display layouts

In the previous chapters, you have explored the main menu with its display modes and functions especially for the experiment view. Maybe you have also created a first personalized work environment. This chapter shall now explain how to save and use multiple of these layouts side by side. This feature enables you to rely on templates created once without having to completely redefine them every time your demands change.

The current way of work within this manual's examples corresponds to the default layout: It is loaded every time ensochemLab is started and saved always when the application is terminated to save your last working desktop. Beside that, you can also save your current display settings separately by clicking on "Options / Display Layouts \ Save Current Layout" in the main menu:



A window will appear where you can enter a name and a description as well as select a save mode for your display layouts. The save mode defines how ensochemLab will save the layout:

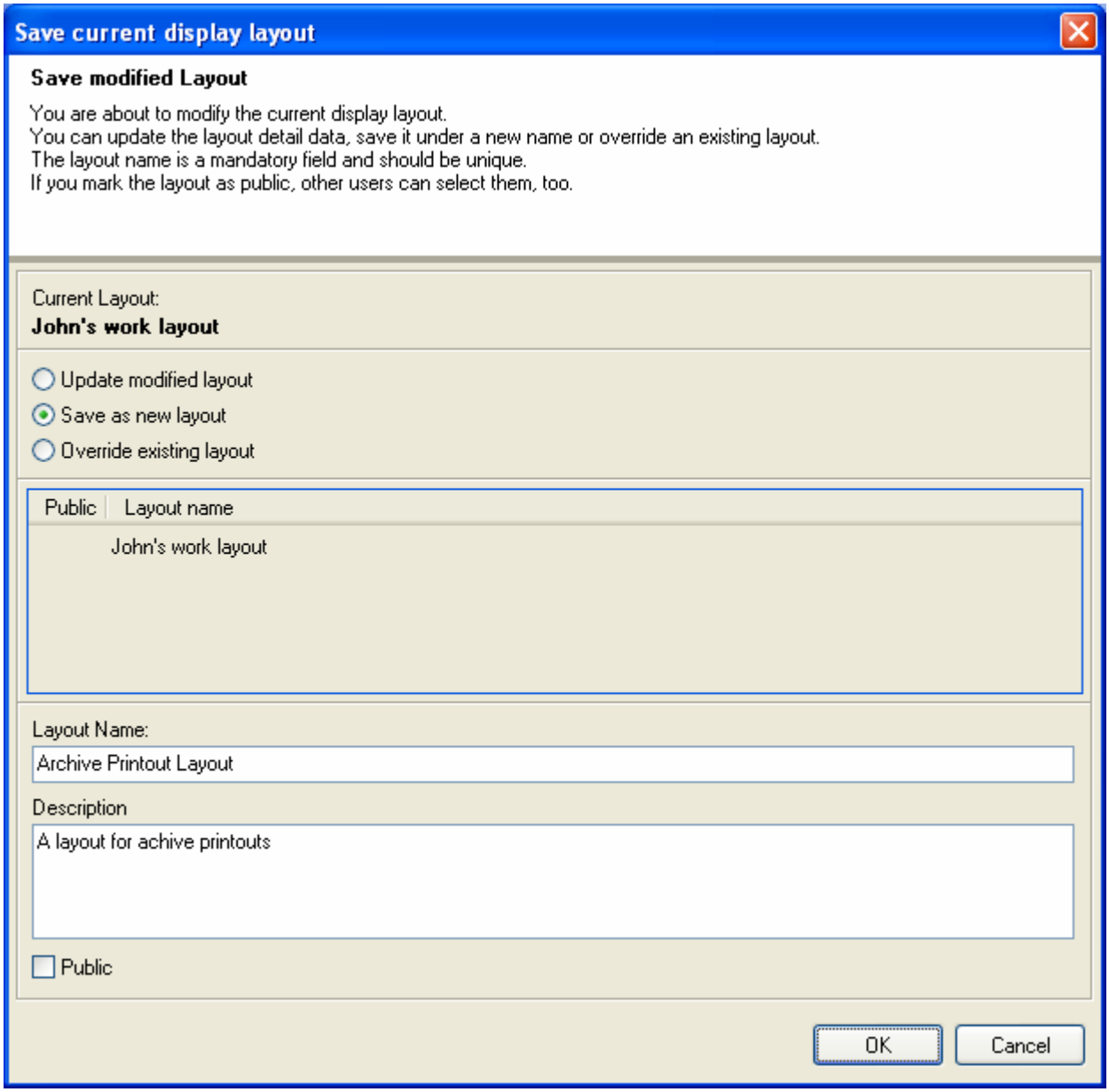
- **Update modified layout**
  The current settings override the last loaded layout. Therefore, you do not need to enter any further data. This option is not available if the predefined standard layout is currently active. It can only be used if the current layout has been modified.

- **Save as new layout**
  This function saves the current display under a new name. Theoretically, you can also use duplicate names for different private records; practically however, this would lead to confusion and is thus not recommended. The names of public display layouts always have to be unique.
  You always have to enter a name. This option is always available.

- **Override existing layout**
  With this function, you can replace an arbitrary existing layout. First select the layout from a list. Then you can change the name and description if you want. This option is only available if there is at least one user-defined layout in the database.
  Of course, you can only use this function for replacing own layouts.

The current layout's name is displayed in the upper part of the window. In the lower part, you can choose whether the new or modified layout shall be public. This option enables other ensochemLab users to apply your template, but not to modify or delete it.
Please note that by default, only ensochemLab administrators can create public layouts. However, this function can also be activated for normal users.

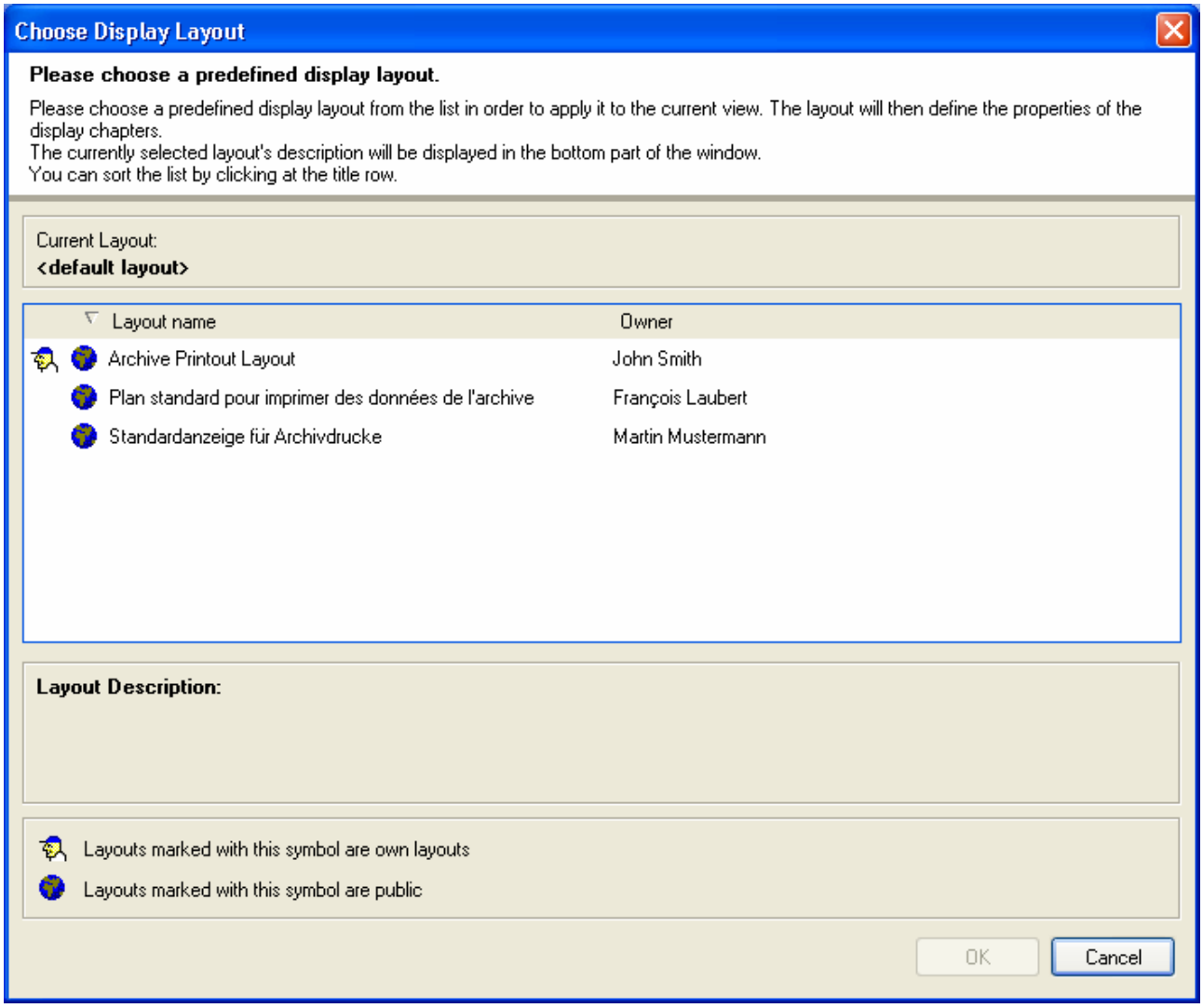
With that, a layout is defined in the following way:



Click on "OK" to save your changes or click on "Cancel" to return to the main window without applying the process to the database.

These layouts are also used for printouts. This enables you to create special printout layouts for example for archiving, applying for patents or other issues. When in need of them at a later time, just activate the corresponding layout.

To apply (use) an existing layout, click on “Choose predefined display layout” ( ) in the main window’s toolbar. A selection dialog will appear where you can select the desired layout from a list that includes your own ones as well as the other users’ public layouts. For every layout, the table shows its name and type (public one, own one):



In the case of questions about a layout or change requests for it, you can contact the specified owner.

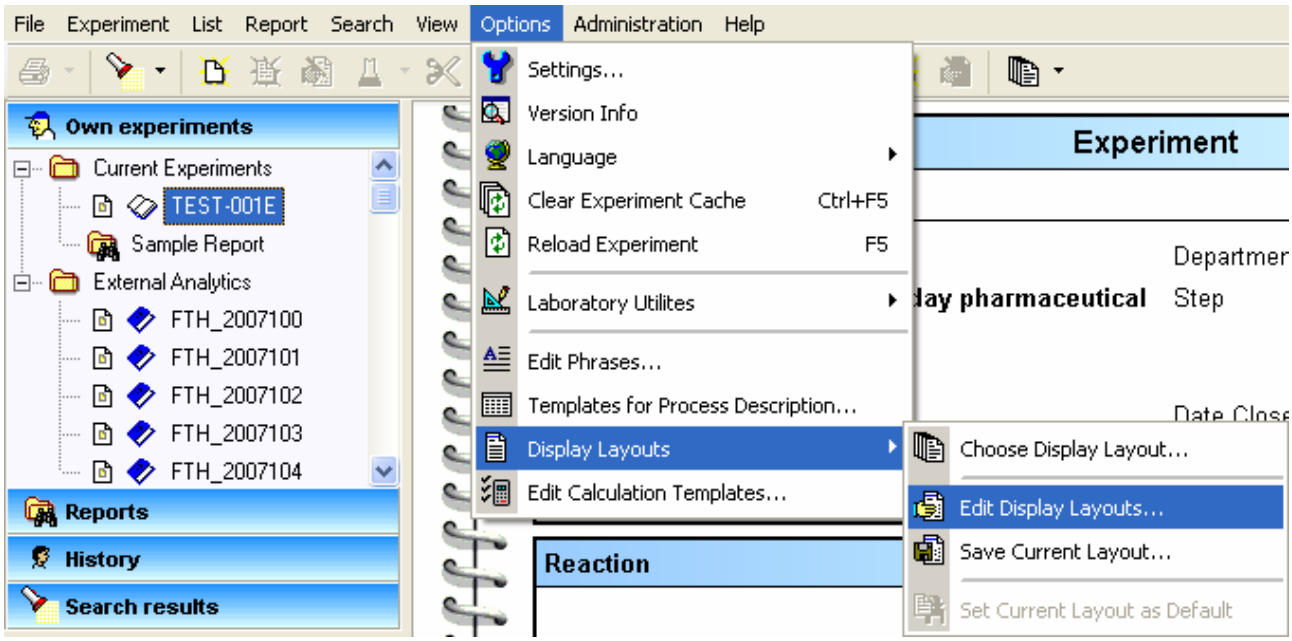
If you select an entry, the corresponding description will appear in the lower part of the dialog. Please note that the currently active layout is not included in the list. With the default layout described and explained above, you can also return to the settings of your last ensochemLab session.

After you have chosen the desired template, please click on “OK” .With the “Cancel” button, you can return to the main window by preserving your current display settings.

If you terminate ensochemLab while a layout is loaded, it will, due to its definition above, override the predefined default layout. Thus, you should never use this “record” for saving view settings.

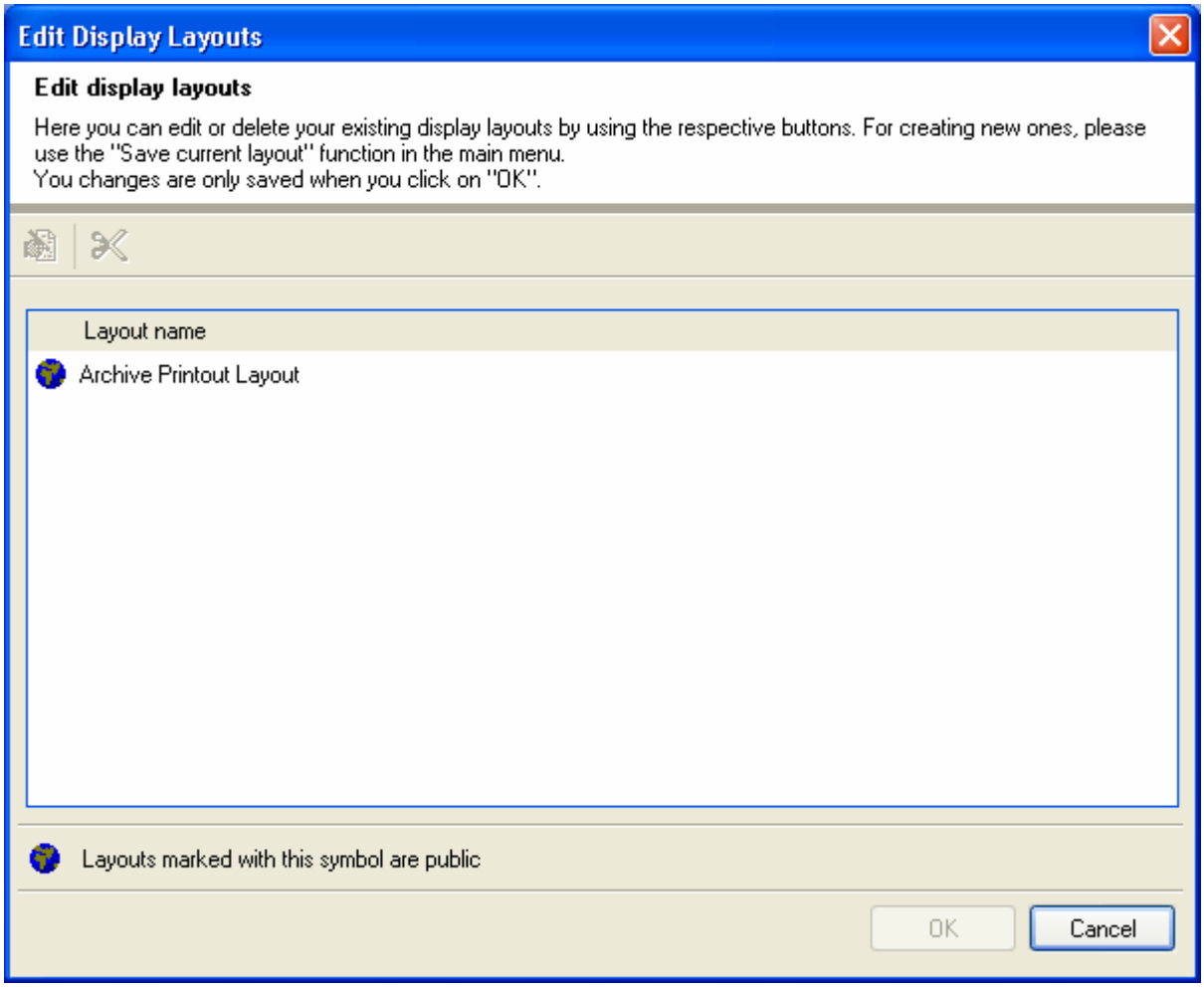
You can save an arbitrary number of display layouts, but you can only use one at a time.

Of course, you can also delete layouts or modify their description data. For this purpose, there is a special edit dialog that can be launched via “Options \ Display Layouts \ Edit Display Layouts” in the main menu:



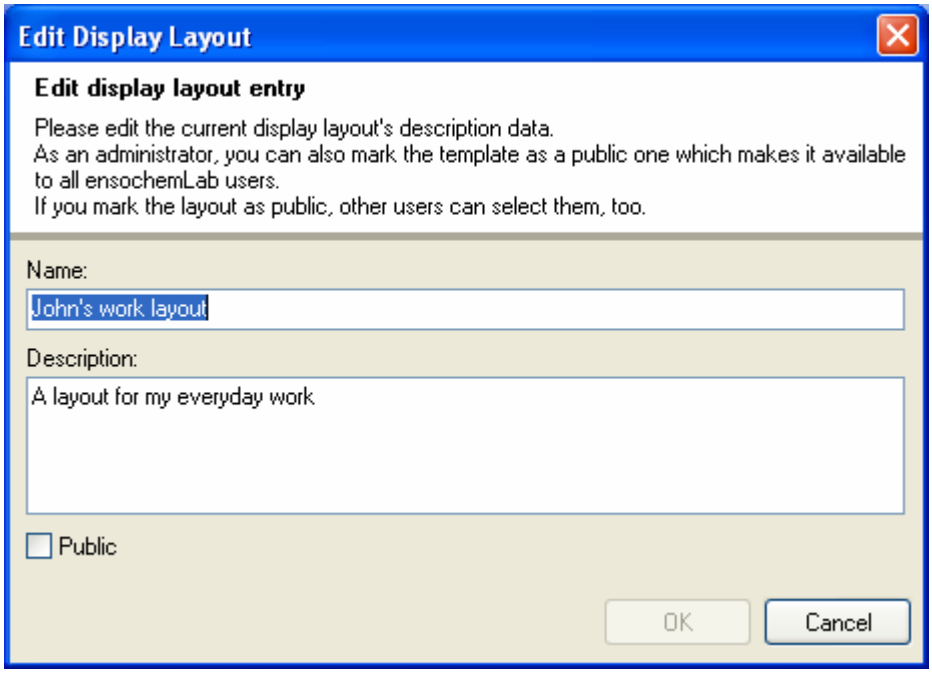
The dialog that will now appear shows all own display layouts. The public ones of other users are not included as you cannot modify or delete them either. Users of previous ensochemLab versions may notice that this has been changed in version 3.2.

This restriction also applies to administrators. For deleting the public or private display layouts of other users, please refer to the “Manage user objects” administration dialog which is explained in the Administrator’s Guide in detail.



The globe ( ) shows whether the currently selected item is a public display layout.

To modify a record please select it from the list and then click on the “Modify layout properties” button ( ).



Now you can modify the description data, but not the content like visible chapters, column widths, … To do so, you have to apply the layout as described above, change your settings in the experiment view and then save it again by clicking on “Options -> Display Layouts -> Save Current Layout” in the main menu, selecting “Save Modified Layout” and then clicking on “OK”.
In this dialog, you can also mark a layout as public or remove this option again (administrators only).

With the “OK” button, you can apply your changes. Using the “Cancel” button, you can return to the layout list without changing anything.

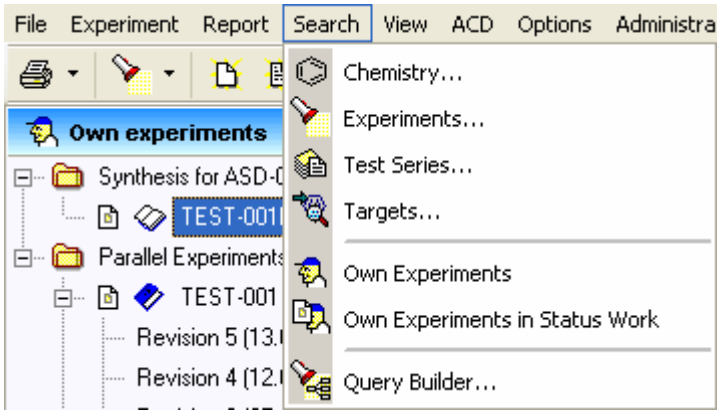
To delete an existing layout, please click on “Delete selected layout” () in the overview dialog (see last page).

Please note that your settings are not applied until you quit the overview dialog with its “OK” button. By clicking on “Cancel”, you can undo all changes made in this module.

Summary:	Display layouts enable you to save your personal display settings within the experiment view. With multiple layouts, you can flexibly switch display options without having to redefine them every time your need change.

9. Search functions

ensochemLab offers multiple ways to search for experiments. You can find them all by clicking at the “Search” entry in the main menu.

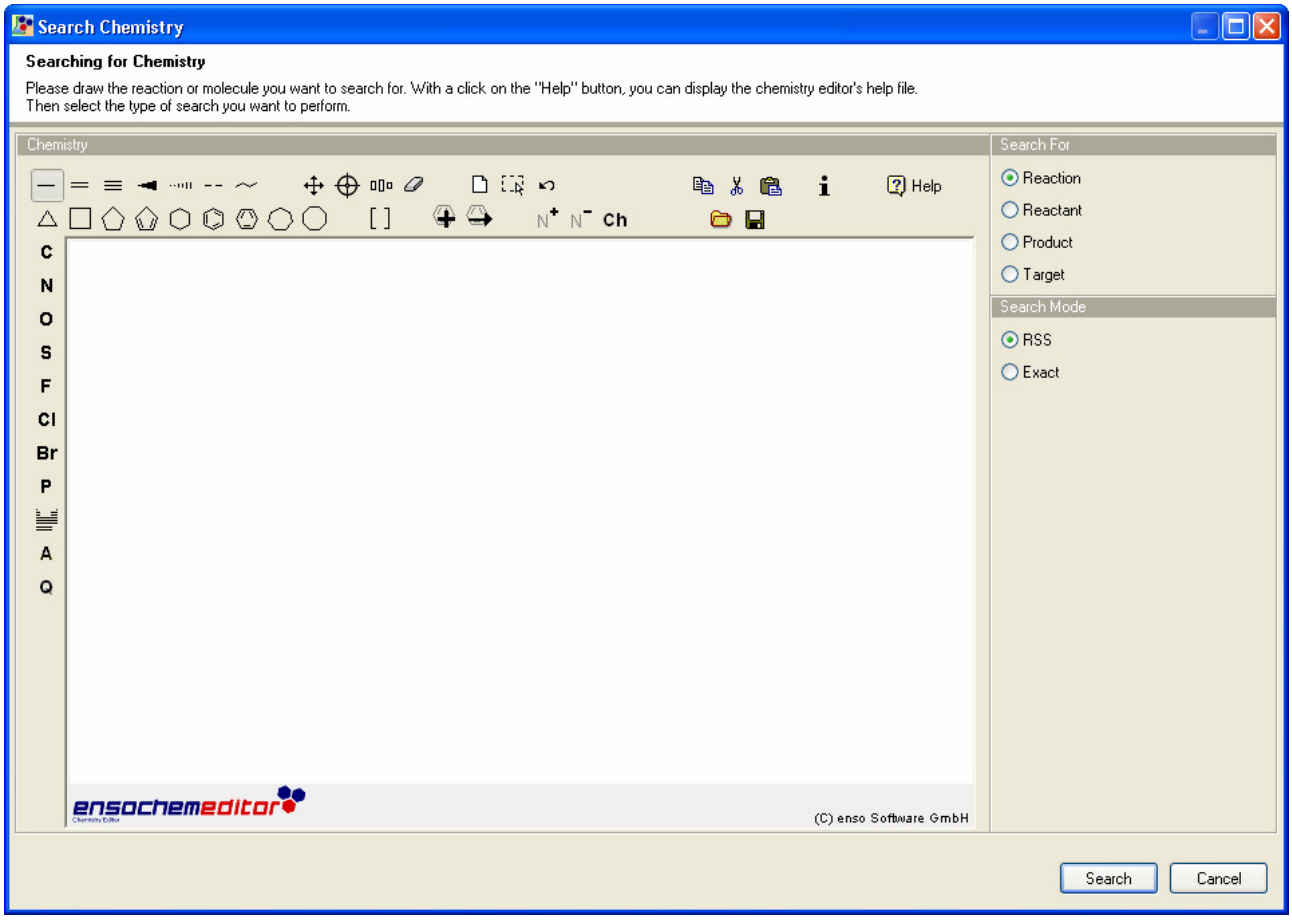


This chapter deals with the search operations themselves as well as the handling of the result lists. In the following text, all different search functions that ensochemLab supports will be explained in detail.

9.1. Chemistry

If you want to search for a specific reaction or molecule, this function is right for you. When you select the corresponding menu entry, the following window will appear. Here you can either directly find ensochemEditor Web Edition or you can use a button to launch your custom chemistry editor. Then please draw the reaction or molecule you want to search for.

The way how chemistry is drawn in ensochemEditor Web Edition has already been discussed in chapter 3 (“Create your first experiment”). For all other editors, please refer to the respective product documentation.



With the two selection fields at the right side of the dialog, you can choose the field in which you ant to search as well as the search mode. You can search for reactions, reactants, products and targets. For each of them, you can perform either an exact comparison or a substructure / subreaction search.

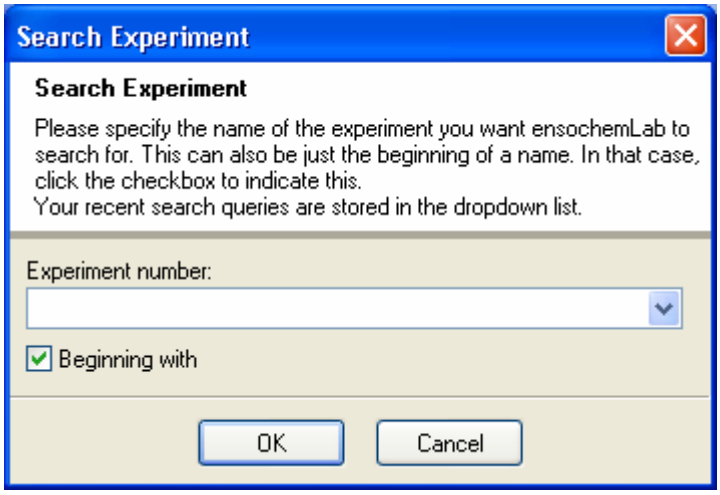
Depending on the installed chemistry search engine, other search modes may be available. The ensochemSearchEngine software which is installed by default offers the exact fragment comparison which performs an exact match of a search structure against all fragments of a molecule. If at least one fragment matches the search query, the respective record is a hit.
For additional information about the chemistry database, please consult your administrator.

Please note that only chemical information is compared, not the way the structure is drawn. Depending on the chemistry database you are using, the detailed result list may vary. For further information on this topic, please consult your administrator or instructor.

After you have drawn your query structure and selected your search mode, please click on “Search” to start the search process.

9.2. Experiments

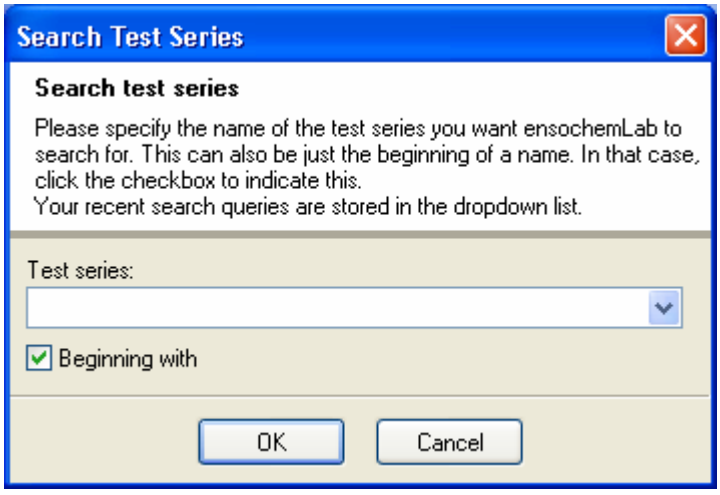
Use this menu entry if you want to search for an experiment number.



You can either search for a full experiment number or for all experiment numbers that start with a given character string. In the second case, you have to select the “Beginning with” checkbox. Click on “Search” to start the search process.
The dropdown list contains your previous search terms used within this ensochemLab session.

9.3. Test Series

The search for test series finds all experiments that have a specific value in the “Test Series” field in the experiment header. When you click on the respective menu entry, the following window will appear:

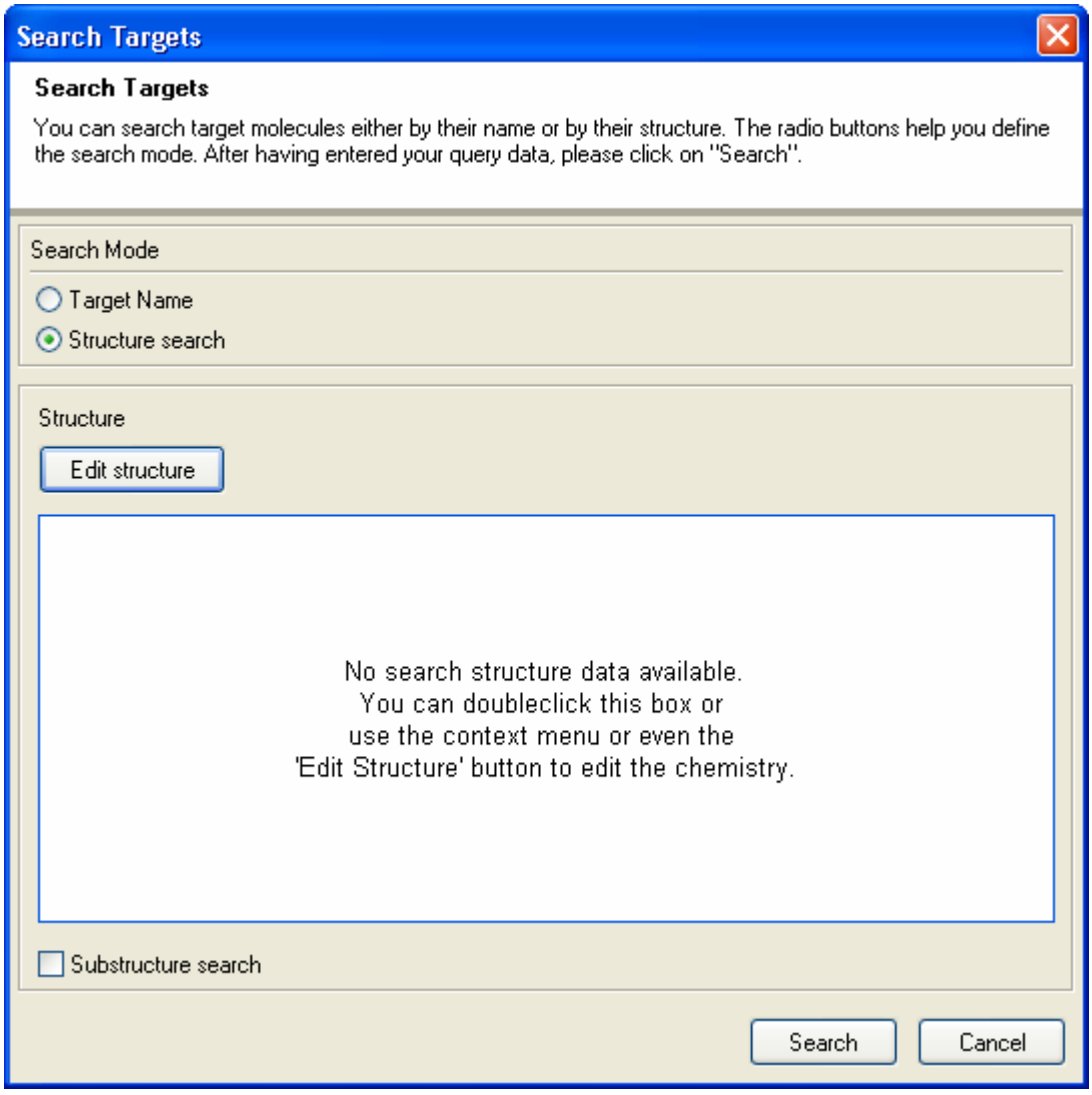


The search algorithm works just like the one for searching experiment numbers. To perform an exact search, please uncheck the “Beginning with“ checkbox. If this option is selected, ensochemLab will find all

experiments whose “Test Series” values start with the text you have entered. An arbitrary number of other characters may follow.
The dropdown list contains your previous search terms. However, as with the search for experiment numbers, you will only find those issued in the current session.

9.4. Targets

When executing this search function, the following dialog is shown:



You already know this dialog as it was shown when defining the target molecule for an experiment by searching an existing record (see Chapter 3. Create your first experiment“).
You can search either for one of the target molecule’s names (synonyms) or for its structure. Please select the desired search mode, enter your query information and then click on “Search” to start the search progress.

As usual, you can launch the chemistry editor by either double-clicking on the structure pane or using the “Start Editor” button.

9.5. Own Experiments

This function searches for all experiments you are responsible for. This means that it finds all experiments you are registered as the owner of, no matter if you have created them personally of if you have taken them over from another user.
This search is automatically performed when you click on the search button in the toolbar.

9.6. Own Experiments with Status Work

This search mode corresponds to “Own Experiments”, but only finds the experiment that have not been finished yet.

9.7. Query Builder

With the Query Builder, you can logically combine a number of search parameters including structure / reaction searches to one query term.
If you do not want to include structures into your search, please select the search mode “Ignore chemistry”. That is the first entry counted from the bottom. You already know how to use ensochemEdit in order to draw structures and you are quite familiar with the search modes, but – where is the editor?
To start the editor, you can click on the “Start Editor” button, use the context menu on the white display pane or double-click on it.

In the lower part of the window, you can create a combined search over nearly all data fields in any chapter of your experiment. At first, please select the desired chapter and then select the field you want to search in. ensochemLab will customize the list of search modes so that you can see only the ones that are appropriate for the field you have chosen. Having selected the search mode, please enter the value you want to search for. Dependent on you field selection, this may also be a lookup list with predefined values.

The search modes for text fields are:

equals exactly	The text in the database has to exactly match the text you have entered.
begins with	The text in the database has to start with the search text you have entered. Afterwards, there may be any other character string.
ends with	The text in the database has to end with the search text you have entered. Prior, there may be any other character string.
contains	The text in the database has to contain the search text you have entered at any position. Prior and afterwards, there may be any other character string.
is empty	The database field must be empty
is not empty	The database field may not be empty

Remarks:	Searches in text fields are generally not case-sensitive.

The search modes for date fields are:

Before	The date in the database has to be before the search date you have entered
after	The date in the database has to be after the search date you have entered
date between (a-b)	The date in the database has to be in the date range you have specified

The search modes for numerical fields are:

equals (=)	The value in the database has to be exactly the same as the search value.
less than (<)	The value is the database has to be lower than the search value.
less or equal (<-=)	The value in the database has to be lower than or equal to the search value.
greater (>)	The value in the database has to be higher than the search value.
greater or equal (>=)	The value in the database has to be higher than or equal to the value in the database.
value between (a-b)	The value in the database has to be in the (open) interval you have specified.
has no value	The corresponding field in the database has to be empty.
has a value	The corresponding field in the database may not be empty.

The search modes for Yes / No fields are:

is true	The value in the database is set (logical value “true”)
is false	The value in the database is not set (logical value “false“)

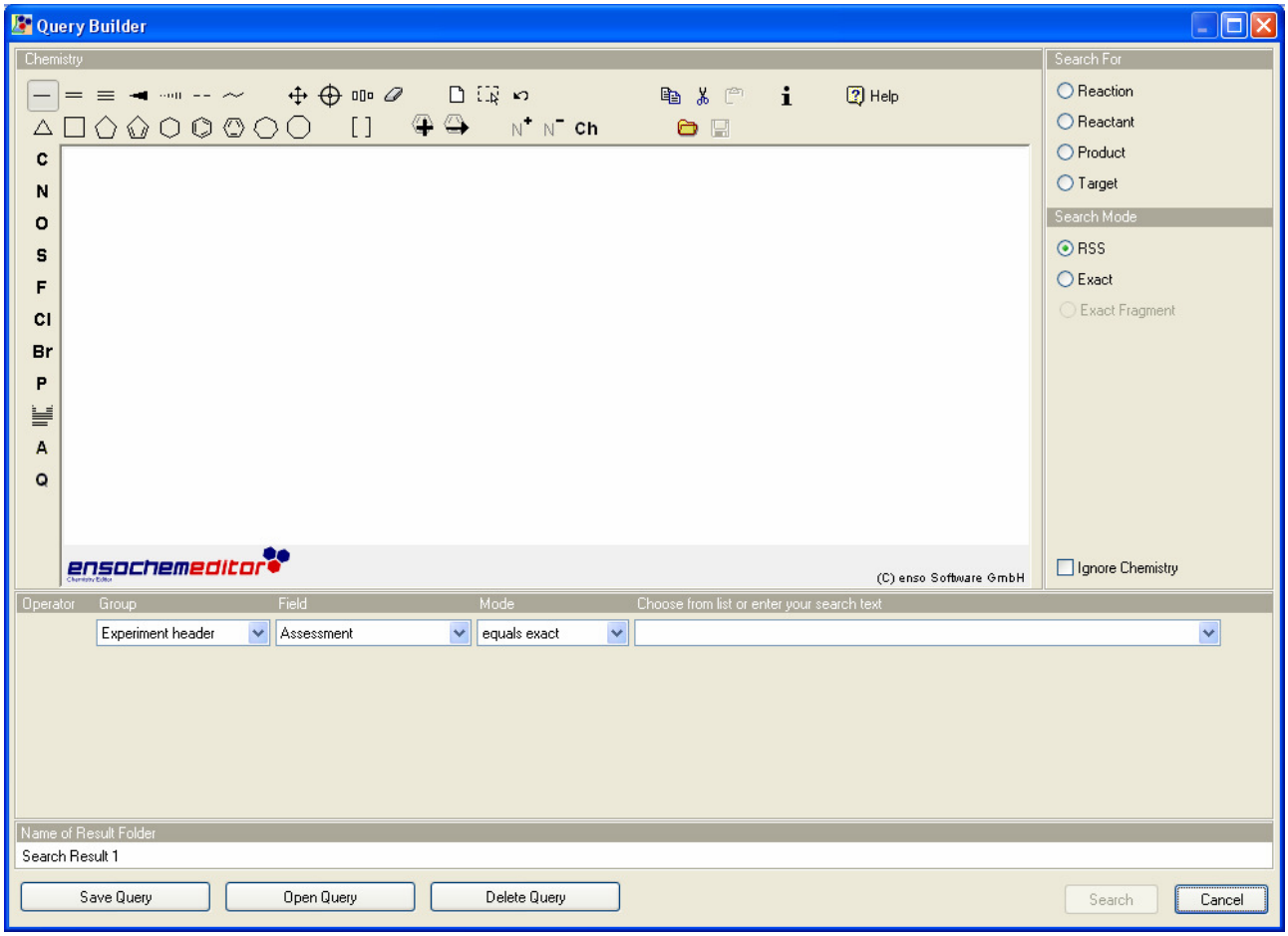
A complete list of all fields and the corresponding search modes can be found in appendix B (“Fields and search modes“). Furthermore, you can also search in the additional data fields defined by the administrator. The respective search type depends on the respective field configuration in this case. Please note that the search modes “is empty” and “has no value” are not available for such data.

After you have filled in a row of query data, ensochemLab will automatically display a new row with empty fields. You can either leave them blank or create the next part of your query. Using the selection box at the left side of the group list, you can specify how you search terms should be combined. The possibilities are the logical descriptors:

and	The query in the current row has to be true as well as the one in the previous row.
or	Either the query part in the current row ort he one in the previous row has to be true.
not	The query part in the current row may not be true. “Not” always implicates an “and not” for combination with the previous row.

For each Query Builder search, you can create a search request that contains at last six different parts. If you do not use all rows that ensochemLab displays, the last row remains empty and will not be included into your search.

Click on “Search” to start the search process.



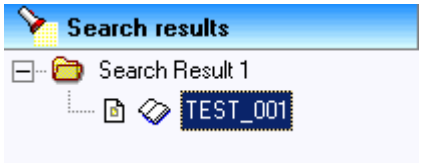
Unlike the other search functions, the Query Builder allows you to specify the name of the folders where the search results should be stored in. The corresponding field can be found at the bottom of the window.

If you want to re-use a query in a later session of ensochemLab, you can take advantage of "Save Query" and "Open Query" respectively. By assigning a short name and an optional description you can easily manage your searches.

To re-initialize the Query Builder, simply click on the button "Delete Query".

9.8. Search Result Management

The results of all search functions, independent from the specific operation you have chosen, are displayed in the “Search results” category in the main window. Each search creates its own folder that is prefixed “Search Result” and then assigned a unique number that is always incremented by one. If no experiments have been found, you will get an error message and no folder will be created.



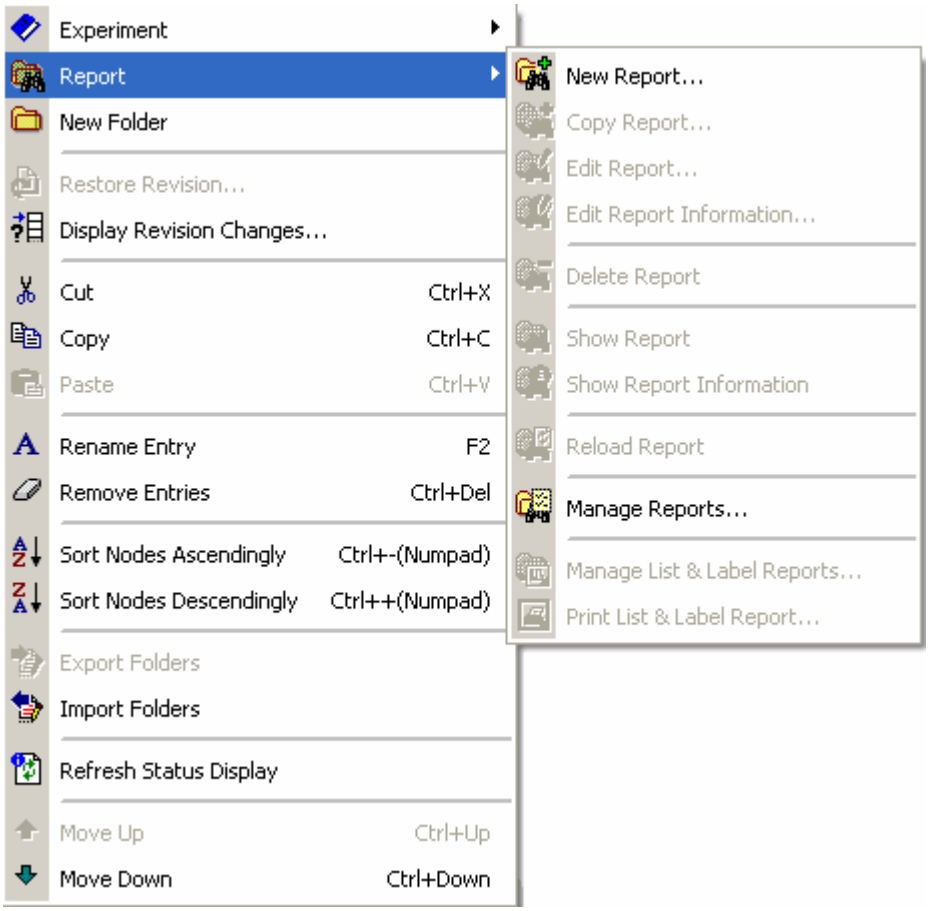
You can copy or move these lists like any other list in the program. Moving them to the “Own experiments” folder, for example, makes sure that they are saved when you terminate ensochemLab.

Remarks:	The menu entry “Experiment -> List operations” can be used to combine search results and other lists using a number of set functions. The chapter „List operations“ will be focused on that topic.

10. Reports

With ensochemLab, you can create reports. A report is a predefined search request whose results are grouped and sorted according to your demands. You can choose which fields shall be displayed as parts of the report. If a report is defined once, you can always execute it in order to perform live reports which your current data.

In order to create a new report, you can use two different functions: In the main menu, there is the “Report Wizard” entry in the “Search” submenu and in the context menu of an arbitrary folder within your experiment list, there is the “Report” / “New Report” option:

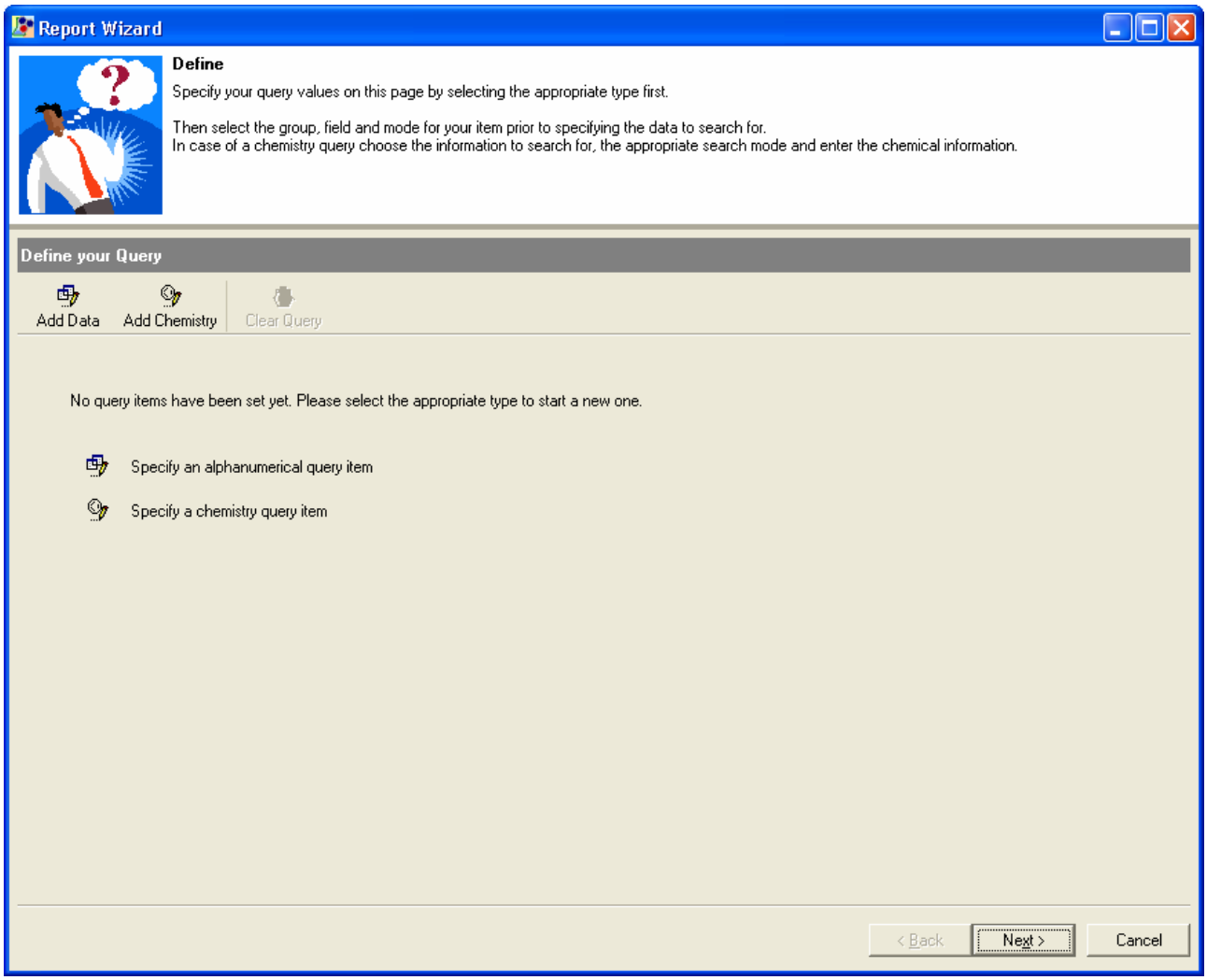


This already hints at the fact that a report is very much alike an experiment reference in the ensochemLab navigator which means hat you will later be able to do all the actions that you know from experiments with your report, too. For a reference, please see the chapter “The main window”. Copying, cutting and grouping are just some of the various possibilities.

Independently from how it was started, the report assistant will appear and guide you through the steps necessary to create an experiment.

10.1. Defining search criteria

The first assistant page looks like this:



On this page you can define your search request. A search request consists of so-called “query items”. A query item is a single criterion that an experiment must fulfill in order to be a hit and thus be a part of the resulting report. ensochemLab supports alphanumerical and chemical query items.

In general, you can search in every data field of your whole experiment. Per report, you need at least one query item. A report can contain an arbitrary number of query items, however please note that one field can only be searched once.

At first, let’s take a look at an alphanumerical search item. In order to add one to your search request please click on the “Add Data” button () in the toolbar. The application will now add a row to your search request:

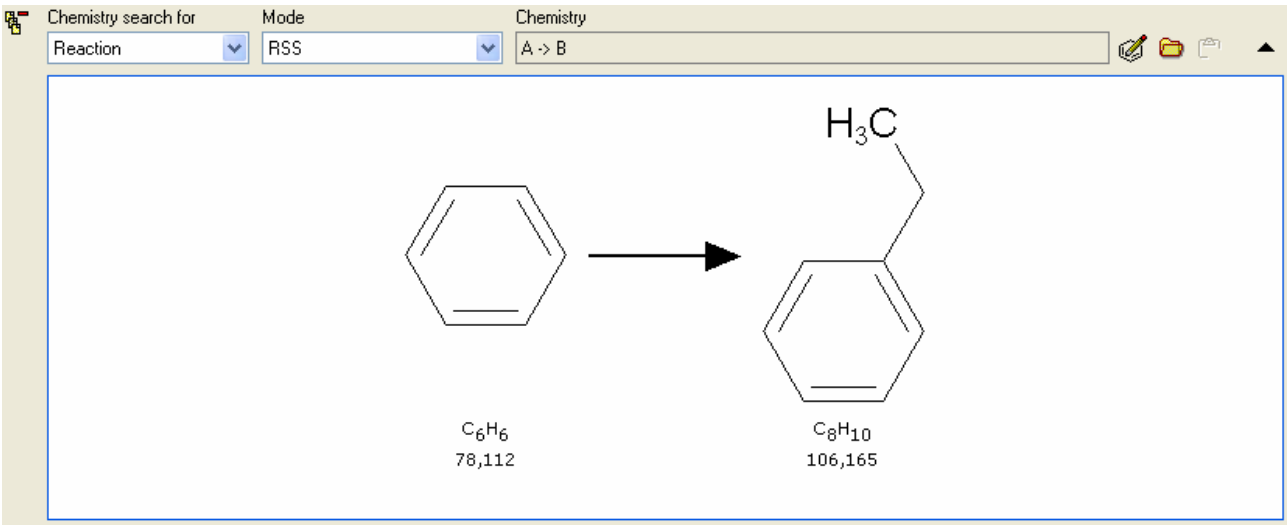
With the selection box on the left side, you can choose the group in your experiment you want to search in. With the next field a bit to the right, you specify the concrete data field. The search mode defines the way in

which the data is to be compared. Additional information regarding the data fields and the respective search modes is available in appendix B to the manual (“Fields and Search Modes”). At the very right side, you can enter the values you want to search for. Depending on the kind of data field, you can also (or exclusively) select values from a list. The possible search value types (text, numbers …) also depend on the respective field.
Besides the normal ensochemLab fields, you can also search in the additional data fields configured by your administrator. They are located in the groups “Additional reactant data” and “Additional product data”. The respective search mode depends on the configured field type.

Nun let’s step over to chemistry query items. Please click on the “Add Chemistry” button ( ) in order to add a new chemistry query item. Again, ensochemLab adds a new row to your search request:

With the selection box on the left side you can choose the data field in which you want to perform the chemistry search. With the field in the middle, you can define the search mode. In order to add the chemical query data, you can either click on the “Past whole reaction / molecule from clipboard” button ( ) for pasting your clipboard contents as search request or use the “Import chemistry from file” button ( ) to import a reaction from an RXN file or a molecule from a MOL file. To directly enter your chemistry with the chemistry editor configured for ensochemLab, you can either double click on the chemistry field (the place where the “< not set >” text is currently displayed”) or click on the “Edit chemistry” button ( ). This opens your chemistry editor where you can draw your reaction or molecule. After the return to ensochemLab, the chemistry field will (depending on the type) either display the schematic reaction layout (“A + B -> C + D”) or the formula:

You can also expand such a chemistry entry to gain an extended view in which you can also see the reaction or molecule. To expand a row, please just click on ”Show chemistry pane” ( ). With a second click on the button, you can return to the much more compact overview display. The depiction of the expanded entry:

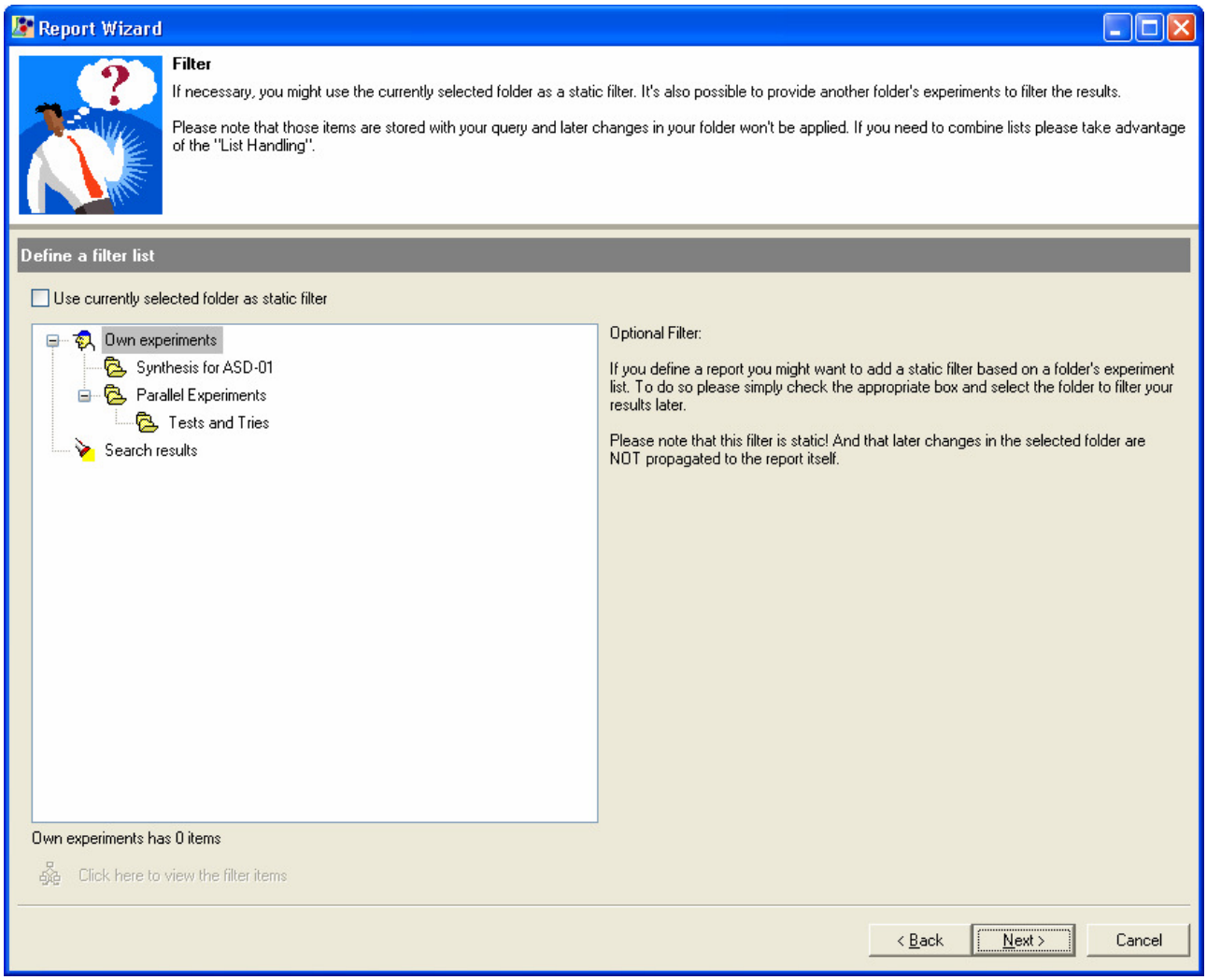


If you want to delete an existing query item, please click on the “Remove query item” button ( ).

After you have defined all your query items, please click on “Next” to continue in the report wizard.

10.2. Static filtering

On the next page, you can now specify a static filter for your report:



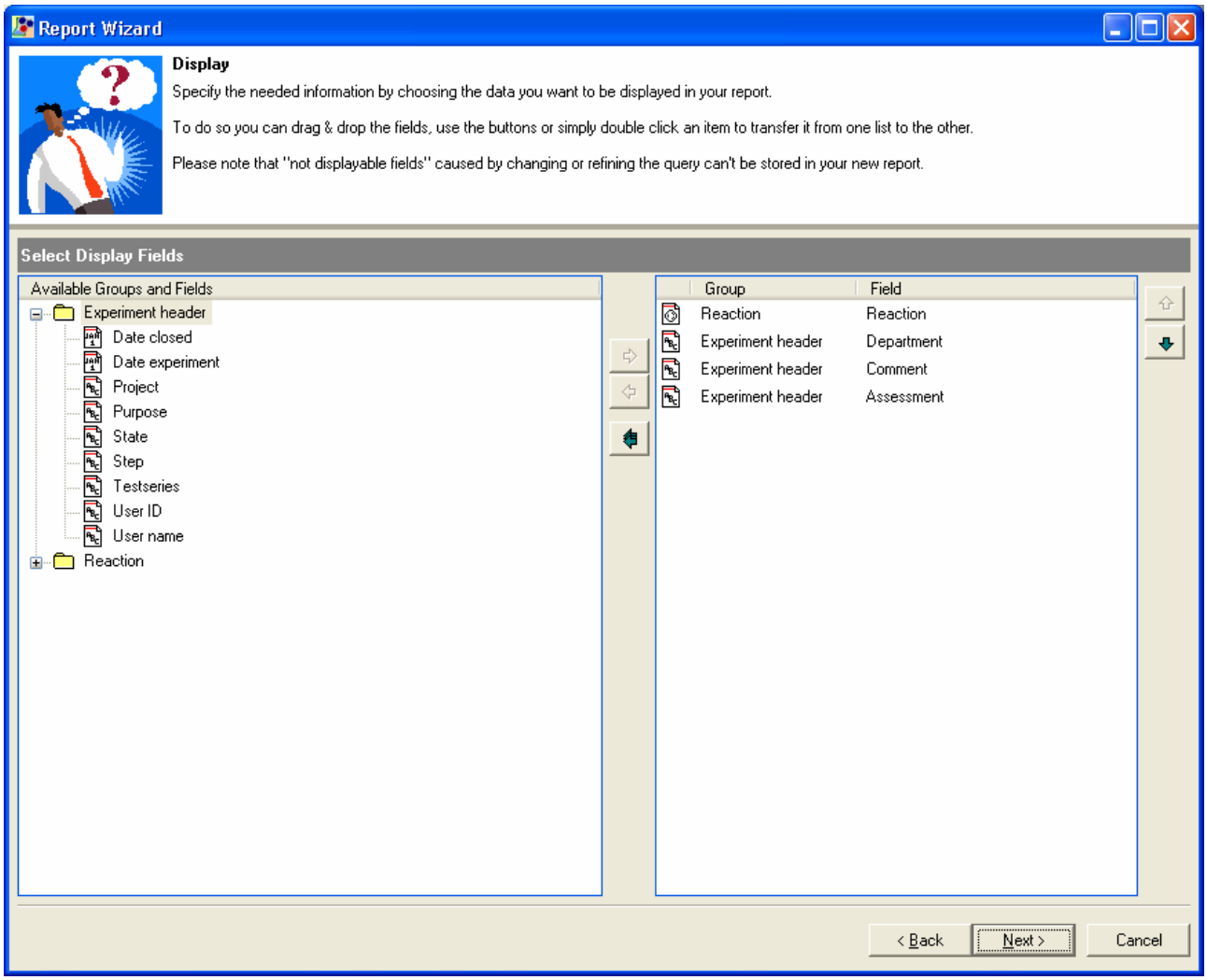
With a static filter, only experiments that are included in the filter list you have defined can be found as results of your search request. In this context, “static” means that the current folder or list is used as reference. If you add experiments to the folder or remove ones from it, these changes will not be applied to your report filter.

If you want to use such a static filter, please check the respective checkbox (“Use currently selected folder as static filter”) and select the desired filter folder from the tree view beneath. Please note that you can only select one single folder. If you want to combine multiple folders to one filter list, please use the “List Handling” module. For additional information, please refer to the respective chapter in this manual. In order to display the experiments in a folder you have selected, please click on the “Show filter elements” button () at the very bottom left corner of the window.

If you are satisfied with your current filter selection or if you do not want to use a filter please click on “Next” to continue creating your report.

10.3. Display fields

On the next page, you can select the data fields you wan to be displayed in your report:



In the list on the left side of the window, you can see a list of data fields that are either predefined (reaction) or that are part of your search request. The additional data fields are also available when their respective chapter is included (e.g. additional reactant data can always be used together with normal reactant data). The list is grouped by chapters. These fields are the only ones you can display in your report. All displayed fields are collected in the list at the right side.

For adding a field to your report, please first select it in the list on the left side and then click on the “Show field” button ( ). The field will now be moved into the list on the right side. If you want to remove a field that is already part of the list, please click on “Hide field” ( ). With the “Delete all fields” button ( ), you can clear the right list (remove all fields).
Of course it is also possible to assign fields via drag & drop. Just drag the desired items from one list into the other.

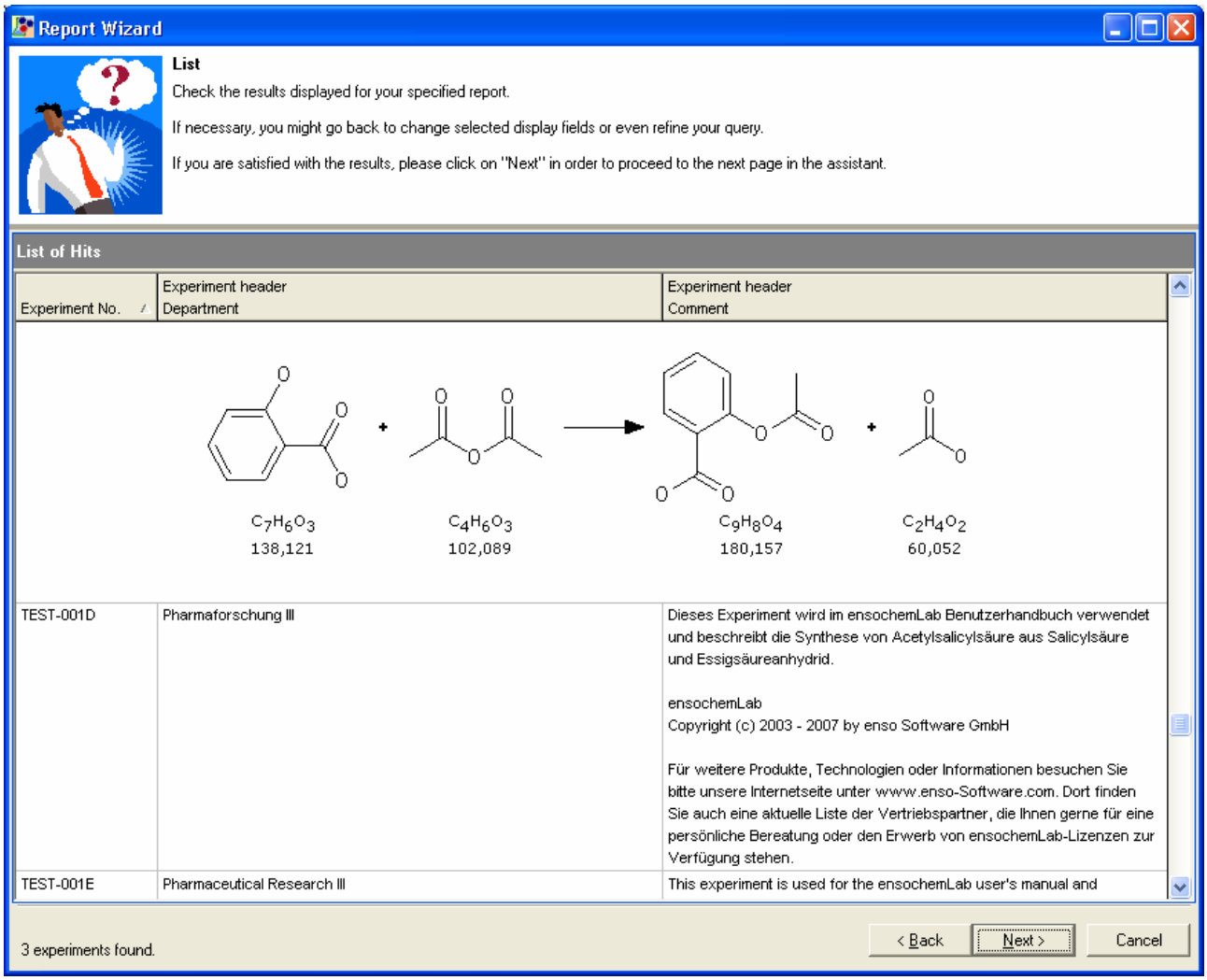
The order of the data fields in the list on the right side corresponds to the field order when the report in the later display. For changing the order, you can either use drag & drop to a move a field to its new position or you can select it and then click on the “Move up” ( ) / “Move down” ( ) buttons on the right side of the list.

Both the features for assigning and removing fields as well as those for changing the display order are also available via the context menu.

When having finished working on this page, you have defined the most important parts of your report. Please click on “Next” to continue.

10.4. Report preview

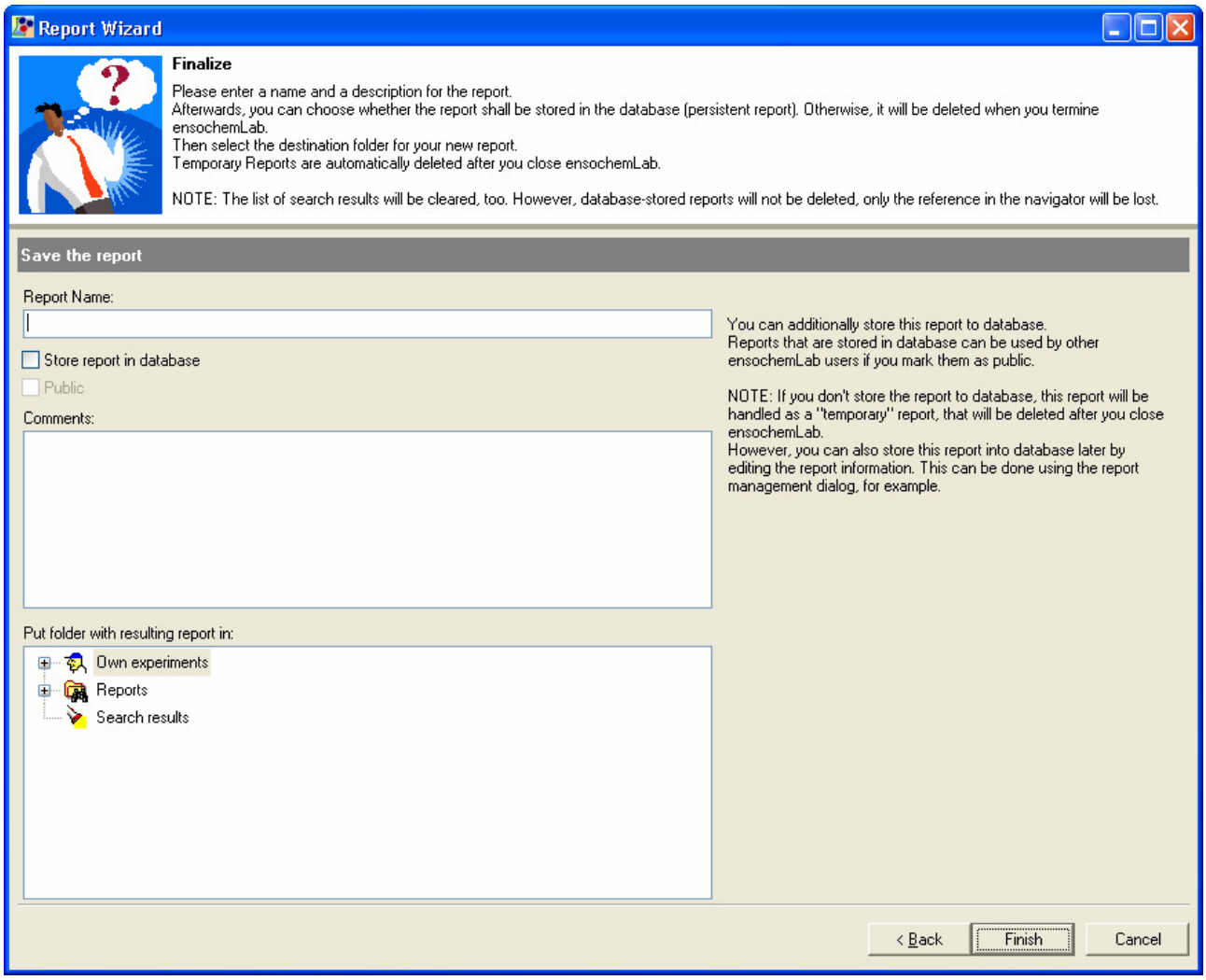
The next page allows you to preview your results before the report will finally be saved.



The hit list contains the experiments that have been found with your search request. Like in the real report, only the fields you have selected for display are visible. Thus, the list is a preview of the real report at the current execution time (e.g. with the current database content). This feature enables you to check the results and, if necessary, click on “Back” in order to return to one of the previous pages and change your search request or display fields.

If you have achieved your desired result and want to keep the current record, please click on “Next” to step forward to the last page of this assistant.

10.5. Saving the report



On this last page, you can define the name under which your new report shall be saved. Furthermore, you can also set the location you want to place it in.
First, please enter an (if possible) unique name into the text field at the top. Then select a storage location from the tree view.

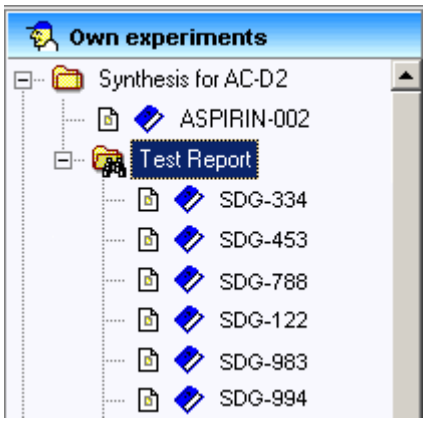
ensochemLab distinguishes between two types of reports: Temporary reports are saved in your navigator and deleted when ending the application. In order to permanently save a report and also having it available in your next session, you have to save it to the database. On this page, you can choose the report type by either selecting the “Store report in database” checkbox or not.
If your report is saved in the database and your administrator has enabled the respective function, you can also mark it as public. In this case, other ensochemLab may also access it in read-only mode. This means that they can view your report with the current experiment data, but they may not change any of its settings. The names of public reports always have to be unique. A temporary report cannot be marked as public.
You can also change both options at a later time. However, please note that database-stored reports cannot be reverted to temporary ones.

With a click on “Finish”, you save your report to the database and quit the wizard.

10.6. Displaying and managing reports

The following part of the chapter will deal with how to work with existing reports and what functions are available to you.

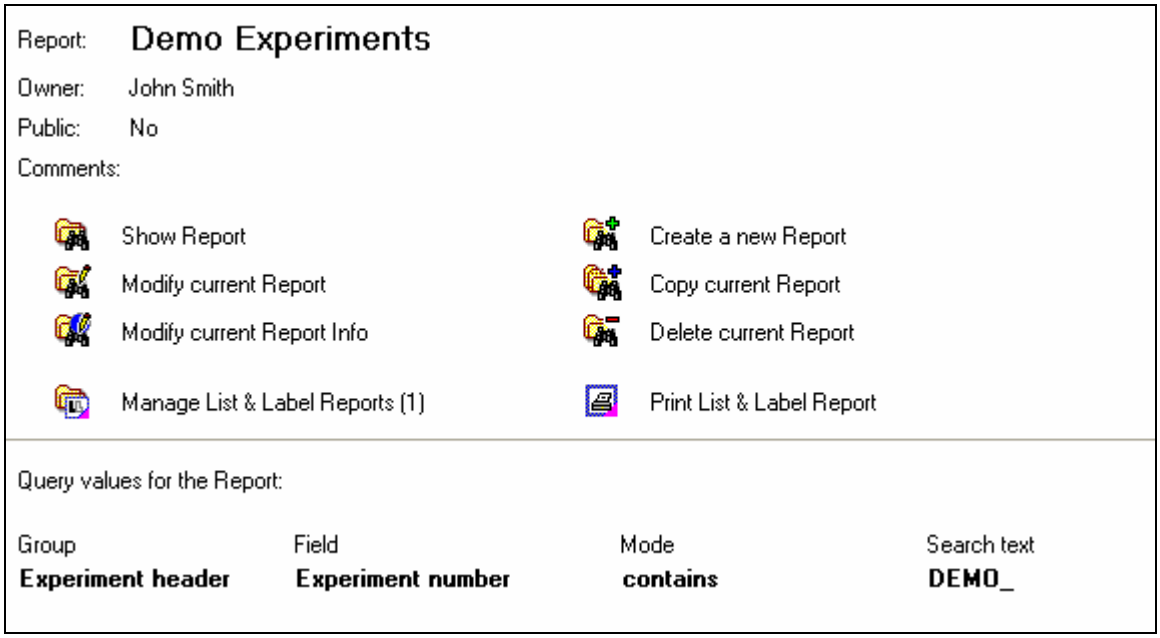
You can select a report in the navigator just like a normal experiment. The only difference is that it contains the experiments which have been found with the respective search request as subordinate nodes:



If you select a report in the navigator, the display pane on the right side of the window where normally the experiment data is shown will display a short overview of your report.

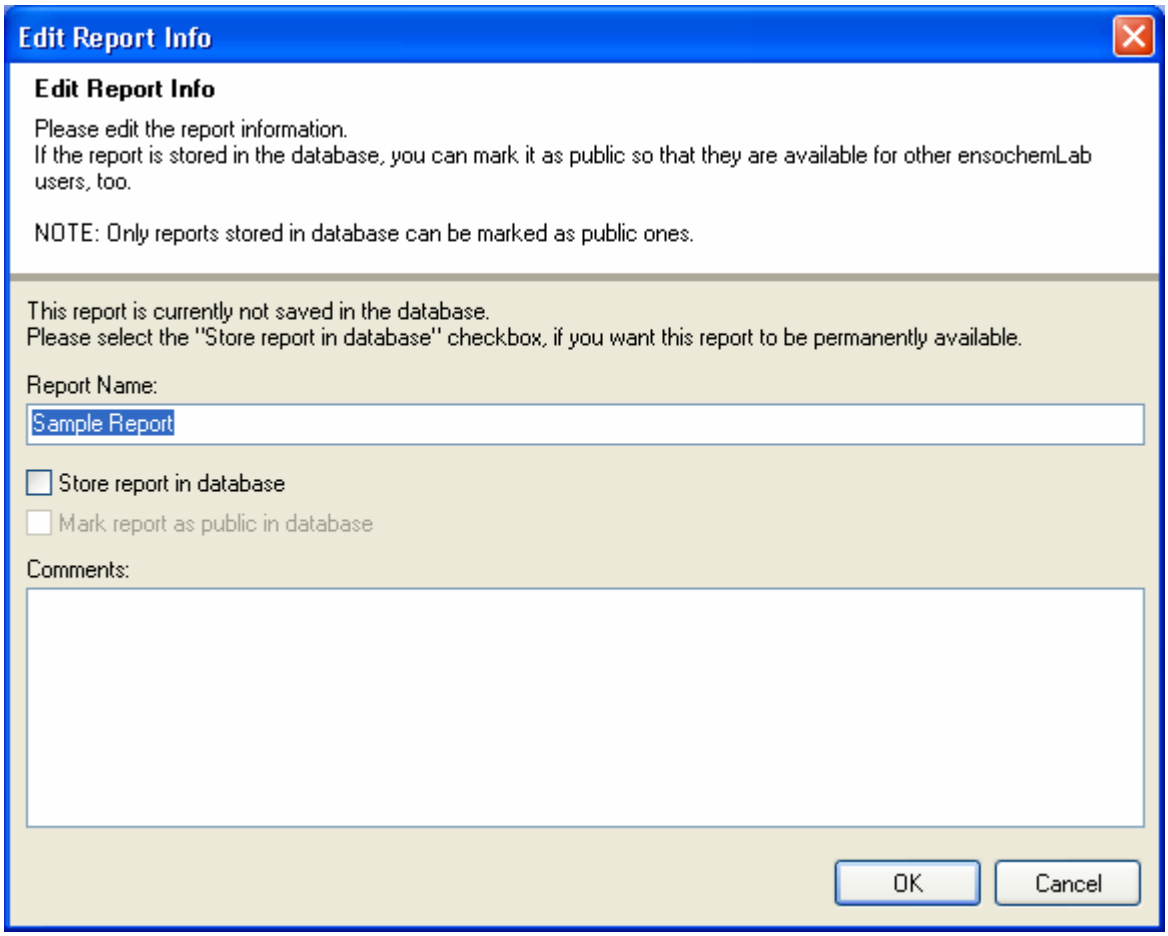
If you have just created the report, you can directly see your report data. In order to display the overview pane you can right-click somewhere in the display frame and then select “Show Report Information” () from the context menu. However, please note that switching the display mode is only a temporary action which means that if (for example) you display a different report and then return to this one, the report data will be shown once more.

On the upper side of the report overview, you can see the actions you can perform with it. In the lower part, ensochemLab displays the search criteria for your request:



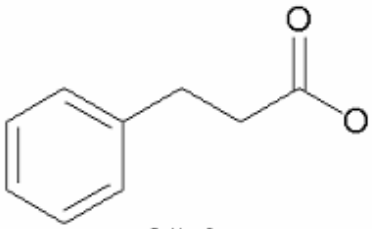
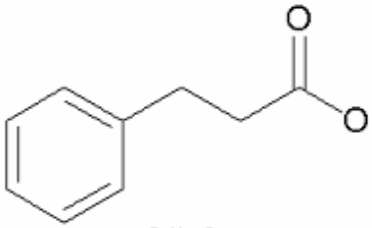
If you want to return to the report assistant for creating a new report please click on “Create a new Report” (). For changing the current report’s search request, please select “Modify current Report” (). With this function, you return to the report assistant with the current report’s data.

If you only want to change some report header data like name or description, you can also do this separately by using the “Edit Report Info” function (). The following window will appear:



You can also mark your report as public here or move it to the database for retaining it for further sessions. Please click on “OK” to save your changes or click on “Cancel” to return to the main window retaining your previous description data.

The most important function is to display the report’s data which is to execute its search request on the current data in your ensochemLab database. You can perform this action by clicking on “Show Report” (). The results will be shown in a table containing the fields you have selected as columns. The table exactly corresponds to the one you have already seen as a preview within the report assistant. With a click on a column header, you can sort the data by this column. A second click on the header changes the sorting order (ascending or descending). Furthermore, it is possible to change the column order by simply dragging a column to a new position.

Experiment No.	Reactants Reactant structure	Experiment header Department
DEMO_001	 $C_9H_{10}O_2$ 150,175	Software-Entwicklung
DEMO_002	 $C_9H_{10}O_2$ 150,175	Software-Entwicklung

The actions from the overview page are also available here by using the context menu.

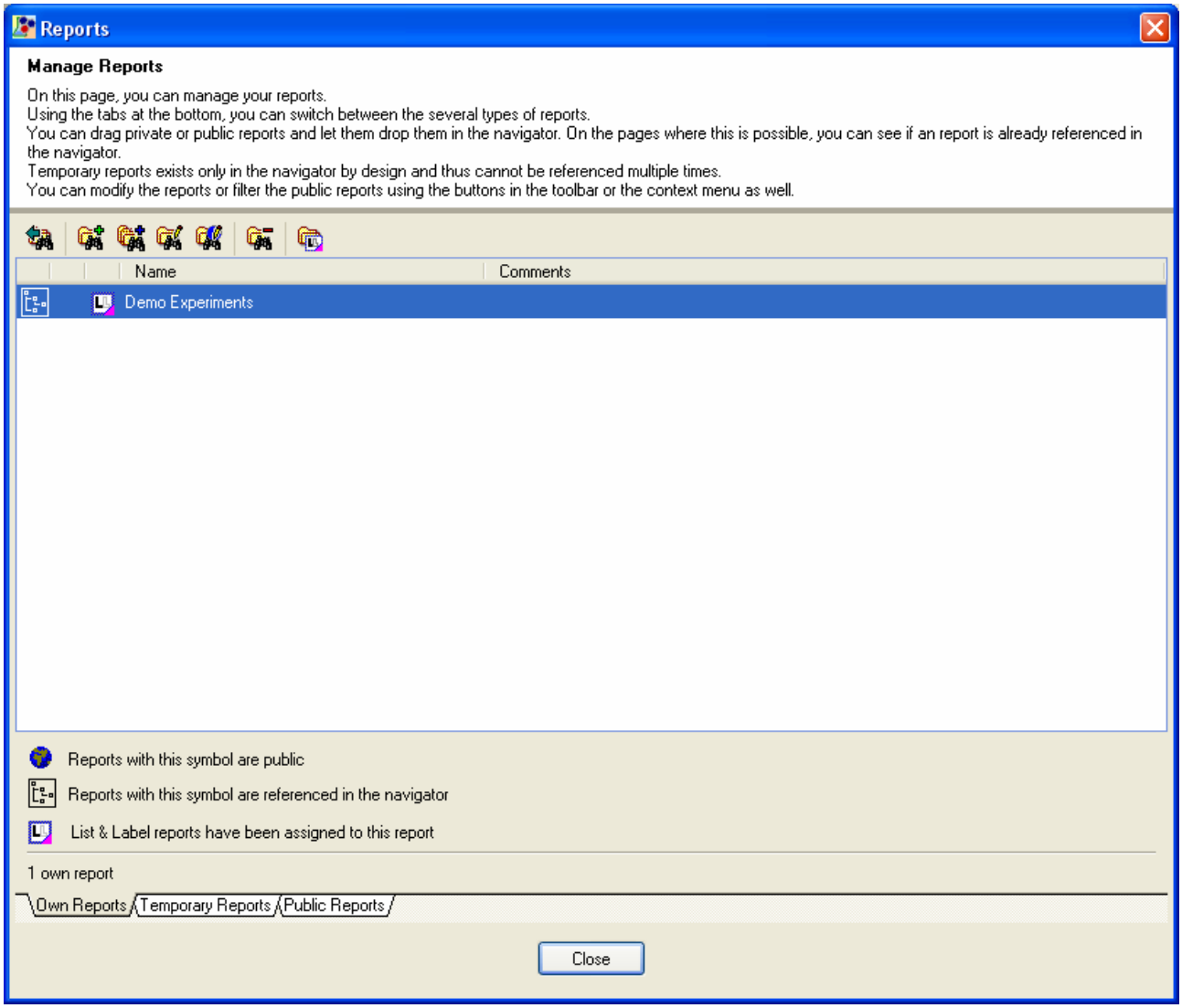
We have already hinted at one very important topic: The character of a report. A report is very much alike an experiment link in your personal navigator. It offers all corresponding features like copying, moving and sorting.

When deleting a report, however, the software distinguishes between the two supported types of reports: If you delete a reference to a temporary report, the report itself will also be deleted. A corresponding warning message will be displayed.

A reference to a permanent report (one stored in the database), on the contrary behaves like an experiment reference in general: Deleting or modifying a reference does not change the report object itself. However, for simplifying your work, ensochemLab asks you whether you also want to delete the corresponding report from the database in a question dialog.

In order to get an overview over all own and public foreign reports that are currently saved in the database and for creating references to them in your navigator, ensochemLab offers a separate dialog for report management. Here you can also modify and delete own reports that are currently not referenced in the navigator.

You can start the dialog by clicking on the navigator with your right mouse key and then selecting “Reports” \ “Manage Reports” from the context menu. The same function is also available beneath “Reports” in the main menu. The management dialog looks like follows:



In the lower part of the window, you can see three tabs. Depending on the currently selected tab, different reports are displayed in the list in the middle of the window. Above the list, there is a toolbar containing the commands that are possible for this kind of reports. Below the list, there is general information (like the total count of reports displayed) and a short legend explaining the symbols used in the list.

If a report is marked with a globe symbol (), it is a public report. Reports marked with the symbol are already at least once referenced in your navigator. The symbol indicates that at least one List & Label report has been associated with this ensochemLab report. List & Label reports are explained later in this chapter.

For creating a new navigator reference to a report, you can either move the respective list entry into the desired folder or navigator group via drag & drop or use the “Add to navigator” () button in the toolbar.

With the “New” button (), you can start the report generation assistant for creating a new report. The “Copy” function () enables you to create a copy of the currently selected report. More information on this topic is available later in this chapter.

If you want to modify an existing one please select it and then click on “Edit” (). If you just want to change the description data (title and comment), you can click on “Modify information” () in order to start the description dialog described earlier in this chapter.
The delete button (), completely removes the selected report from the database. This will also delete associated List & Label reports independently of their respective owner.

Please note that you can only delete or modify own reports. The List & Label reports are no exception to this rule as they are only defined in combination with the respective ensochemLab report on which they are based. The existence of subordinate objects does not change the permissions defined for the parent report.

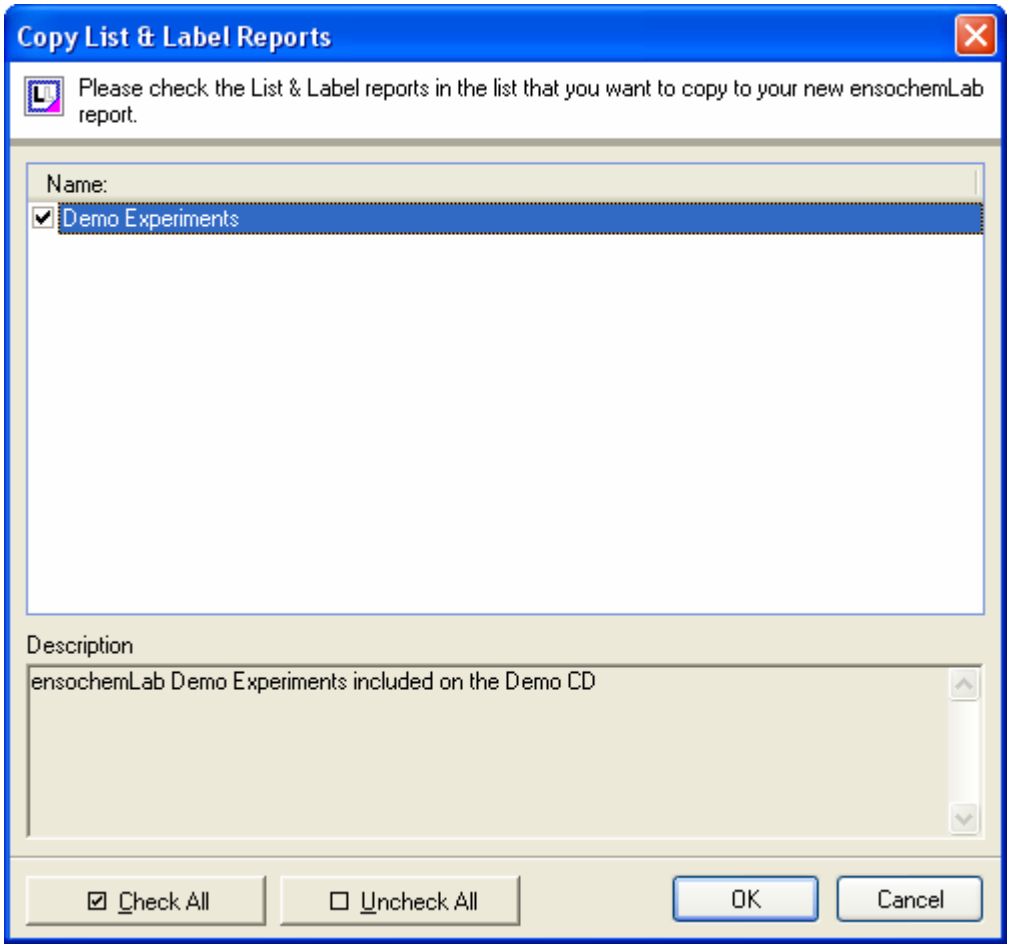
With a click on “Manage List & Label Reports” () you can open the management dialog for List & Label reports which is covered in detail in a following part of this chapter.

Since there may be a great number of public reports, the corresponding page also supports two filter functions for displaying only the records you want. The respective commands can be found in the filtering menu (). With “Filter by name”, you can display only the records which contain a specific text in their name. “Filter by comment” lists only those whose comment includes the text you enter.
For displaying all reports - this means removing the current filter – please click on “Filter nothing”.

With a click on “Close”, you can return to the ensochemLab main window.

This chapter has already shown a number of places where you can copy reports. Copying a report means that the report wizard is opened with a copy of the current report's data. You can the normally use all functions within the dialog to freely modify your copy. On the last page, we recommend entering a different name, for public reports you have to. Then click on "Finish" to complete the wizard.

If List & Label reports have been associated with the original ensochemLab report, a dialog is displayed in which you can select the List & Label reports you want to copy:



Your ensochemLab report has already been created at this moment. For not copying any of the List & Label reports, you can thus simply click on "Cancel".
Otherwise, please select the List & Label reports that you want to copy. With a click on "Check all", you can select all entries in the list. A click on "Uncheck all" removes all marks. Afterwards, please click on "OK" for completing the operation.

10.7. List & Label Reports

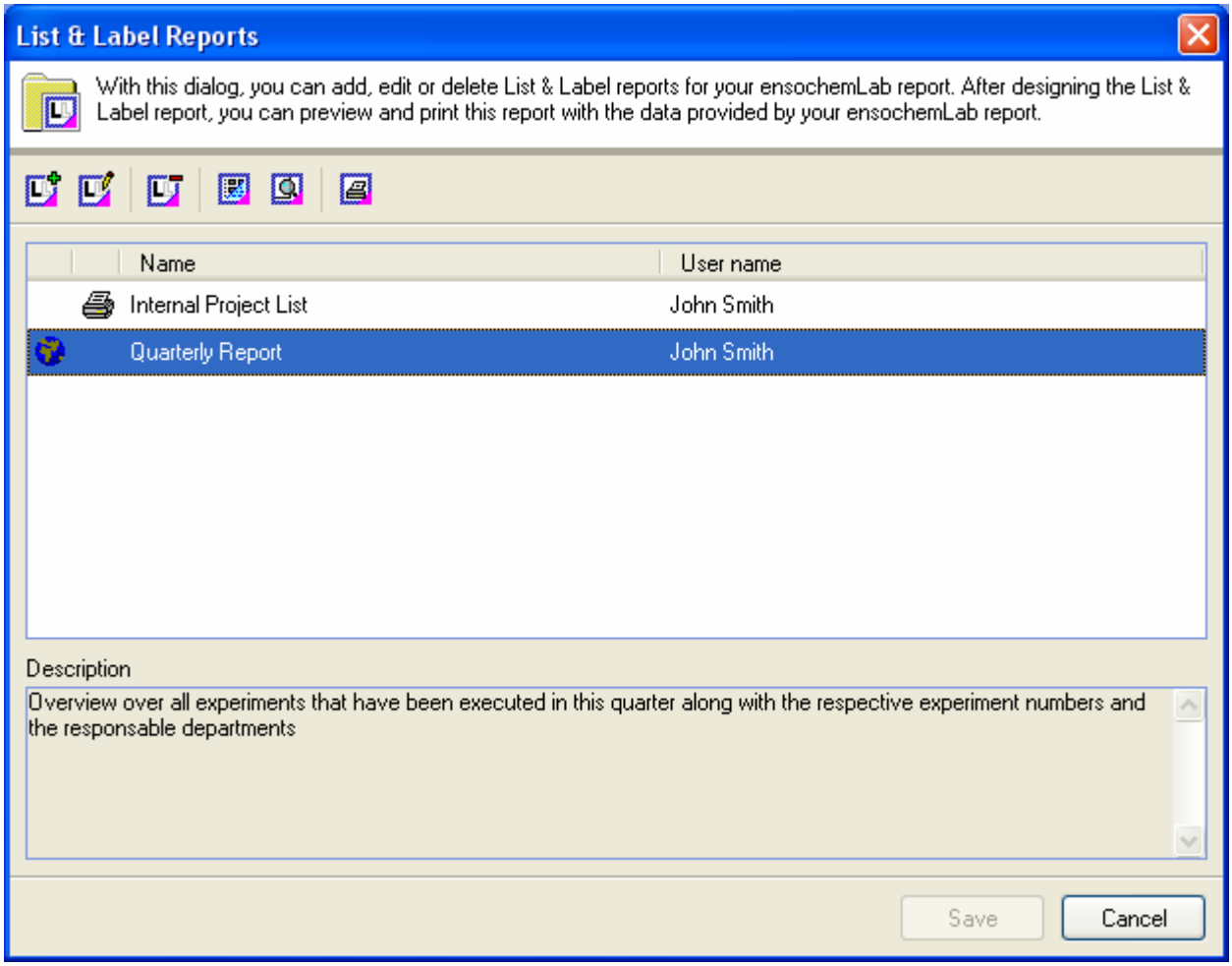
Up to now, you have only used normal ensochemLab reports. These reports have a vastly predefined table layout that you cannot directly modify. For example, you cannot change the table to have an alternate color scheme, maybe even depending on the respective row's data.

In addition, the software also provides so-called List & Label reports that are based on an existing ensochemLab report from which they retrieve their respective data. All other (display) options are freely configurable. The following example creates a simple multi-colored table layout.

For starting, please select the report you have created earlier in this chapter in the navigator. You then have a couple of possibilities to launch the management dialog for List & Label reports:

- Display the report information page and click on the "List & Label" reports link there.
- Use the report entry's context menu in the navigation pane and click on "Report" \ "List & Label Reports".
- Change to an arbitrary display mode for your report and then open the "Report" entry within the main menu. Choose the "List & Label Reports" function.

Independent from the method you use, the following dialog is displayed. In your case, it will most likely be empty.



For creating a new List & Label report, please click on “New List & Label Report” (). ensochemLab will then launch the List & Label report designer which is an external application including an own dedicated documentation (help file) that you can launch by using the “?”, “Contents” menu entry. Additionally, you can press the F1 key in order to directly display the help topic associated with the current function or setting. This is why this manual will only explain the creation of the sample report, but will not detail with any other features provided by the designer.

When creating a new report, the designer helps you with a wizard. The first step is selecting the correct printer you want to use. Elementary settings like paper format and size are taken from this device when calculating the preview. Furthermore, you can also select how you want to format your data table and whether you want to include a title row or a summary.

The most important step is the selection of the fields you want to include in your table. You can use all data fields contained in your ensochemLab report. As already indicated, a List & Label report always processed the data provided by the ensochemLab report on which it is based. Due to that reason, it is not possible to add other data fields. If you want to do so, please modify your ensochemLab report accordingly before you create your List & Label report.

After you have completed the wizard, the designer’s main window becomes accessible where you can perform all further changes to your report. For this example, you can try to perform the following modifications:

1. Change the list title to “Project Results 3rd Quarter”
2. Create a new text field stating “Results of the 3rd Quarter – Project Status Overview” below the main title edited in the first step.
3. Add an ellipsis with a blue border (1cm border size) at the right side of the title and create a text field stating “Confidential” inside it.
4. Change the table columns to “Experiment number”, “responsible department” and “reaction”.

The report designer of course enables you to perform much deeper changes to your layout. This means that you can, for example, include picture files, apply more complex table layouts or change arbitrary object properties. Additionally, you can take advantage of dynamic elements which includes displaying certain objects only under certain (data-dependent) conditions (for example highlighting rows with unfinished experiments), dynamically calculate field values (the count of unfinished experiments etc.), generate barcodes (the barcode for the flask in which the product is delivered etc.) and much more.

In order to ensure that your report will be correctly displayed later, it must contain a data table. However, it is not necessary that this table contains any rows.

When you have finished creating your layout, please close the designer and answer “Yes” to the question whether you want to save your changes. Then, please select an arbitrary folder and file name on your local computer where you want to save the layout definition file. Of course, you can also save at any prior point during the design process.

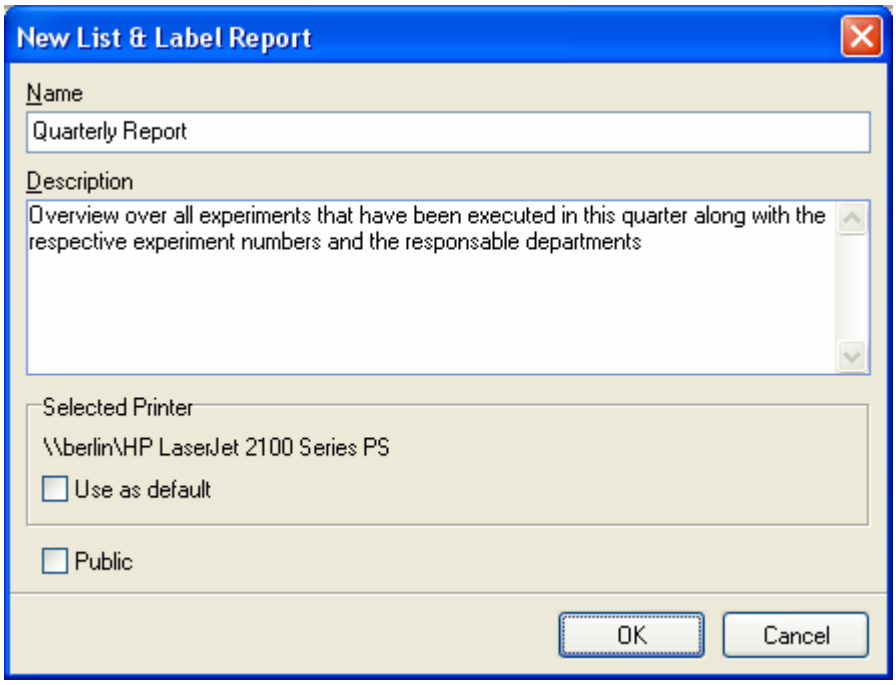
Please note that your report will be registered in the ensochemLab database in the next step. Afterwards, your local file is no longer directly necessary. Therefore, you will be asked whether you want to retain the file you have just created or whether you want to delete it. In general, there is no need for keeping the file unless you want to use it for any other purpose outside ensochemLab. On the other hand, you can also use this method to create local template files for more, slightly modified reports.

However, please note that your chosen option will be directly executed. If you select “Delete”, the file will be deleted no matter if you cancel the report creation process later.

You may have noticed that, strictly speaking, there is not one, but three report definition files on your hard disk. If your file is named “Quarterly Report”, these files are called “Quarterly Report.lst”, “Quarterly

Report.lsv" and "Quarterly Report.lsp". Still, inside ensochemLab and the report designer as well, these files are always treated as one.

The next dialog that appears deals with the save process itself:



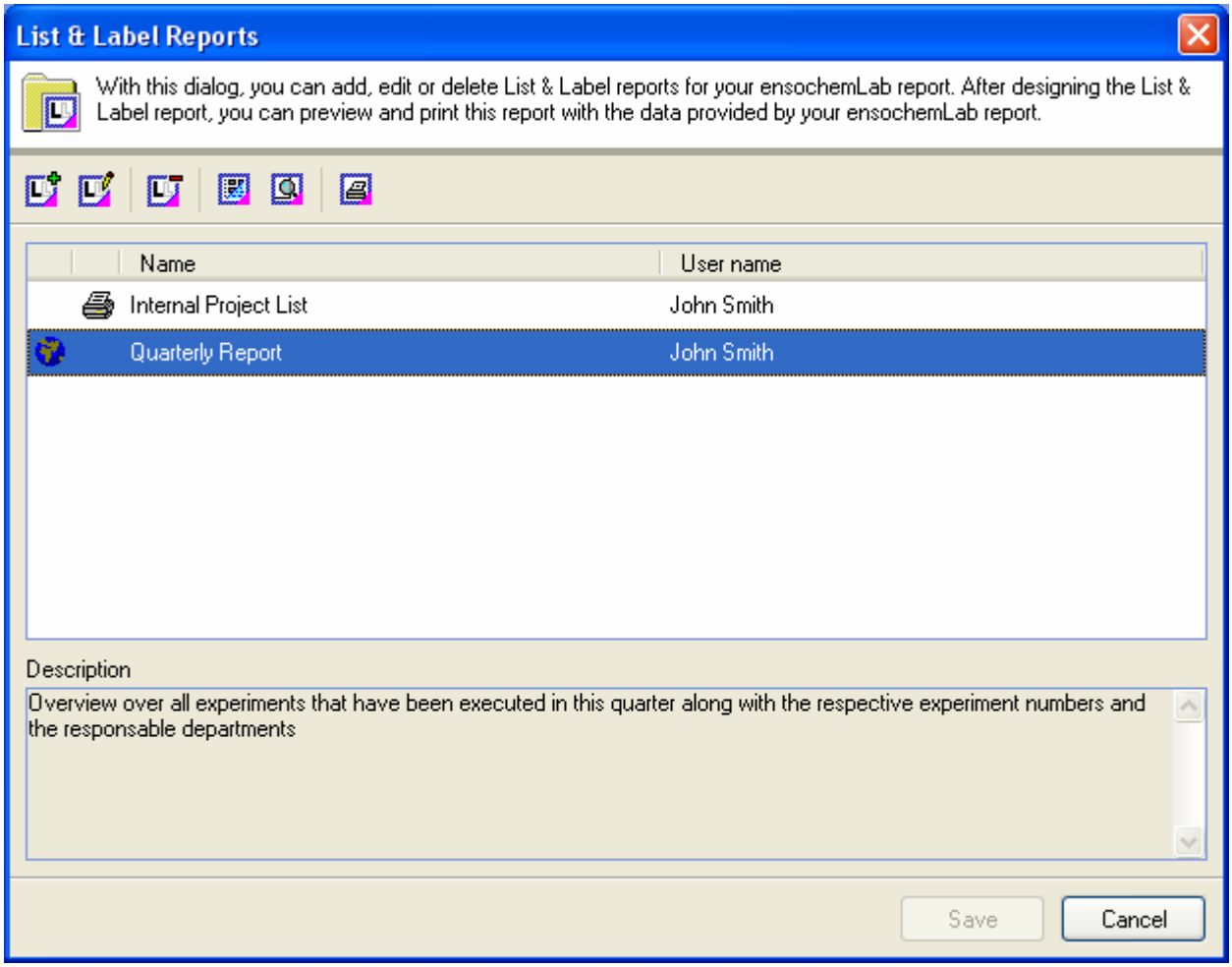
Here you can enter a name and a description under which you want to save your new List & Label report into the database. If your administrator has enabled the respective function, you can also mark your report as a public one so that it is available to all ensochemLab users. However, please note that the names of public reports need to be unique.

Additionally, you can configure whether you want to set the printer you have used when designing the report as the default one for your record.

With a click on "OK", you apply your report to the overview list. If you click on "Cancel" instead, you return to the report management dialog without applying your new report.

When creating new reports, you can of course also cancel the initial configuration assistant and load an existing layout definition file from your local hard disk in order to apply this one to the database instead.
If you modify an existing report's layout and load a local definition file meanwhile without modifying the layout you have originally been editing, a confirmation dialog is shown. Therein, you can decide whether to replace the current record in the database with this different file. If you modify both files, the confirmation dialog gives you the options to load either file or completely abort the process.

Your administration dialog for List & Label report now contains an entry. This means that the time has now come to discuss its remaining features.



For every existing report, you can see the respective name and owner. Generally, you can also create List & Label reports for foreign ensochemLab reports. When planning to do so, you should however keep in mind that you have no control over the original base report. This does not only mean that you cannot change the data fields available to your List & Label report, but also that the owner may change his report in a way rendering your List & Label reports invalid at any time. Such a change can, for example, happen if a used data field is removed from the base ensochemLab report. Furthermore, he can always delete his report which removes your List & Label report, too.

When using own base reports, you should still keep in mind that changing the base report later may cause undesired malfunction of the associated List & Label reports.

You can avoid both problems by creating copies of the base reports and then using them instead for List & Label reports of the original ones.

If a record in the management dialog marked with the globe symbol, it is a public one. A printer symbol indicates that a default printer has been configured. After a click on an entry, its description is visible in the lower pane of the window.

For modifying a report's description data, please select the respective list entry and then click on "Edit List & Label Report" ( ). The dialog that you already know from creating a new report will appear.
If you want to return to the designer for altering your report's layout, then click on "Design List & Label Report" ( ). If you use ensochemLab in multiple languages, the designer will contain the data field names in the

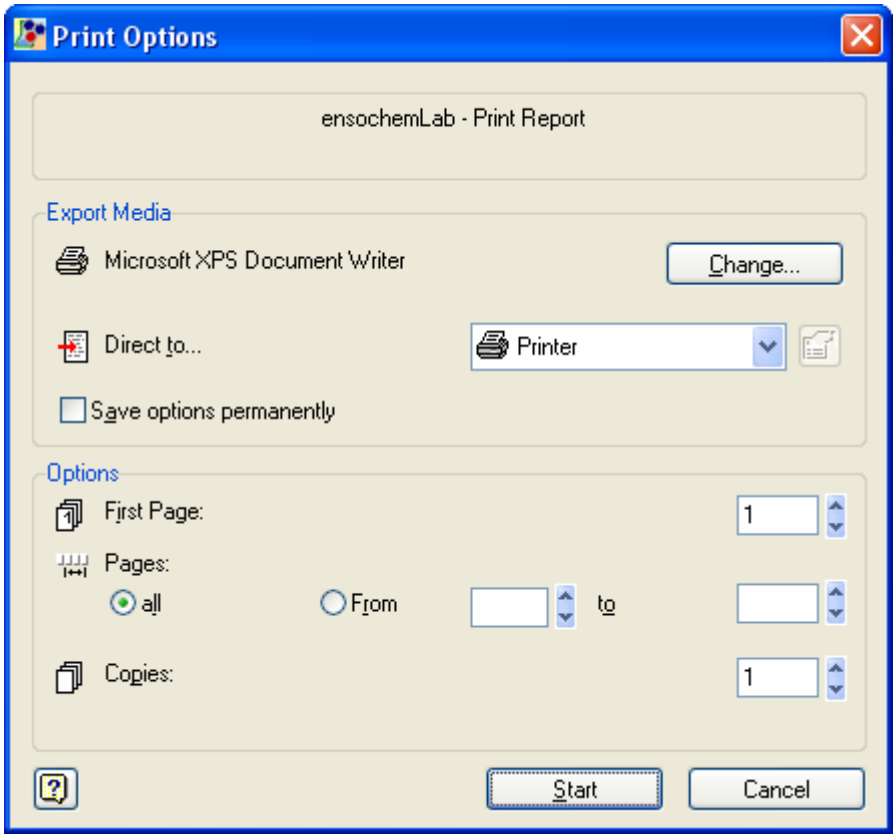
language originally used for creating it. The data field language cannot be changed once the report exists and only applies to the designer.
With a click on “Delete List & Label Report” you can delete the current report.

Just as with normal reports you can only modify or delete own records. When editing, this applies to the description data as well as to the layout.

Please note that no data has actually been saved up to now. This means that if you close the dialog with a click on “Cancel” now, all changed your have performed are undone. You can save your changes with a click on “OK”.

For printing a List & Label report or displaying the associated print preview, please click on the “Preview List & Label Report” button ( ). In this window, you will find features for printing your report, saving it in different file formats (including PDF), switching between pages and changing the display’s zoom factor.
You can either use the default printer for your printout by normally clicking on the printer toolbar symbol with your left mouse button or open a printer selection dialog by right-clicking on it.
After you have finished working with the preview dialog, just close it in order to return to the List & Label report management dialog.

Of course, you can also directly print a List & Label report without having to open the preview dialog first. This feature is provided via the “Print List & Label report” ( ) button. The following dialog in which you can select a target for your printout will appear:



By default, the output option for normal printers is initially selected. You can change or configure the printer you want to use with a click on “Change”. In this context, configurations means setting the correct options for paper size, printing quality and other features offered by your printer. Additionally, you can select to take a different printer for the first page than for the remaining ones. As an example, this enables you to print the

cover sheet in color on an inkjet printer and the tabular data on a monochrome laser printer for reduces costs.

Besides creating a paper printout, there is also a couple of other media available on which you can “print”. The following table contains a short overview. Due to a limitation of the List & Label component, some of the entries in the software are in German; you can find an English translation in the table.

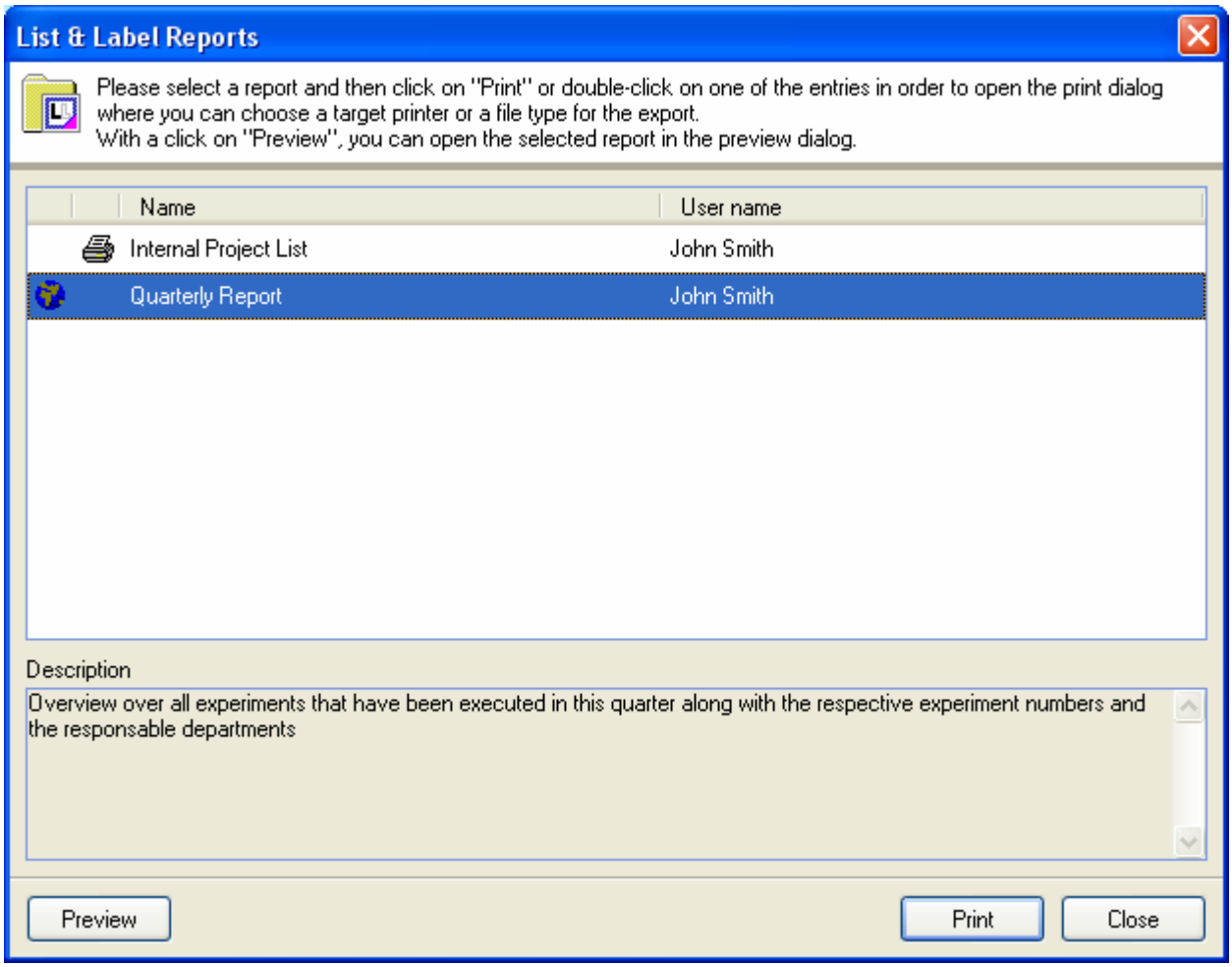
Export Media	English Translation	Description
Printer		The report will normally be printed on the selected printer, see description in the chapter text.
Preview		The preview dialog will be opened containing your report data. This corresponds to a click on the “Preview list and Label report” button.
File		A printer output file will be created.
HTML Format		A website possibly containing multiple files will be created.
Multi-Mime HTML Format		A website totally included in one file will be created.
Adobe PDF Format		A PDF document containing your report data will be created.
Bitmap		Your report data will be saved in a picture in the Bitmap format.
Metafile (EMF)		Your report data will be saved in a picture in the Windows Metafile format.
JPEG-Grafik	JPEG Graphics	Your report data will be saved in a picture in the JPEG format.
Multi-TIFF-Grafik	Multi TIFF Graphics	Your report data will be saved in a picture in the Multi TIFF format.
TIFF-Grafik	TIFF Graphics	Your report data will be saved in a picture in the TIFF format.
Rich Text Format (RTF)		Your report data will be saved in a document in the Rich Text Format.
Nadeldrucker (TTY)	Dot Matrix Printer	Your report data will be prepared for printout on a dot matrix printer. You can either save the result into a file or directly send it to a compatible printing device.
Text Format		Your report data will be saved in a normal, unformatted text file.
Microsoft Excel Format		A Microsoft Excel worksheet will be created with your report data.
XML Format		An XML file containing your report data will be created. This format can be used for exporting data into different applications.

Depending on the output media you have selected, the outward appearance of your report may vary, maybe some of the contents cannot be displayed at all in the chosen file format (for example an embedded company logo when saving as a plain text file).

However, with this command sequence you have to open the management dialog for List & Label reports every time you want to print such a report. Thus, we shall now take a look at a much more comfortable procedure. First, please select a report in the main window’s navigator. Then, there are three different options that are all marked with the  symbol and lead to the same result.

1. Open the context menu on the respective navigator entry and select “Report” \ “Print List & Label report” there.
2. At the main menu, click on the “Print List & Label report” entry located in the “Report” menu.
3. Open the report’s overview display and click on the “Print List & Label report” link there.

If only one List & Label report has been associated with your ensochemLab report, the printing dialog explained above is directly opened. If there are multiple List & Label reports, the software shows you a selection dialog. For this decision, it does not matter who has created the records. This can either be you or a different ensochemLab user (for public or administrative List & Label reports).

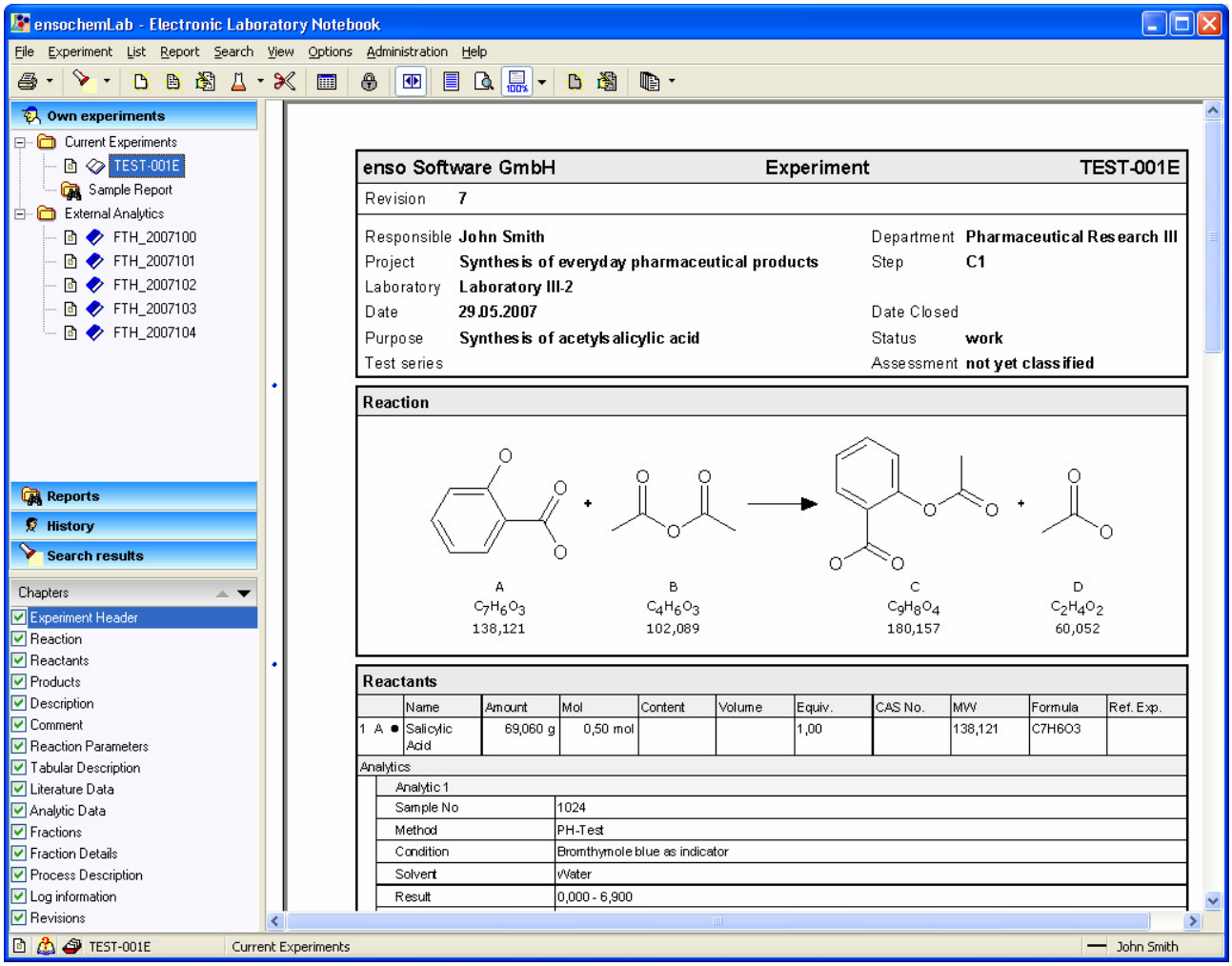


In general, this dialog is very similar to the management dialog explained earlier in this chapter with all modification features removed. Selecting a report is thus completely the same.
After you have selected an entry, you can either directly print the respective report with a click on “Print” or select “Preview” in order to show the preview window that you also already know.
After printing your report or closing the preview dialog, you return to this selection window so that you can print more reports. With a click on “Close”, the dialog is closed and you return to the main window / the management dialog.

Summary:	With the aid of reports, you can save arbitrary database queries and generate a current and user-defined overview display of the results at any time. This enables you to get a summary of all your experiments with only little afford. With public reports, you can make your queries available to all users.

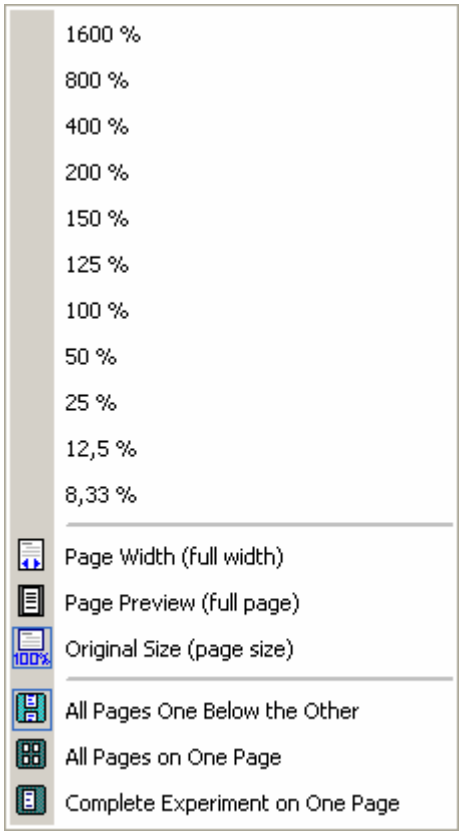
11. Printouts

Click on the „Print preview“ button ( ) in the main window’s toolbar. ensochemLab will now show the current experiment as a print preview:



This is the print preview on actual page width which is selected by default. In this mode, the experiment is shown exactly in the size it would have if it was printed on paper. Binary attachments for the description or for the analytic record are displayed each on an additional page in the addendum. Besides that, the print preview exactly corresponds to the experiment view in the normal display mode. If you close or completely hide a block of data there, it will also be closed or hidden in the print preview.

To change the print preview mode, please open the corresponding menu (beside the “Print Preview” button ( ) in the toolbar):



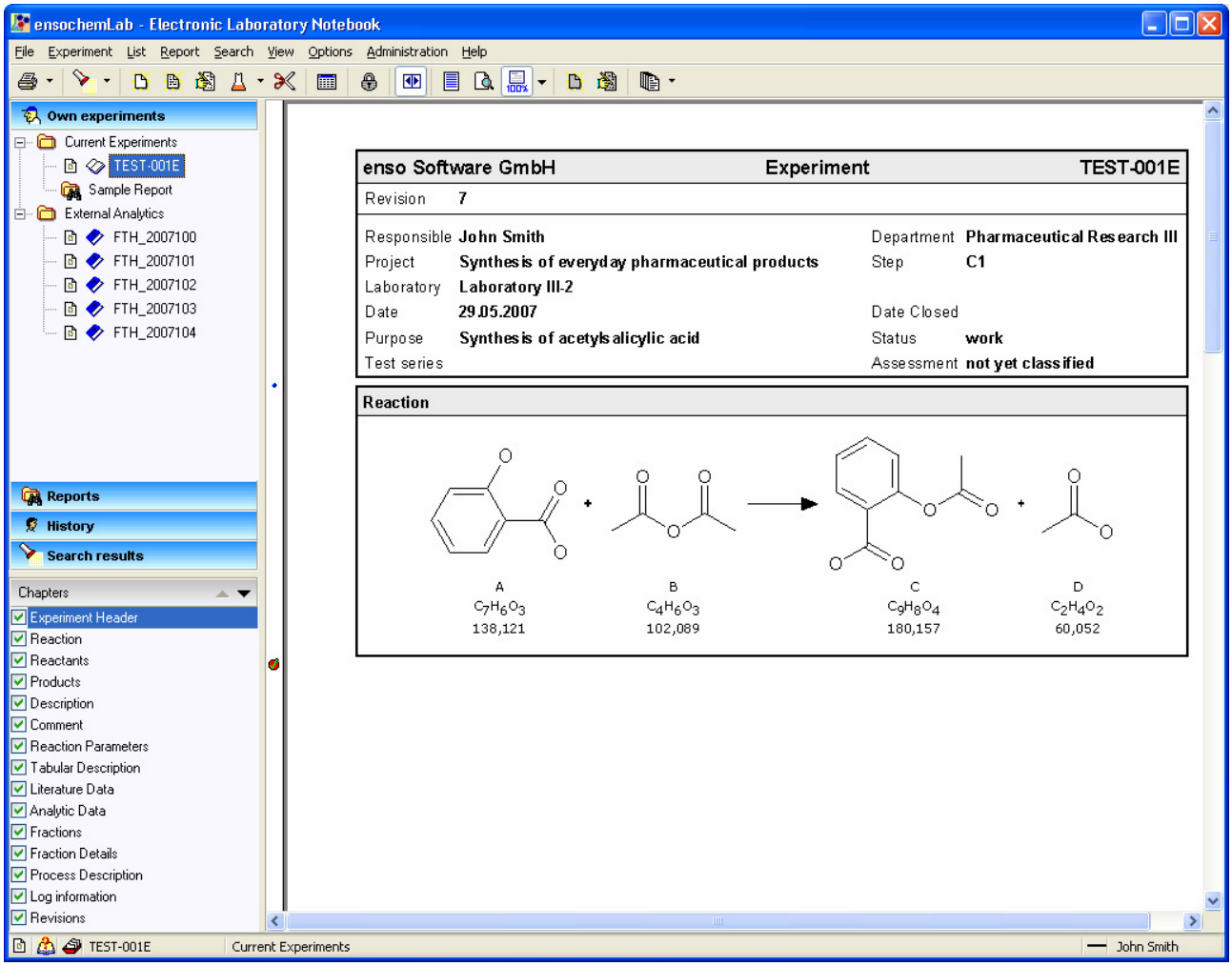
In the upper section, you can select the size in which you want the experiment to be displayed. However, please note that there may be deformations when displaying attached binary data if these image files have a rather different size that has to be scaled accordingly.
As an alternative, you can also choose one of the three predefined display modes:

1. The print preview on page width scales the experiment so that it is shown completely in the width of the main window and that you don't have to scroll horizontally.
2. The "Page Preview" option scales your experiment so that it is fully shown (horizontally and vertically) on one page within the main window.
3. The print preview in original size is the default mode and has already been discussed above.

Besides that, you can also change the page arrangement by using the selection options in the lower menu part:

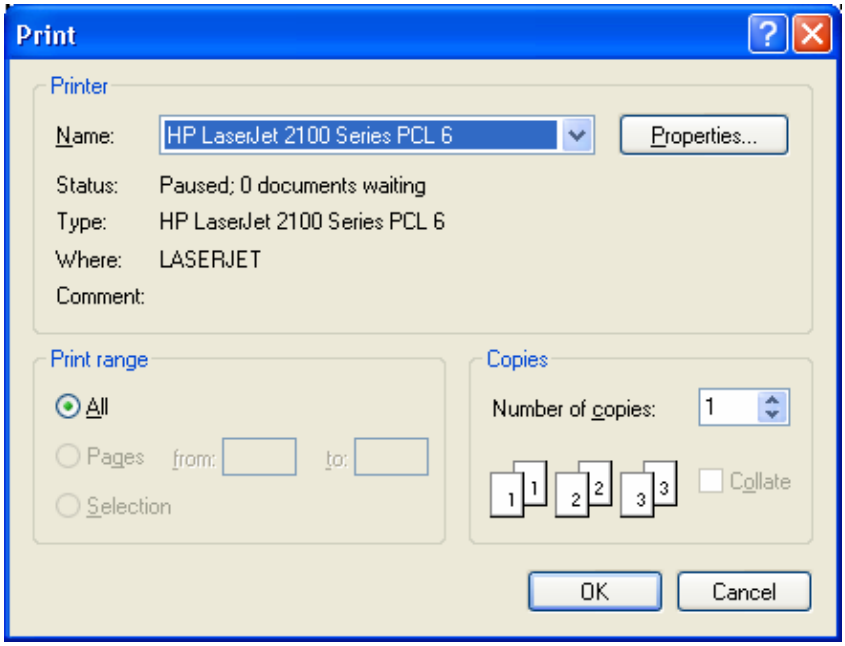
1. All pages one below the other
   All pages are displayed one below the other, each one on an individual page. The printout will need several sheets of paper.
2. All pages on one page
   All pages are scaled down and displayed in columns on one physical page. The printout will therefore only need one sheet of paper.
3. Complete experiment on one Page
   The whole experiment will be scaled down so that it can be displayed continuously on one physical page. Columns are not used and the printout will need one sheet of paper.

In addition to the pages breaks automatically created by ensochemLab, you can also define own manual page breaks. In general, this is possible between two blocks of data and within the experiment description. To define a break, please click on one of the blue points at the left side of the experiment display. ensochemLab will show a red circle with a green check in order to indicate the break. If you want to remove a manual page break, just click the circle again:



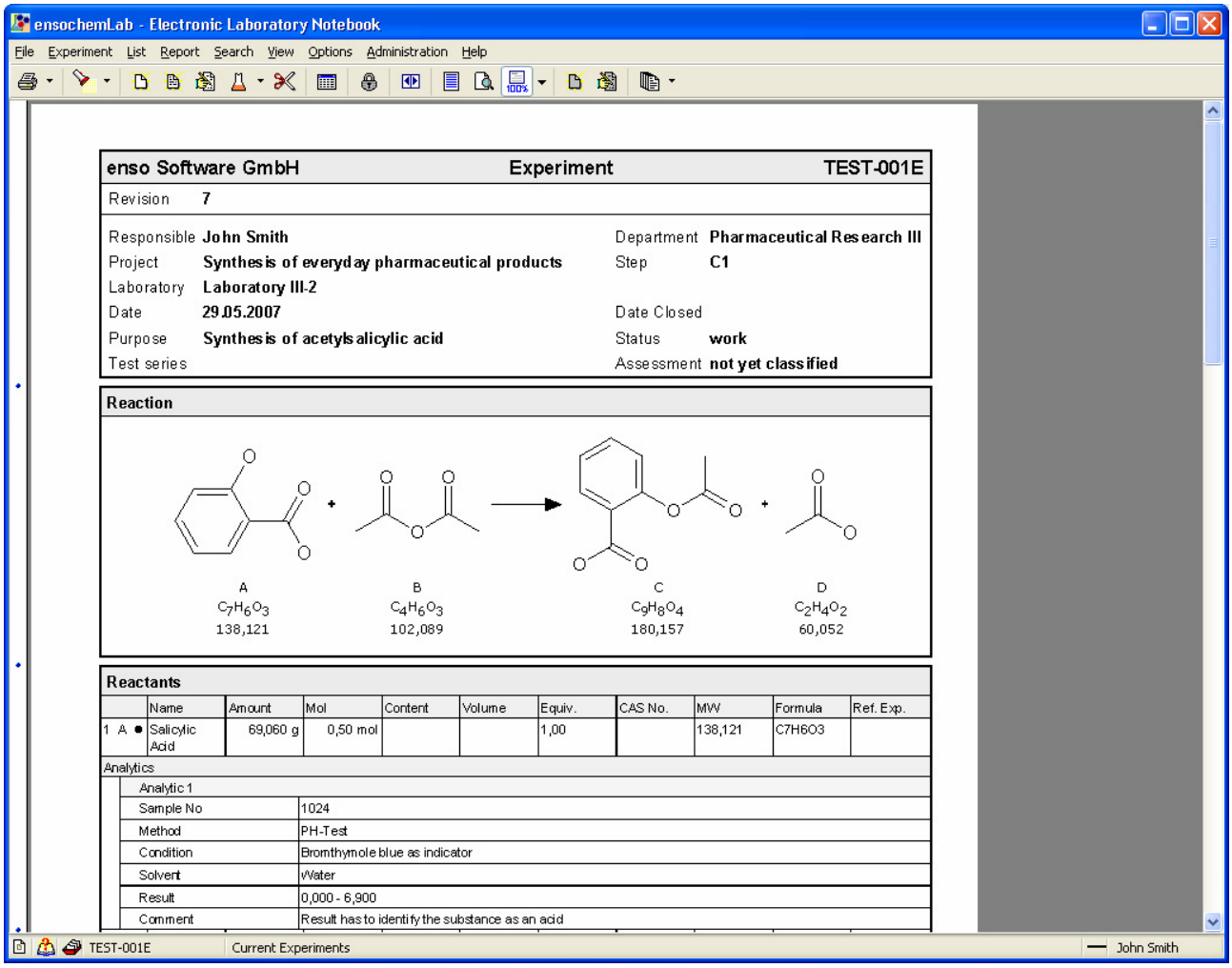
To actually print your experiment, you can either use the menu by first selecting on “File” and then on “Print” or clicking on the button in the toolbar. ensochemLab automatically detects whether you have selected an experiment or a folder for the printout. If you want to override the program’s decision (as you might have selected the first experiment in a folder, but want to print the folder overview), you can use button’s dropdown menu. It appears when you click at the small arrow beside the print icon:

When you click on one of the entries, the following dialog appears. Here you can select the printer you want to use and specify other data like the paper format or the number of copies you want to print:



If the respective feature has been enabled by your administrator, you can also print out single pages from within your experiment.

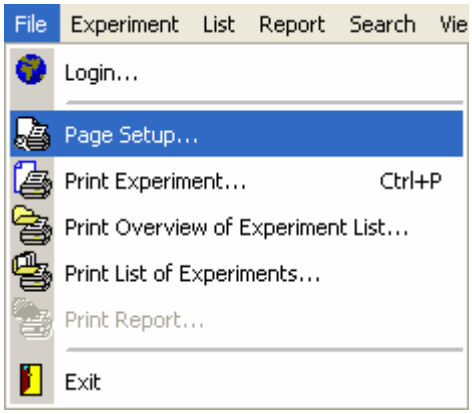
By the way, if you need more space for the experiment display, you can hide the navigator. Just click on the button in the toolbar:



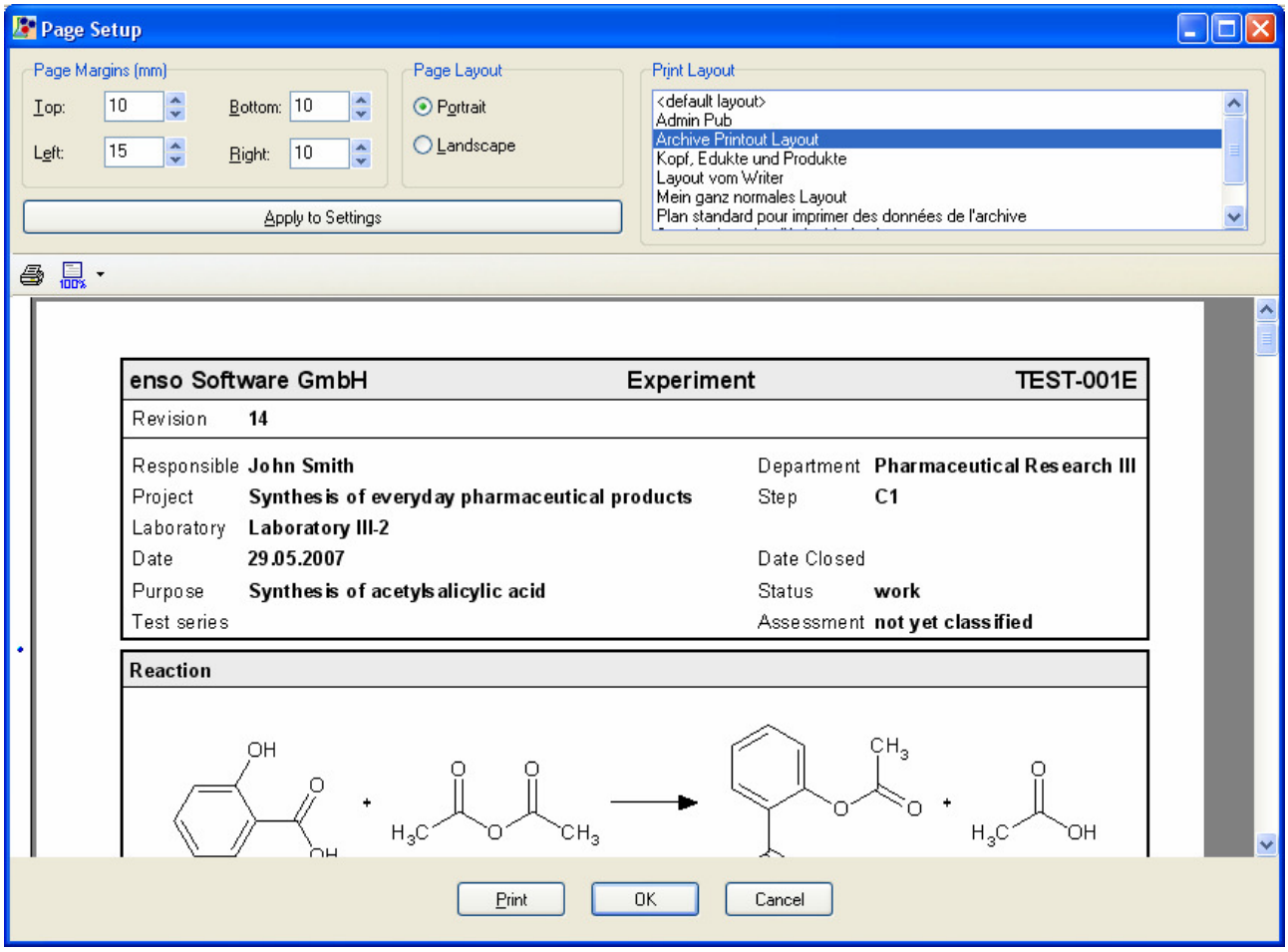
As you have seen, you can change the way an experiment is displayed in the normal view mode by either deciding to show reactants and products below each other or side by side, by changing the visible columns or by altering the column widths. In the print preview, on the contrary, the experiment page is displayed just like it will look when it is actually printed out. However, if you want to alter the page layout, you need a mode which combines the two sets of features. Always switching between the normal view mode and the print preview would be quite unhandy.
That is why ensochemLab is able to display the whole experiment in the width of a sheet of paper when you click on the respective toolbar button (). In this mode, all features of the normal view mode are available and the experiment is already scaled to match the paper size.

Use a Print Layout

Further more ensochemLab assists you to select a layout without being forced to change the currently selected one for display. Depending on usage and workflow the preferred display and specified printout may differ. To ease your work and preset the required layouts you can either set a print layout in your user settings or you first click on "File" in the main menu and after that on "Page Setup".



In case you selected a dedicated print layout in your settings, the appropriate "Page Setup" dialog will show up any time you initiate printing, e.g. by clicking on the button in the toolbar. This is done to allow you controlling page breaks, etc.



Available functions and course of action to specify the print out is as described before for the "Print Preview" in the main window. If you want to save the currently set values for "Layout" or "Page Margins" respectively to keep them for later printing, simply click on the button "Apply to Settings" and they are directly transferred into your user settings.

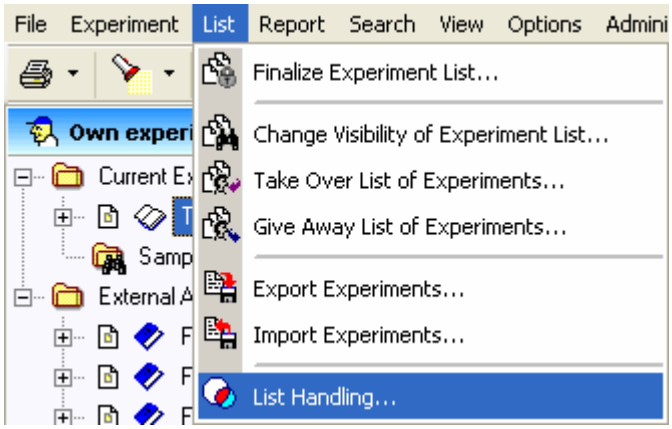
Summary:	ensochemLab offers a number of different print previews that can be used to check the result that is to be expected. Click on “Print“ to start the actual printing process.

12. List operations

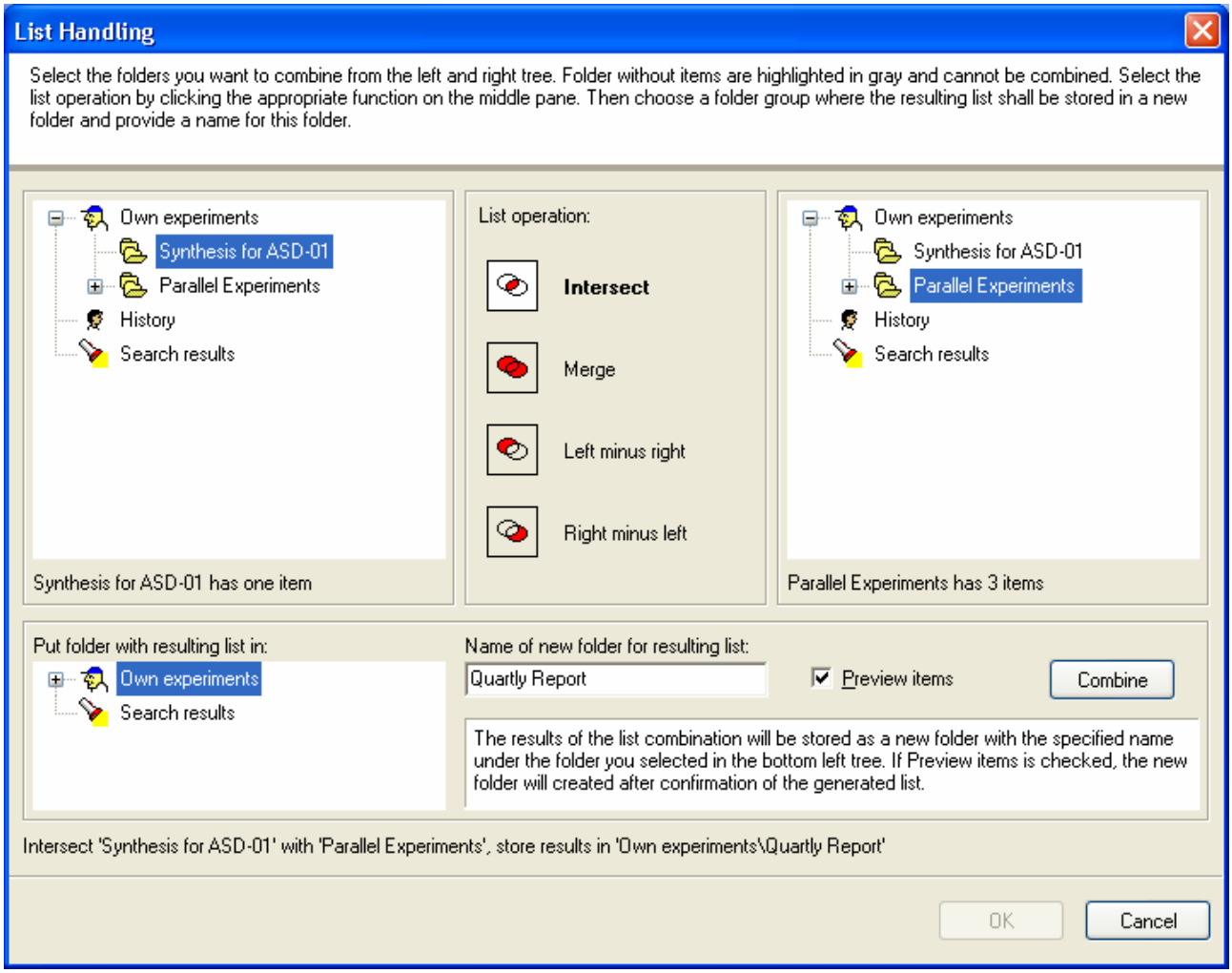
In previous chapters, we have already discussed the topic of basic list management. However, these functions were not very efficient and comfortable when dealing with huge amounts of experiments or folders, especially not with hierarchical structures.
Therefore, will now take a look the list handling functions integrated in ensochemLab.

To process the steps described in this chapter, you should have already at least 5 experiments in your database that should be grouped into several folders.

You can find the functions in the main menu. Just open the “List” entry and then click on “List Handling”:



The following window will appear:



The fields at the right and left side of the window show your folder structure in all navigator sections. This includes the folders “Own experiments”, “History” and “Search results”. Please select your first folder at the left side. Then proceed to the right side and choose your second folder. Please note that you may not select one folder twice. The order of your folders (which folder is to be selected on which side) depends on the list operation you want to perform. We will discuss this later.

Now you should choose the folder where you want to save your result list in. To do so, just select a parent folder in the list at the bottom left of the window. In the field right beside it, you can enter the name of a new subfolder that ensochemLab shall create. However, please note that the whole “Search results” category is deleted when the program terminates! To avoid this, you should save your new folder in “Own experiments”. The “History” folder is write-protected and thus not available for results.

Now it is time to take a look at the final step in this dialog, the selection of the list function. In the middle of the window, you can see a list of all functions that are available in ensochemLab. The selected one is displayed with a white background. To change the selection, just click on another entry. The functions are:

Intersect	All experiments that are part of both lists (the right one and the left one) are added to the result folder. Experiments that are only located in one folder are ignored.
Merge	All experiments from the list on the right side and the list on the left side are added to the result folder, no matter if they can be found in both folders or only in one of them. Each experiment is added only

		once, duplicates are not transferred.
	Left minus right	All experiments from the list on the left side that are not part of the list on the right side are added to the result folder.
	Right minus left	All experiments from the list on the right side that are not part of the list on the left side are added to the result folder.

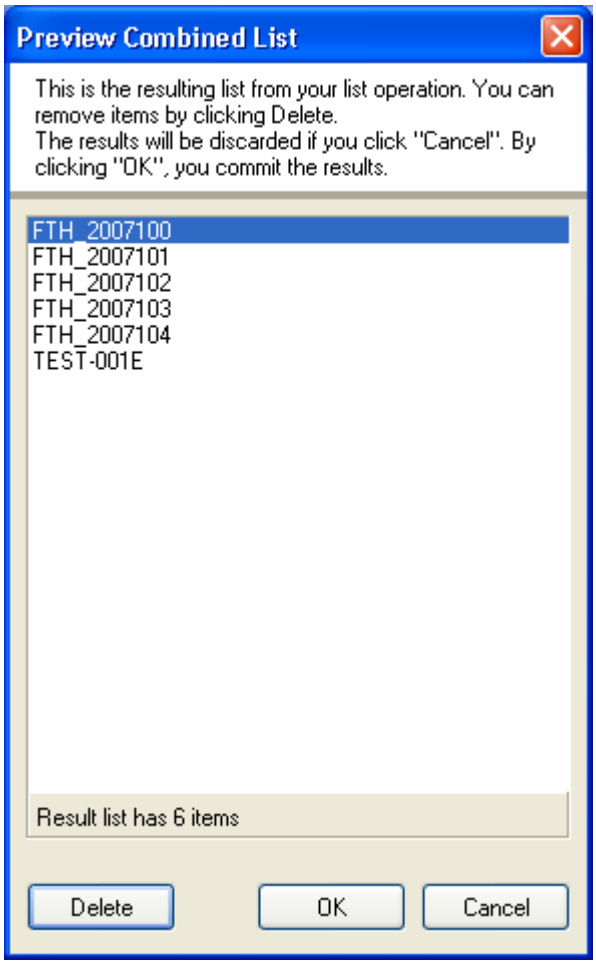
When using the functions “Intersect” and “Merge”, the order of the selected source folders does not matter. With “Left minus right” and “Right minus left”, however, it is very important!

Having selected your search mode, you have to choose whether you want to preview the result list before it is actually saved. This enables you to remove entries much faster than you could do in the main window. To use this function, mark the “Preview items“ box.

Now click on “Combine“ to start the process.

This manual will continue with the “Preview” function. If you have not selected the function, you just will not see the following window, everything afterwards is the same again.

Now take a look at the preview window:



To accept the list without changes, just click on “OK”. If you want to return to the list operations dialog to change your source folders, the search mode or cancel the whole operation, please click on “Cancel”.

If you want to delete an entry from the list, please select it and then click on “Delete”. Please note that this function has no impact on the experiments themselves or their references in the source folders. However, you should leave at least one item in the list or ensochemLab will cancel the operation even if you click on “OK”.

As you surely have noticed, list handling cannot be used to manage experiments that are not part of at least one list. To include an experiment in an existing list, used to context menu command “New” within the navigator as described in chapter 4 (“The main window”).

Summary:	The list operations offer easy and comfortable functions to manage folder structures with the aid of logical operators. The result ill be placed in a new directory. Use this function to manage your experiment hierarchy.

13. Working with experiment lists

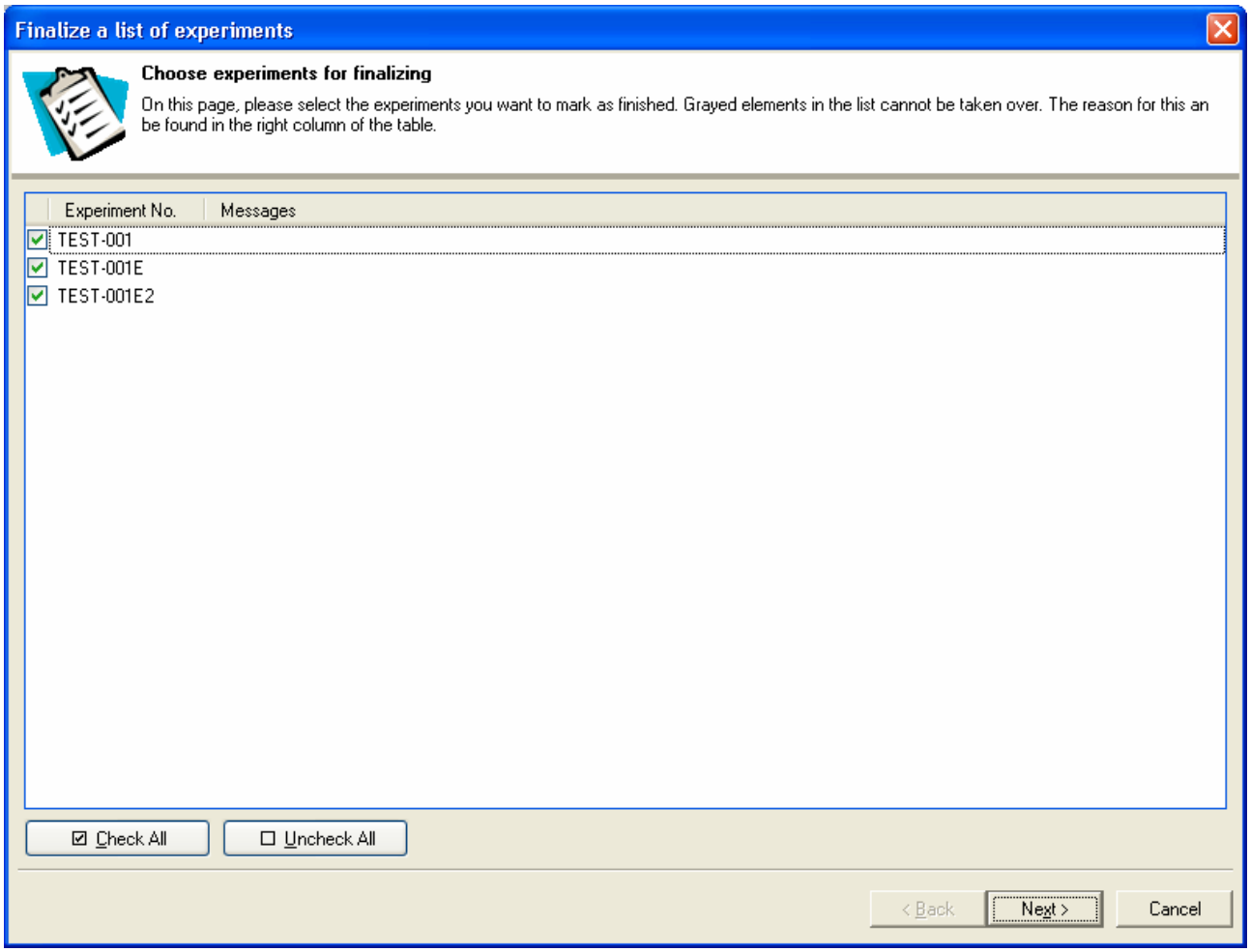
In the former chapter, you have seen how single experiments and also experiment lists can be combined or divided – in short: managed. However, the result of all these functions has always been a new list; the experiments themselves have never been changed. In some cases, though, it is useful or even righteous necessary to modify some experiment header data like the owner or the current state for quite a larger number of experiments. This can for example be the case with an automatically created set of experiments for one test series. This chapter describes the comfortable options ensochemLab offers fur such a task.

One issue is the same for all these operations: All experiments have to be in the same folder. Subfolders are automatically included. If your experiments are shattered among several folders, use the list operations from the last chapter to combine them with the “merge” option in one working folder.

13.1. Finalize experiment list

If a whole set of experiments has automatically been performed by some laboratory robot or a just slightly different try has been performed in multiple experiments, you have to finalize a list of experiments.

The corresponding function can be found in the main menu under “Experiment” \ “Finalize experiment list” after you have selected a folder in your navigator. ensochemLab will now open the following window:



On the first page of this wizard, you can select the experiments you want to finalize. The list contains all experiments from the currently selected folder as well as those from its subfolders.

For continuing, you have to select at least one entry.

With the two buttons at the left side beneath the experiment list, you can select or deselect all entries in the list with one single click.

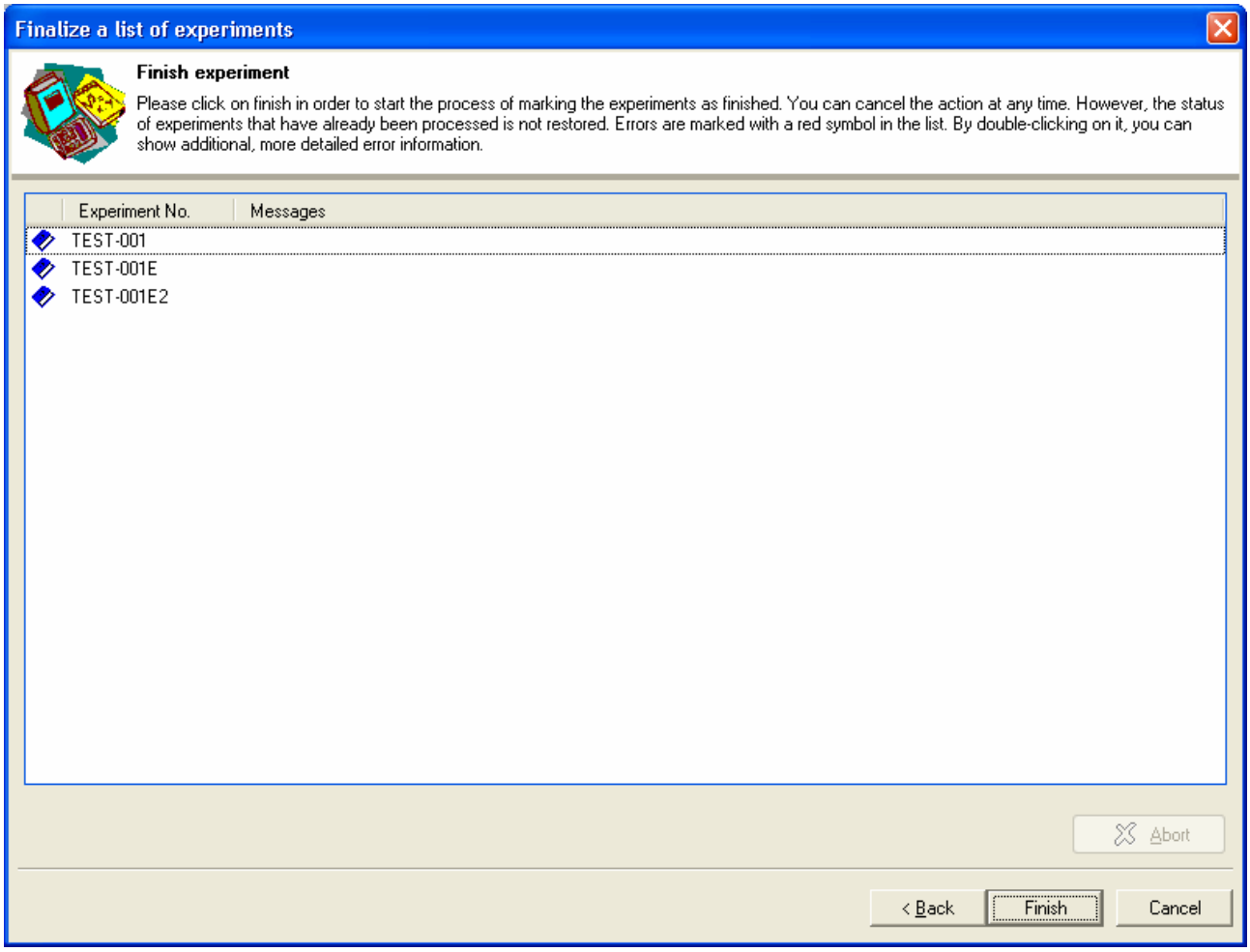
If an experiment in the list has a gray background, it cannot be finalized. The reason for this can then be found in the right column.

After you have chosen your experiments, please click on “Next” to continue.

Here you can see the list of your experiments once again; however, ensochemLab has now already filtered those entries that can definitely not be finalized. Still, this does not mean that there might not be errors later. Colleagues might have changed or deleted one or more of your experiments in the meantime, for example.

After a last check of your experiment list, please click on “Finish”. ensochemLab now processes the list from top to bottom. The symbol with the open book indicates the experiment that is currently being processed. A green mark indicates an experiment that has successfully been finalized whereas a read X stands for an error. The reason for the failure can be found in the right column of the table in such a case.

While the process is running, you can see a process bar at the lower edge of the list along with an “Abort” button with which you can cancel the process at any time. However, please note that experiments which have already been finalized will not be reset.



After the whole operation is finished, you can see a complete text (the number of experiments that have been finished and the number of failures) instead of the progress bar.

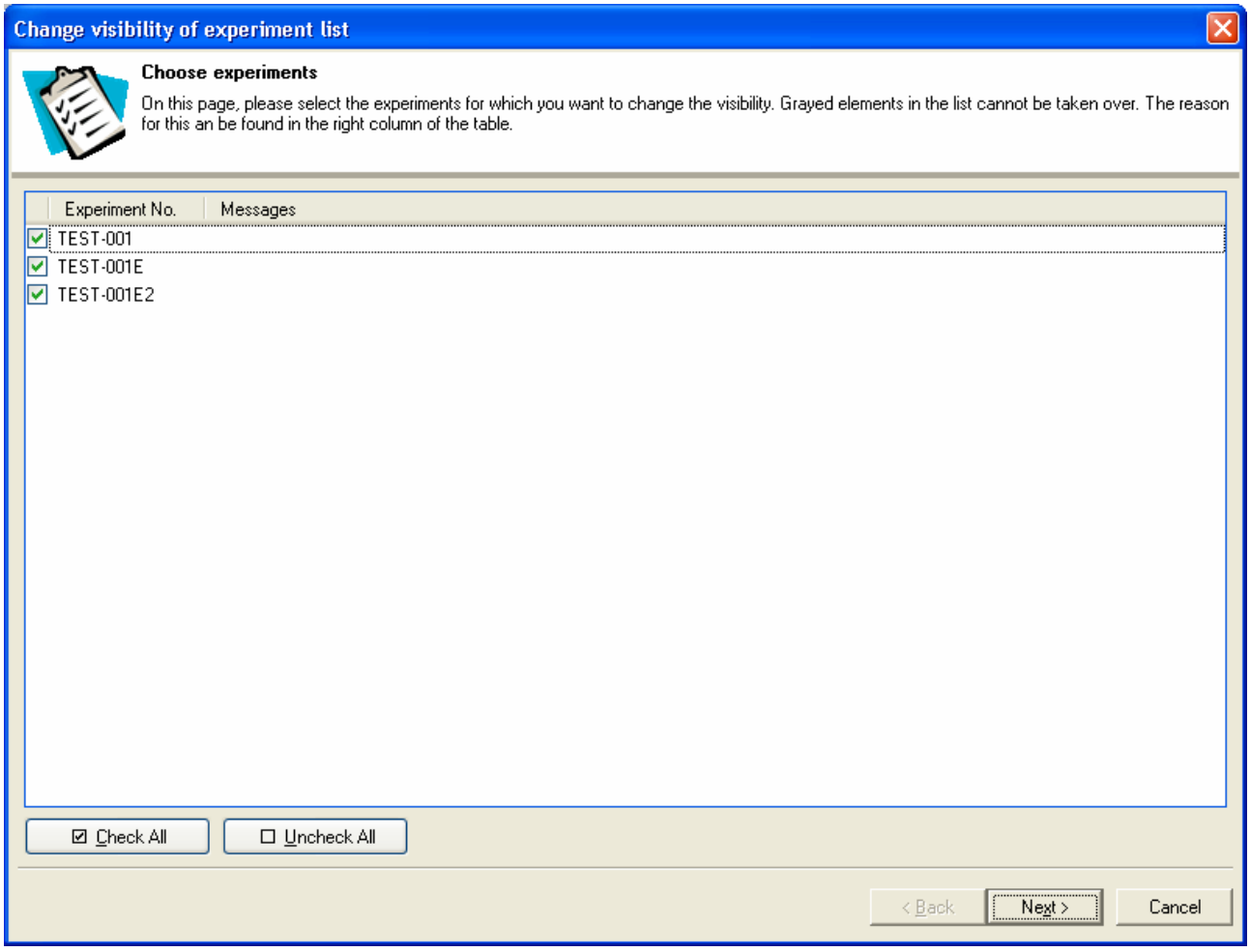
Then please click on “Close” in order to return to the main window.

13.2. Change visibility of experiment list

This function is only available if you use the default user administration module. For further information, please consult your administrator or supervisor.

If the policies for the visibility of experiments in your enterprise have been changed or if you have to activate a list of experiments that have been private ones of your colleague up to now, you can use this list operation feature.

For launching the corresponding module, please click on “Experiment” \ “Change visibility of experiment list” in the main menu. The following window will appear:

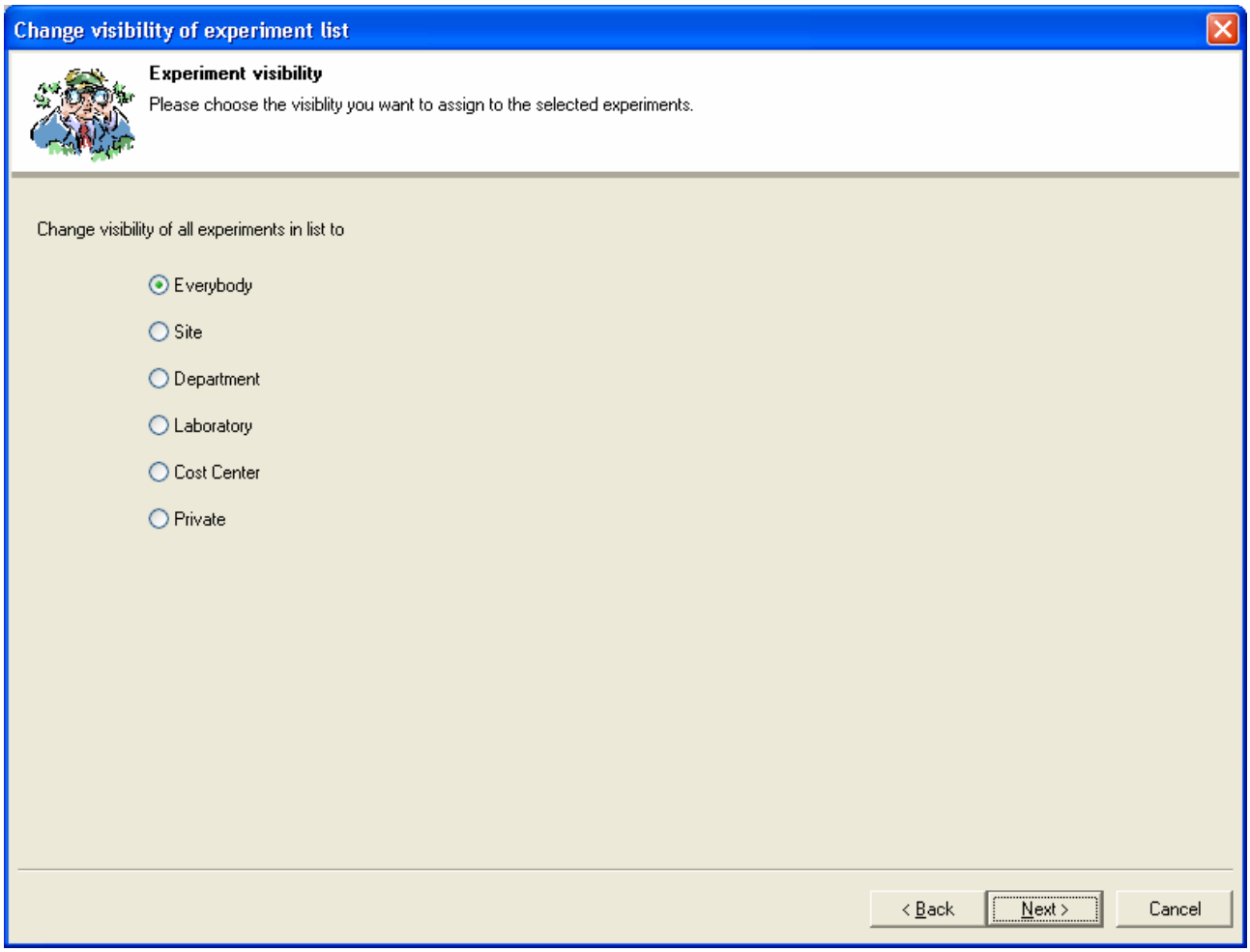


Just like the first page in the wizard for finalizing a list of experiments, this page displays all experiments within your currently selected folder. The visibility of experiments displayed in gray cannot be changed; the reason for this is available in the column on the right,

More information regarding the selection of experiments can be found in part 1 (“Finalize experiment list”).

Click on “Continue” in order to proceed within the wizard.

On the next page, you now have to select the new visibility for all experiments. Please note that you can only select one visibility that is applied to all experiments. If you want to apply different visibilities to certain experiments, you either have to use the function related to single experiments or split your list with the list operation feature discussed in the last chapter.

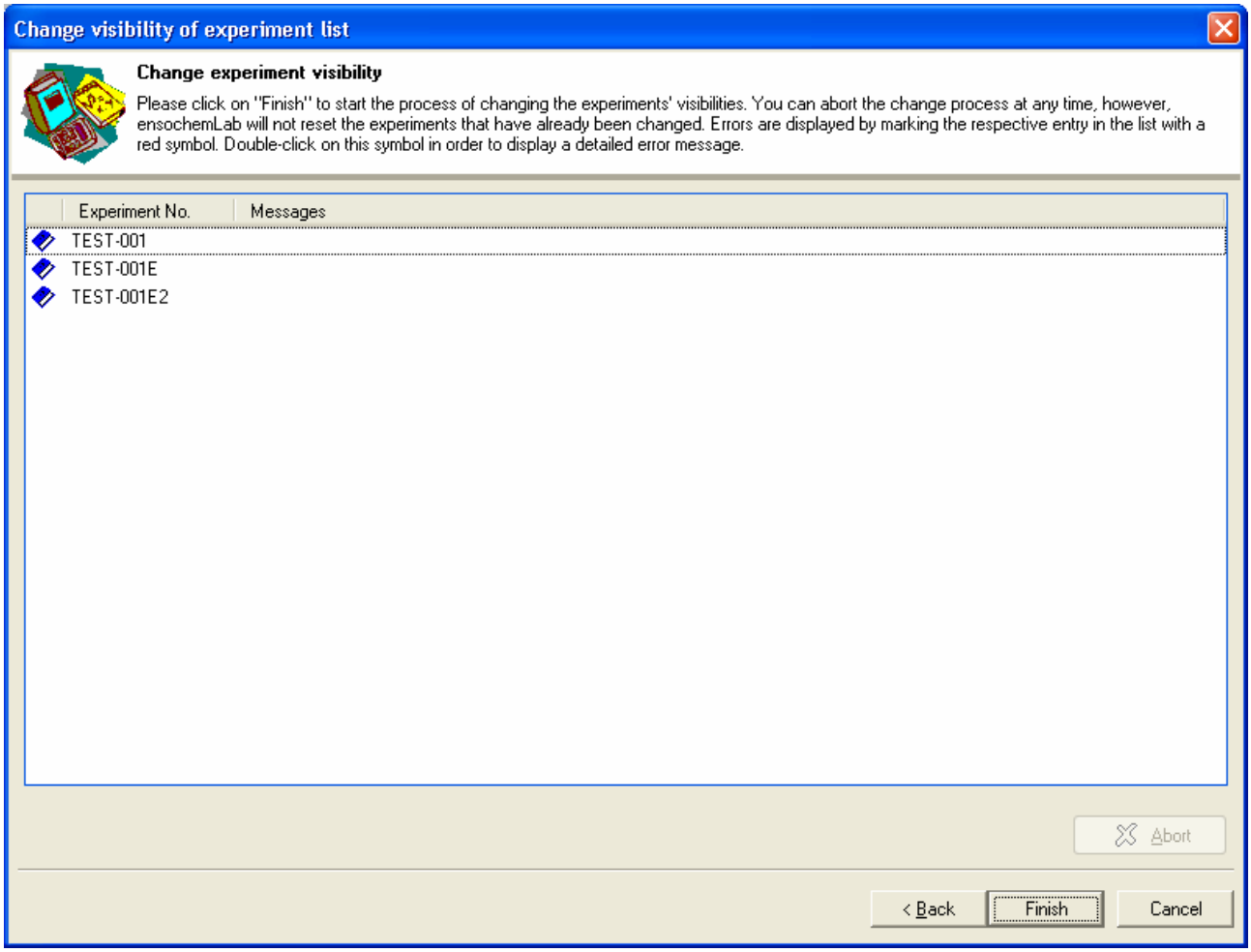


The available experiment visibilities are exactly the same as those you can define in the experiment header.

After you have selected your decision, please click on “Next”.

On the last page of this wizard, you can see the process page you already know from the first part of this chapter. It contains the part of the experiment list that can be processed and that you selected for changing the visibility.

After a click on “Finish”, you can watch ensochemLab perform the necessary operations. The symbols for indicating the progress and the result are also the same as those in the previous part of this chapter. As usual, the right column contains the error messages.

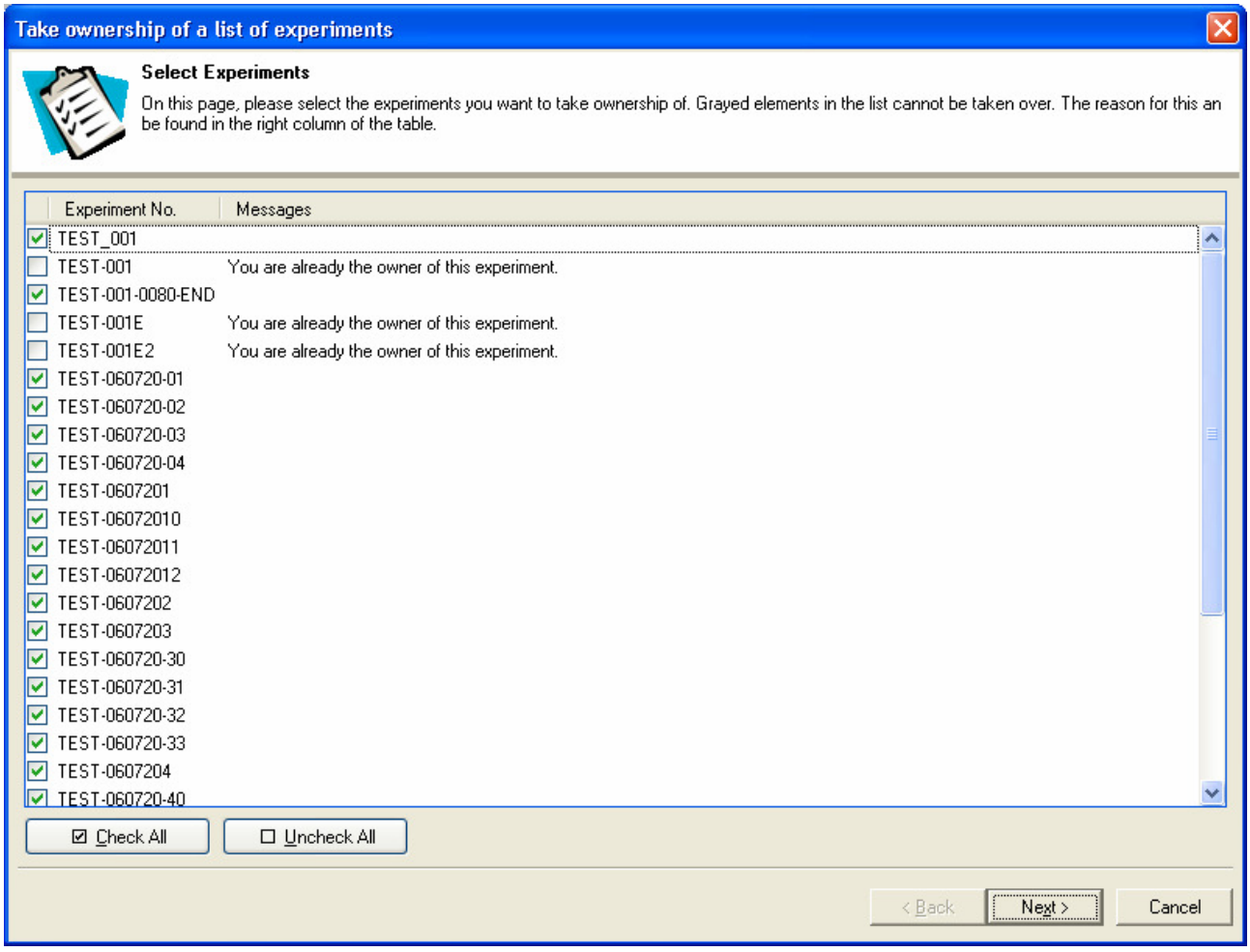


After the whole operation is finished, you can click on “Close” in order to return to the main window.

13.3. Take over list of experiments

If a colleague leaves the company, moves to another division or department or if he cannot perform his work for a longer period of time due to an illness, you need to be able to gather not only reading, but also writing access to his experiment. For doing so, you can take the ownership of his experiments if the administrator has enabled this function.
As with the rest of the features in this chapter, you don't need to manually change every single experiment, but you can use a comfortable list operation.

The corresponding module can be launched via the entry "Experiment" \ "Take over list of experiments" in the main menu. The following window will appear:



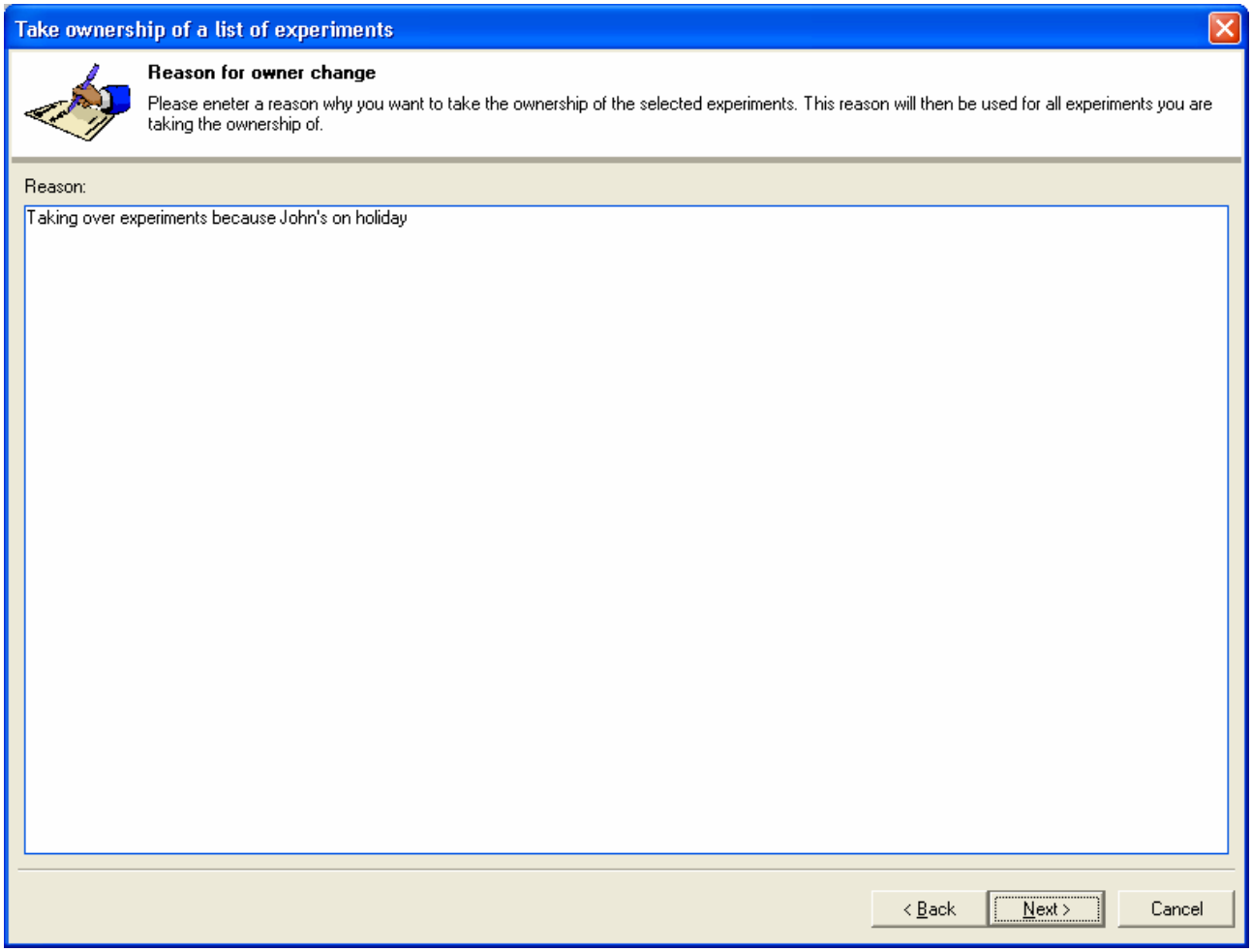
Just as with the two preceding list operations, the first page in the wizard is used to select the experiments you want to modify. The buttons at the lower edge of the window, you can select or deselect all entries in the list at once.

If you cannot take over an experiment (if it is already yours for example), it is displayed in gray. In the column on the right side, as usual, you can see the corresponding reason.

More information regarding the selection of experiments can be found in part 1 ("Finalize experiment list").

Click on "Continue" in order to proceed within the wizard.

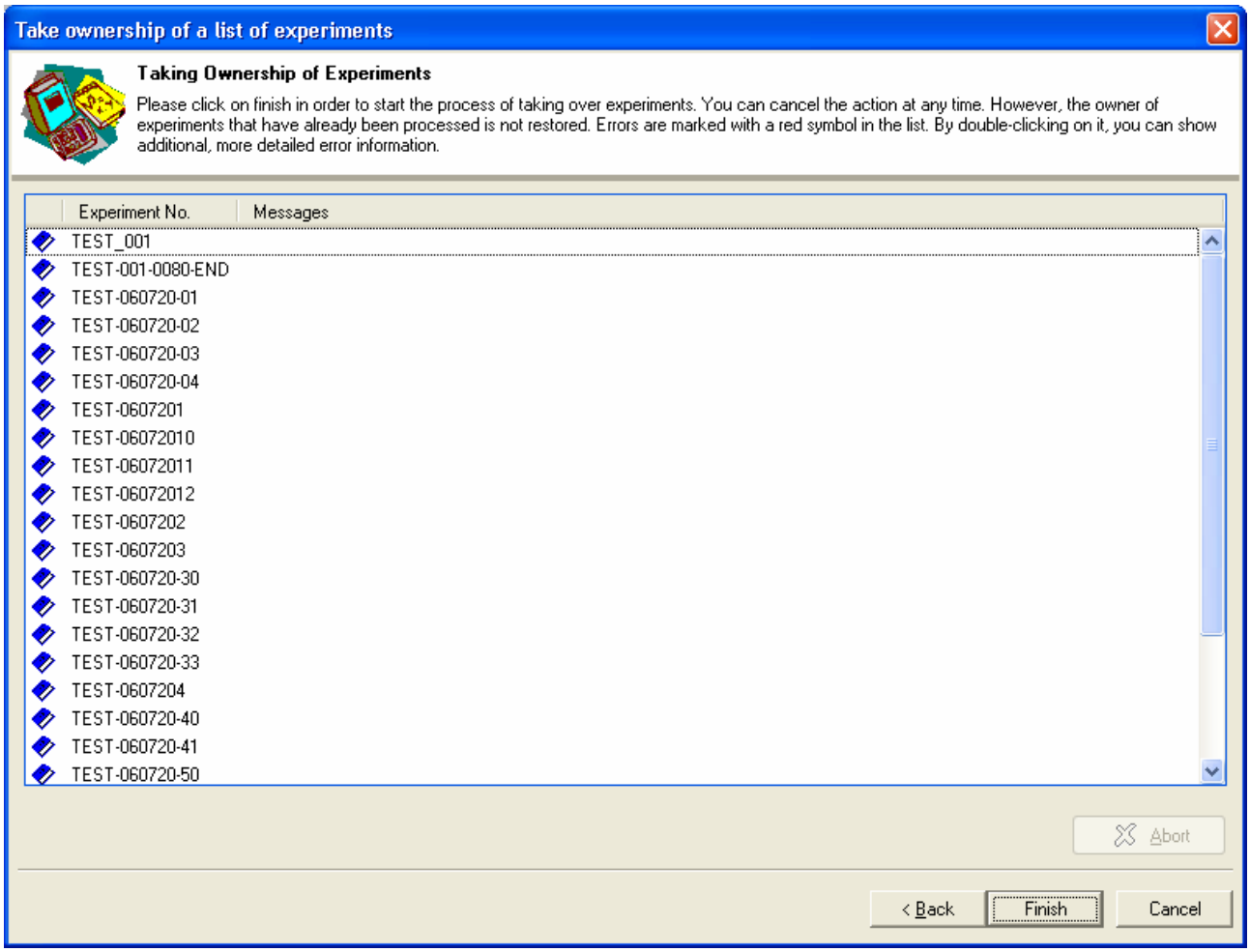
The wizard now shows this page:



On this page you have to enter a reason why you wan to take over the experiment. This reason will be stored in the protocol information data for every single experiment in the list.

Afterwards, please click on “Next” to continue.

The last page in this wizard is the processing page. It is exactly the same as the ones of the preceding list operations.



After a click on “Finish” you can watch how the operation is being performed on your experiments. The result and processing symbols are the known ones. The column on the right side contains the error messages.

After all experiments have been processed, you can click on “Close” and return to ensochemLab.

13.4. Give away list of experiments

Instead of having another user take over your experiments, you can also give them to him using the “give away experiment” function. This can, for example, be useful when you leave for a longer business travel.

The function can be found in the main menu under “Experiment” \ “Give away list of experiments”. In the principle, it works in the same way as the one for taking over a list of experiments. That is why it will not be discussed in detail here.

Summary:	ensochemLab offers a number of utile functions with which you can perform certain operations like taking over an experiment, passing it to another user or changing its visibility on all experiments in the current folder instead of having to change every single experiments on its own.

14. Working with fractions

The documentation of reaction processes, cleaning steps or product batches of products is covered by the ensochemLab fraction module.
It is possible to document probes of reaction processes or several specific workup steps as well as to enter different batches of one synthesis.

How to use the fraction module is demonstrated in three examples that are all based on the synthesis of acetylsalicylic acid (See Chapter 3).

Example A: Detailed documentation of a reaction process using analytic methods like HPLC
Example B: Simple documentation of cleaning steps without HPLC.
Example C: Simple documentation of purification steps considering a byproduct.

Example A:

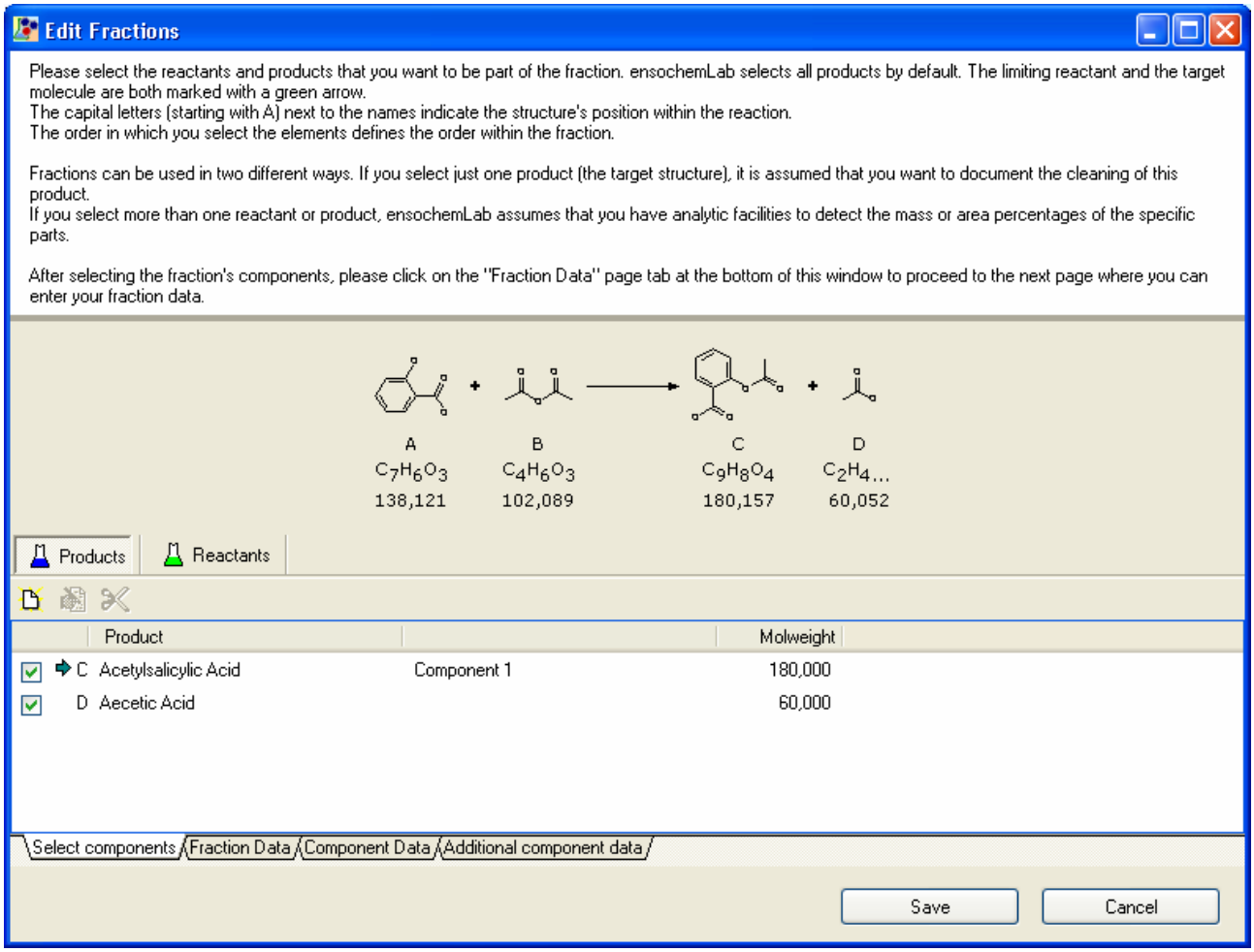
To reproduce this example, we recommend creating a new experiment by copying the experiment “Synthesis of acetylsalicylic acid” described in chapter “Create your first experiment” into a new one. The copy procedure is described in the chapter “The main window”. Choose a unique experiment no and save the experiment

Reactant amounts are:

salicylic acid	0,50 mol	69,05 g
acetic anhydride	0,74 mol	75,21 g

To create a fraction, please click on the “Edit Fractions” menu item in the “Experiment” menu or press the corresponding button in the toolbar ().

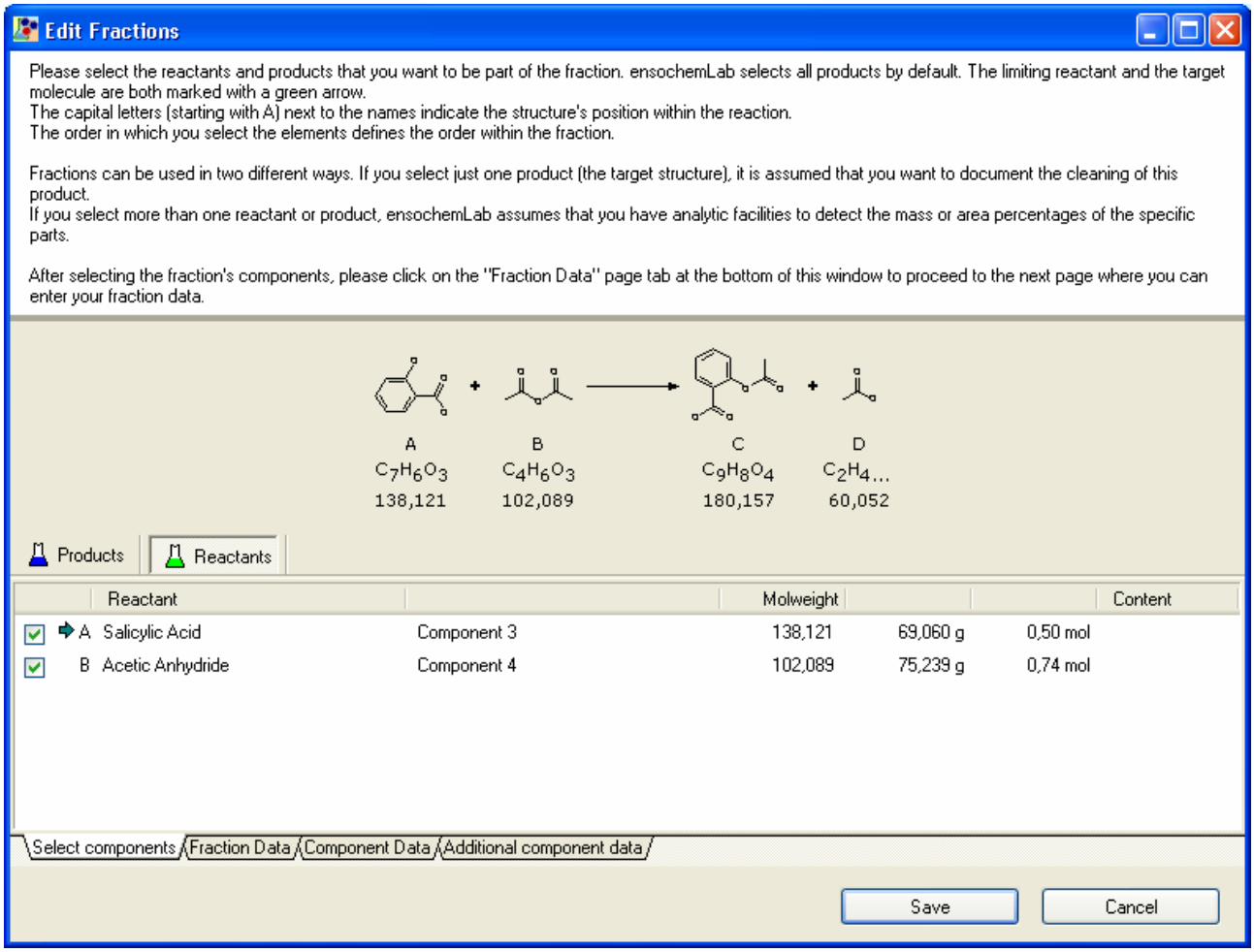
The following window will appear:



You are on the „Component selection“ page by now. On this page, you can define which reactants and products should be included in the fractions. Please check the desired entries with a mark in the list.
The first column of the table shows the name of the respective molecule, the second one shows the order of the components. The third column is used to display the molar mass. When dealing with reactants, there are three more columns for the reactant amount, the amount of substance and, if applicable, the content.

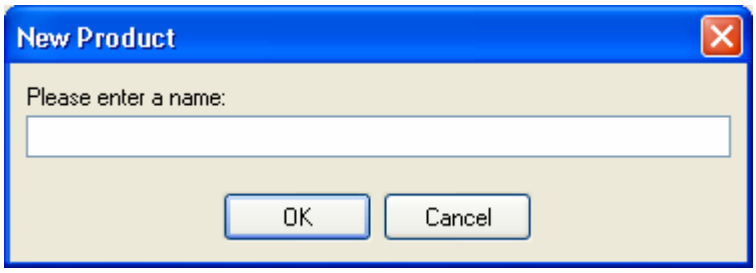
With the button at the top of the list, you can change between products and reactants. The symbols used there are displayed in the whole fractions dialog to indicate the kind of a molecule:

- for products
- for reactants



In the upper part of the page, you can see the experiment's full reaction. All reactants and products are displayed, no matter if they are selected for fractions or not.

You can also create new products. To do so, you can either use the context menu or the toolbar. Just click on "Add Product" ( ). The following window will appear:

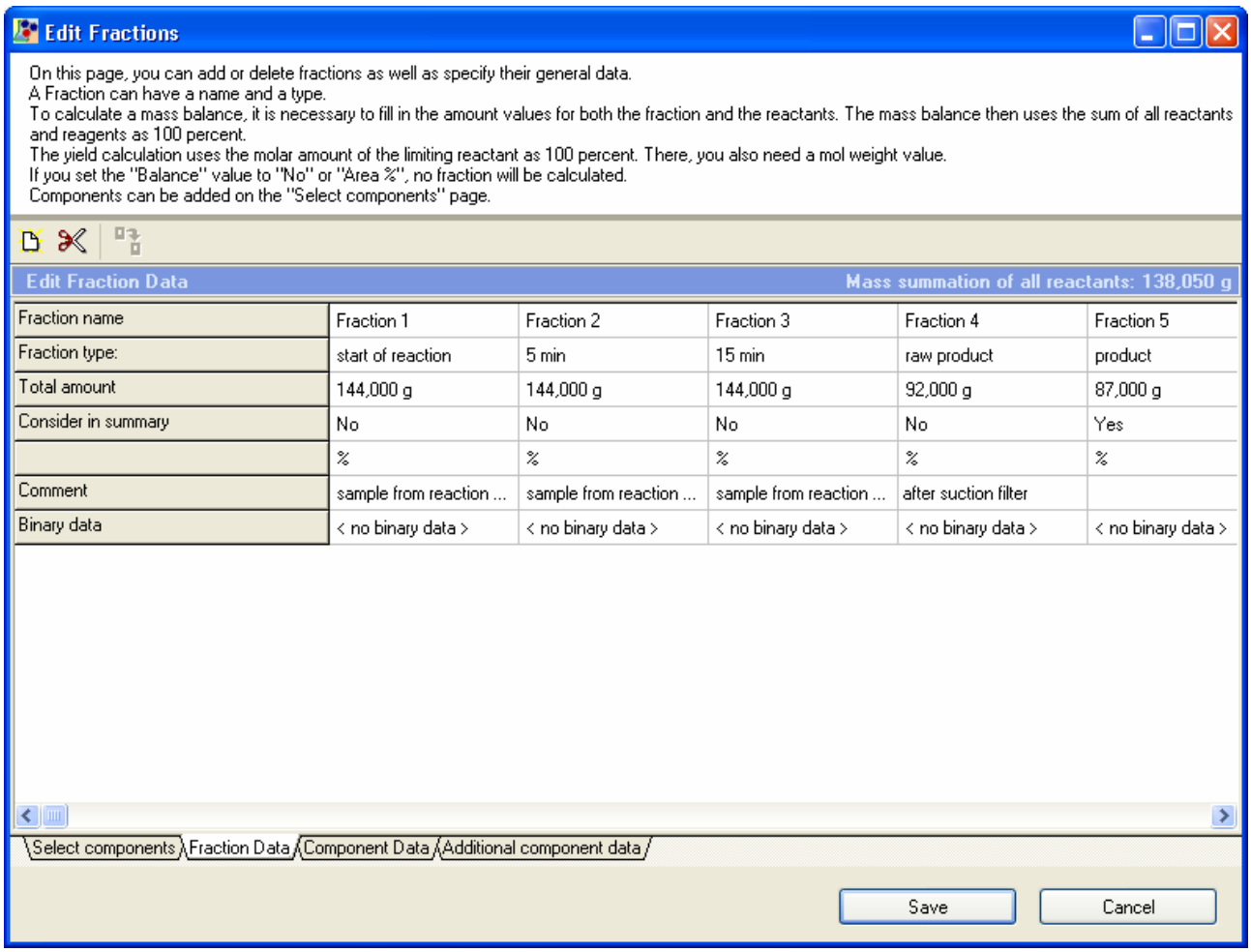


Now please enter a name for the new product and then click on "OK". It will be added to the list of existing products, but will not be visible in the reaction display as it has no structure at this moment. You can add a structure by using the experiment wizard. For further information, please refer to chapter 3 ("Create your first experiment"). There, you can also enter additional data like substance code or batch.

Please note that the “Change product name” ( ) and “Delete product” ( ) functions are only available for products just created in this dialog. Already existing products have to be deleted r altered via the experiment wizard.

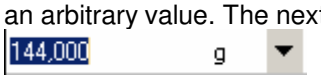
The fractions module cannot create new reactants. It is also impossible to modify or delete existing ones.

After marking all reactants and products, you can go on to the “Fraction Data” page:



On this page, you can assign a set of general data to your fractions. These data include the fraction name, the fraction type and the mass of the fraction, which will be analyzed by HPLC. From the HPLC run you will get either area percentage or mass percentage. If you get mass percentage form your analytic system further calculations will be possible. You can summarize the calculation values of several fraction by choosing “Yes” in then input field “Considering in summary” for the appropriate fractions. In case of this example it is useful to choose “Yes” only for the last fraction which contains the end product.

A description for the fraction and an arbitrary number of binary records can also be stored.
To edit one of the fields, please navigate to it by either clicking on it or selecting it with the arrow keys on your keyboard, and then click into it or press the return key. The first two fields are text fields where you can enter an arbitrary value. The next field is divided into a numeric field and a field with a selection list.

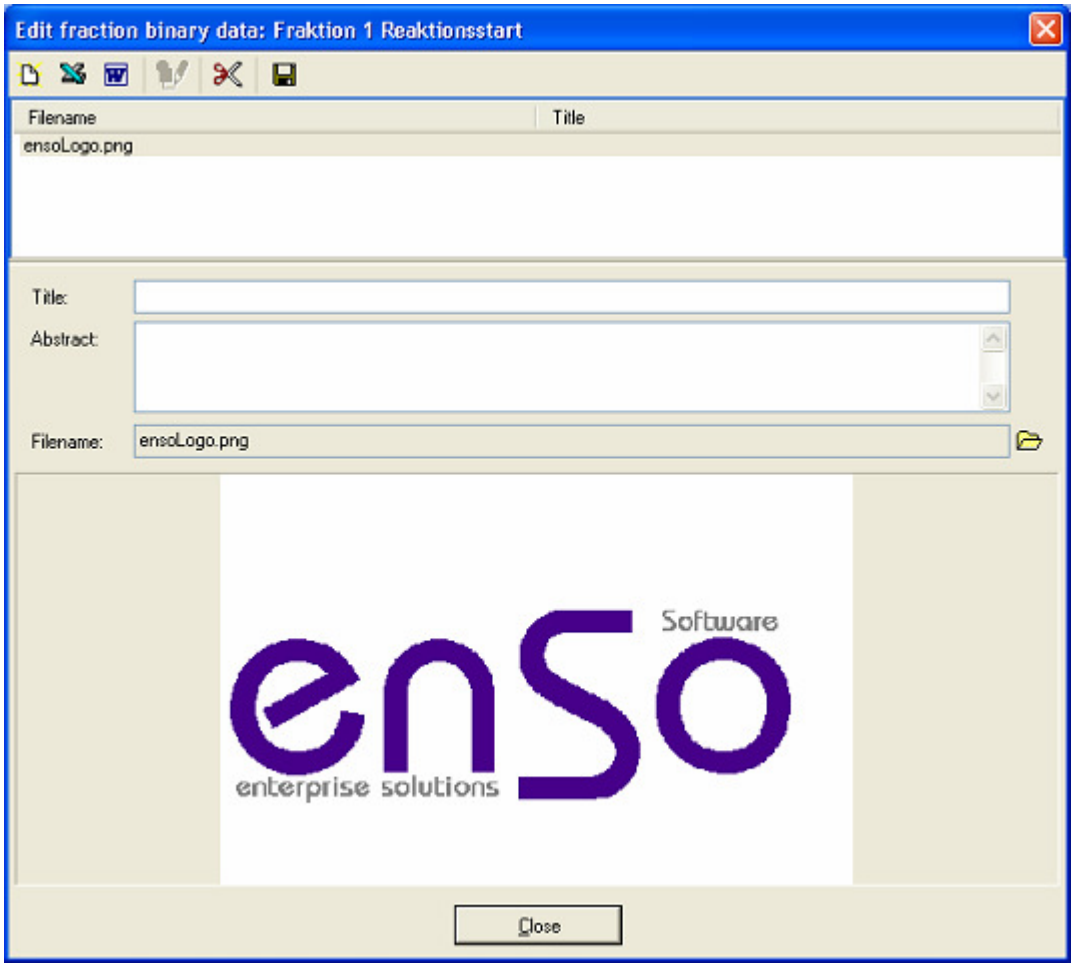


On the left side, you can enter the value. By using the selection list at the right side, you can specify the corresponding unit.

The “mass percentage/ area percentage” -field is a selection field that does not support free text entries. The Yes/No field “Consider in Summary” is just alike. The comment is another text field.

To create a new fraction, please click on the “Add fraction“ button ( ) in the toolbar. ensochemLab will then create a new column in the table. An existing fraction can be deleted by clicking on the “Delete fraction” button ( ).
Both functions are also available via the context menu.

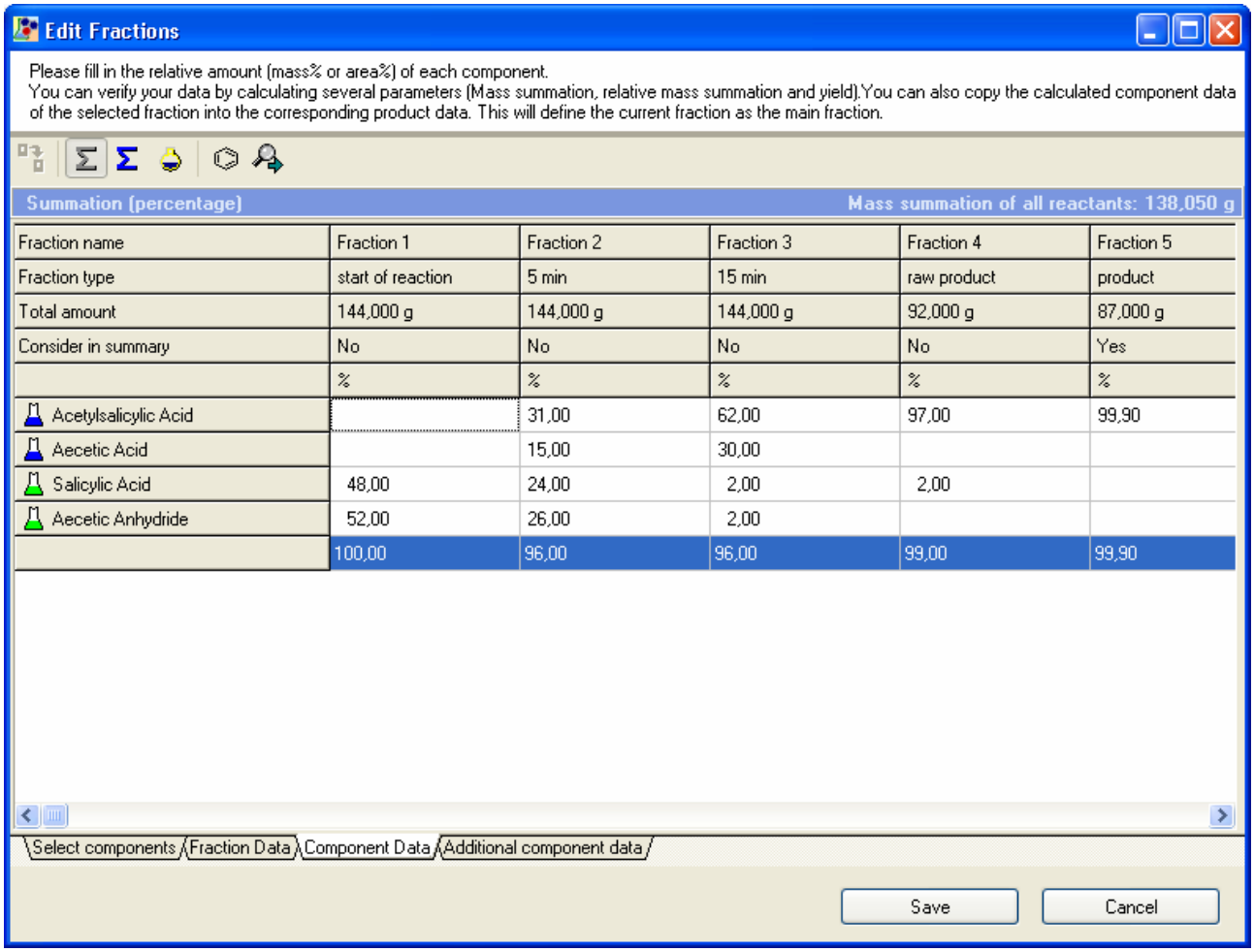
The “Binary data” field cannot be modified directly in the fraction dialog, but opens a new window instead:



Please click on “New binary record“ ( ) to create a new binary record. By doing so, you will be prompted to select a file on your local hard disk. After the file has been imported successfully, you can enter a description for the binary record.
To view a preview image for a binary record, just select the corresponding entry in the list. The image will then be displayed at the bottom of the window. Please note that a preview is only available for images in the bitmap (*.bmp), PNG (*.png) and JPEG (*.jpg) format if no other display module is installed on either the server or the local computer.
To delete the current record, please click on “Delete binary record” ( ).

Having imported all binary records, you can return to the fractions dialog by clicking on “Close”. The field “Binary data” in the table will then show the number of binary records inserted.

We are now ready to move on to the “Component Data” page:



On this page, you can enter the distribution of the reactants and products in the fractions created in the previous steps. These values are all percentage values that correspond to masses or areas, depending on your selection on the second page (“Fraction Data”). The values are provided by an analytical system like HPLC, GC…

At the beginning of the reaction there are only reactants found in the fraction. The proportions of the reactants increase during reaction time (until fraction 3). Fraction 4 shows the situation after suction filtering and fraction 5 contains the almost pure product.

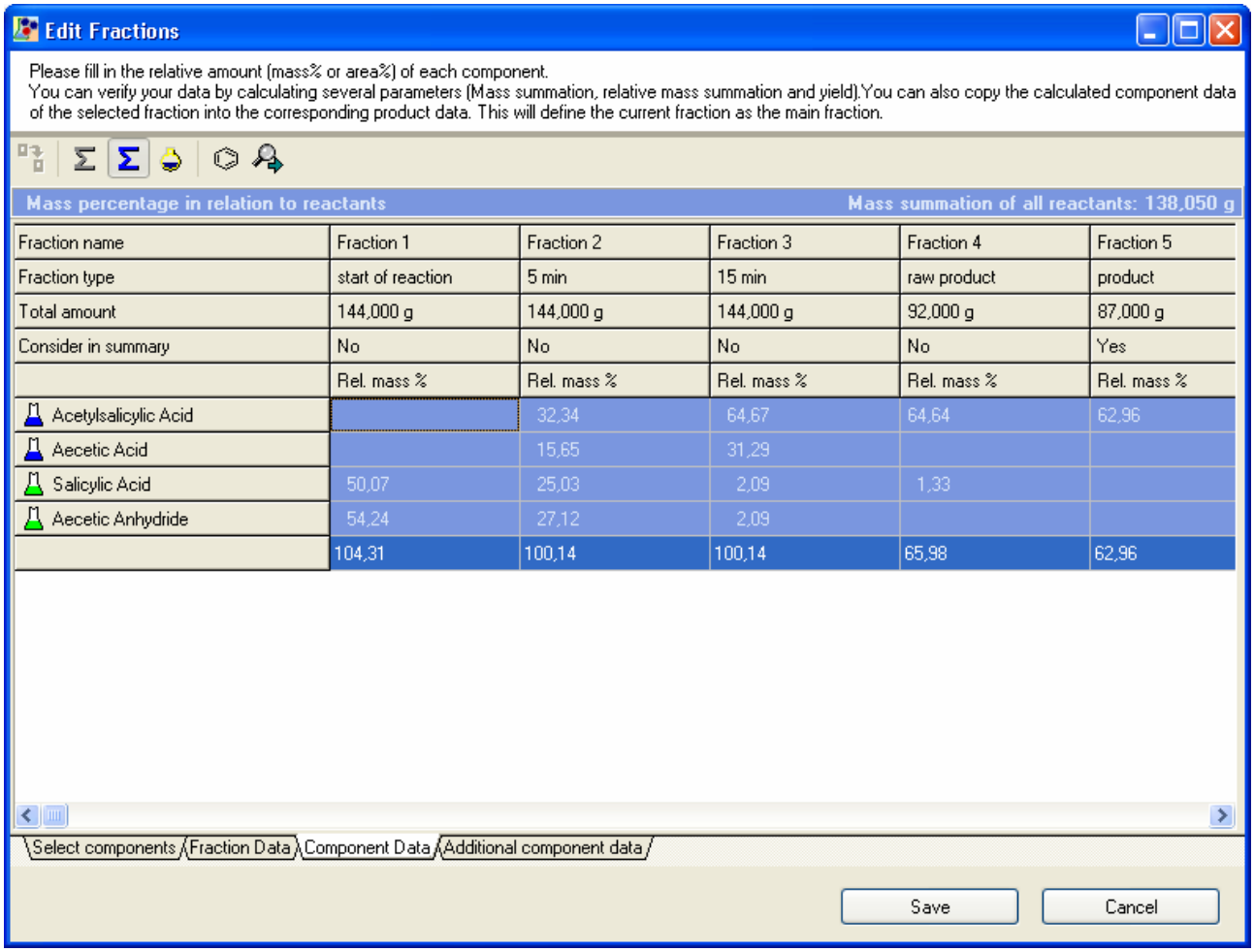
Optionally summation of all percentage values of each fraction is shown in the last line (button Σ). Normally it should be 100% if all peaks of the HPLC elution profile are taken into account.

The “Show molecule structures“ button can be used to toggle the display of the molecules’ structures in the grid (visible / invisible). All structures are shown in a separate column at the right side of the component name.

The “Show reference data” ( ) function displays a new window at the right side of the component table that contains the most important limiting reactant data (Name, molar mass, Mol amount and used amount). You can hide the display by clicking on the button once again.

Please note that you cannot change any reactant data in this overview. To modify data, please launch the experiment wizard. Further information can be found in chapter 3 (“Create your first experiment”).

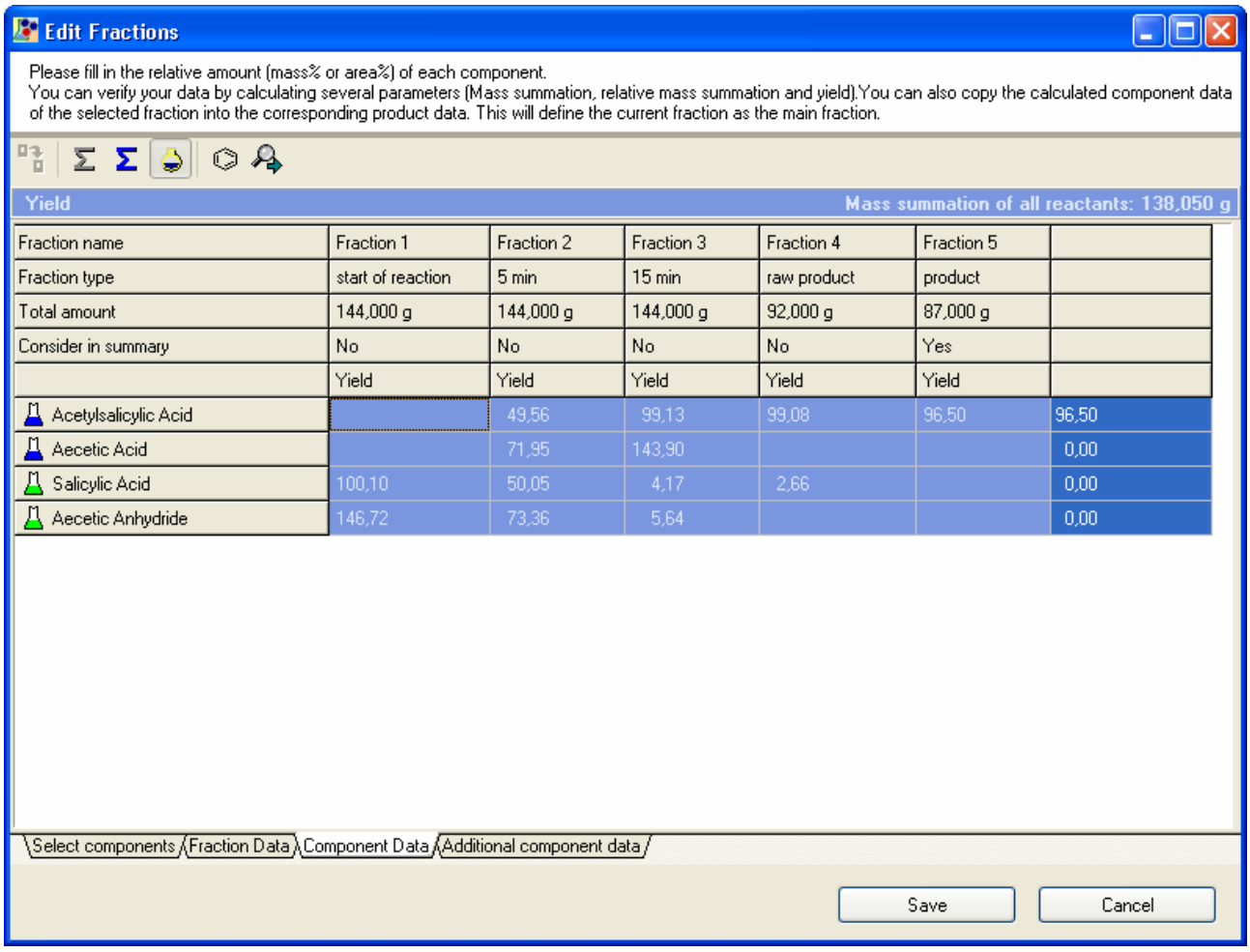
The third function, “Mass percentage in relation to reactants” ( ), calculates the relation of each product amount to the overall reactant amount. It does so by calculating the absolute amount of every product and then comparing it to the sum of all absolute reactant amounts. The calculation is the same for area percents. For display purposes, the whole table is restructured. At the right side of every row, there will be a summation of all calculated percentages of a component within all fractions, which are defined as “Consider in summary”. Beneath the last row, ensochemLab will also show the column summation you already know from the summation function.



Calculation of the mass percentage is done as follows:

Mass of reactants	salicylic acid	069.05g
	acetic anhydride	075.21g
Total mass of reactants		**144.26g**
Total mass of fraction 5	87,8g	
Mass% of acetylsalicylic acid	99,9%	
Calculated mass of acetylsalicylic acid	**87.71g**	
Relation	**87.71** / **144,26** =	**60.8%**

When you click on the “Yield“ button, ensochemLab will calculate the yield of every component in relation to the limiting reactant.
The program also shows the full yield of a component over all fractions. This value is displayed on the right side of the respective row.



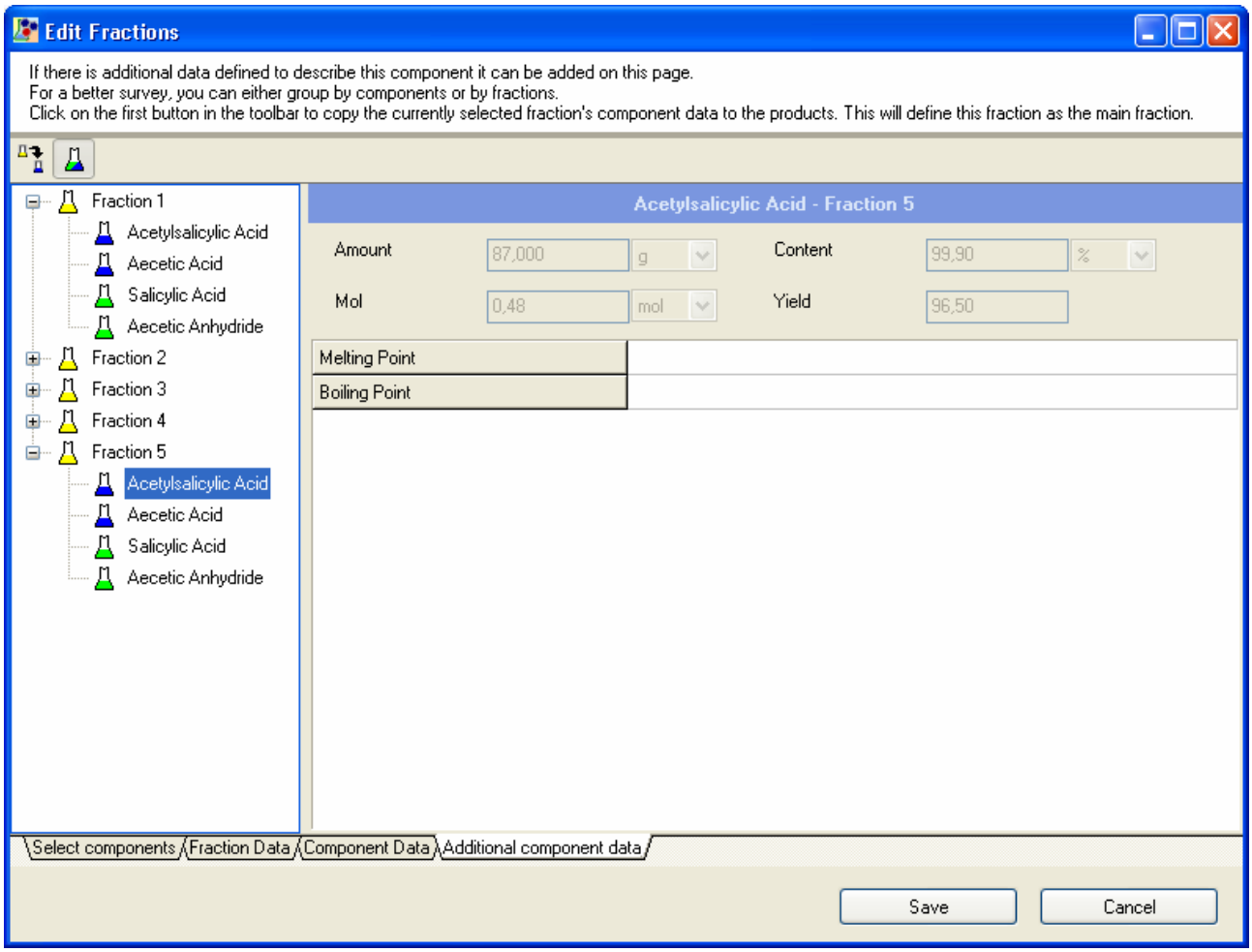
Calculation of the yield is done as follows:

Limiting reactant salicylic acid	069.05g	**0.500 mol**
Total mass of fraction 3	144.00g	
Mass% of acetylsalicylic acid	62%	
Calculated mass of acetylsalicylic acid	89.28g	**0.495 mol**
Yield % of acetylsalicylic acid in fraction 3		**99%**

By the way: ensochemLab displays the reactants' mass summation in the upper right corner of many pages in the fractions dialog. This can be useful when calculating spreading on basis of experimental results or tabular data, for examples. You can then use the value without having to switch back to the experiment display in the main window.

You may have already noticed that not all reactants are available in the fraction dialog: Components that have been marked as solvents or catalysts in the experiment wizard may not be part of a fraction. They will not be included in the calculations either.

Now it is time to take a look at the last page in the fractions dialog, the "Additional component data" section:



On this page, you can enter additional data for the reactants and products in a specific fraction. With respect to this, ensochemLab offers you a tree structure at the left side of the window that contains all reactants and products once per fraction in the default display mode. This means that the acetic acid used in this example can have different melting points in every fraction.

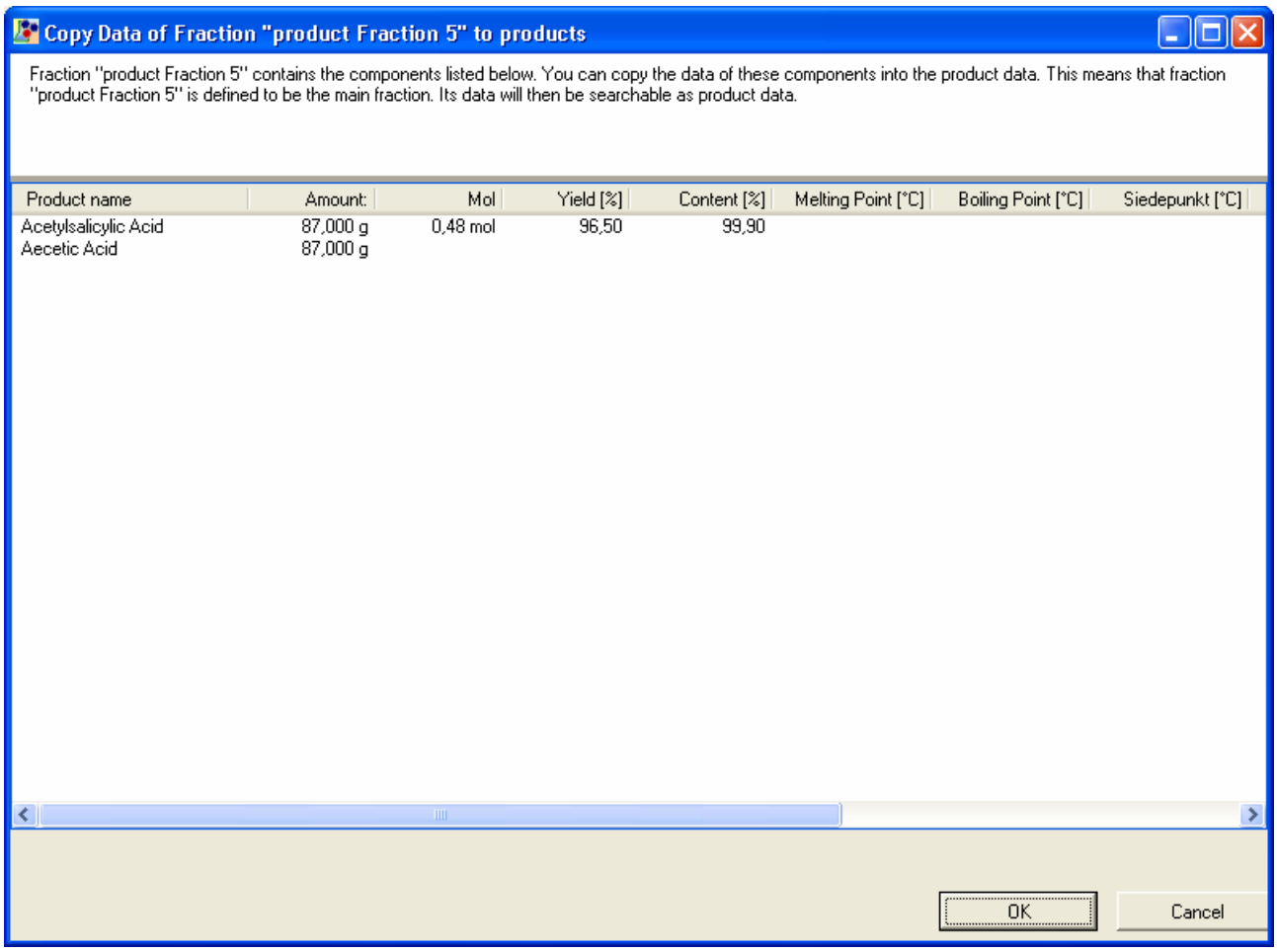
To simplify entering data, ensochemLab shows the most important data from the previous pages with the current entry from the tree.
The data field "Text data" is a normal text field that can contain any arbitrary value. The fields "Melting Point", "Refraction" and "Boiling Point" already have predefined data masks for the respective format. The boiling point, for example, is automatically added a "°C" indicator. For the two other fields, you can enter an optional condition (e.g. "at room temperature", "at 1.32 bar air pressure", …).

However, these additional data fields may vary a lot from the values used in this manual's examples depending on the specially customized ensochemLab version your company has purchased. If you have questions, please contact your system administrator or supervisor. Additionally, the data fields may not be displayed in the language you have selected in the application: All field definitions are stored and managed on the server centrally. This means that they are always created in the installation language of your ensochemLab web server.

The tree view also supports another display mode with a different entry placement. Please click on "Group by components" ( ) to take the specific components (reactants and products) as root nodes and place the fractions and their data beneath them.

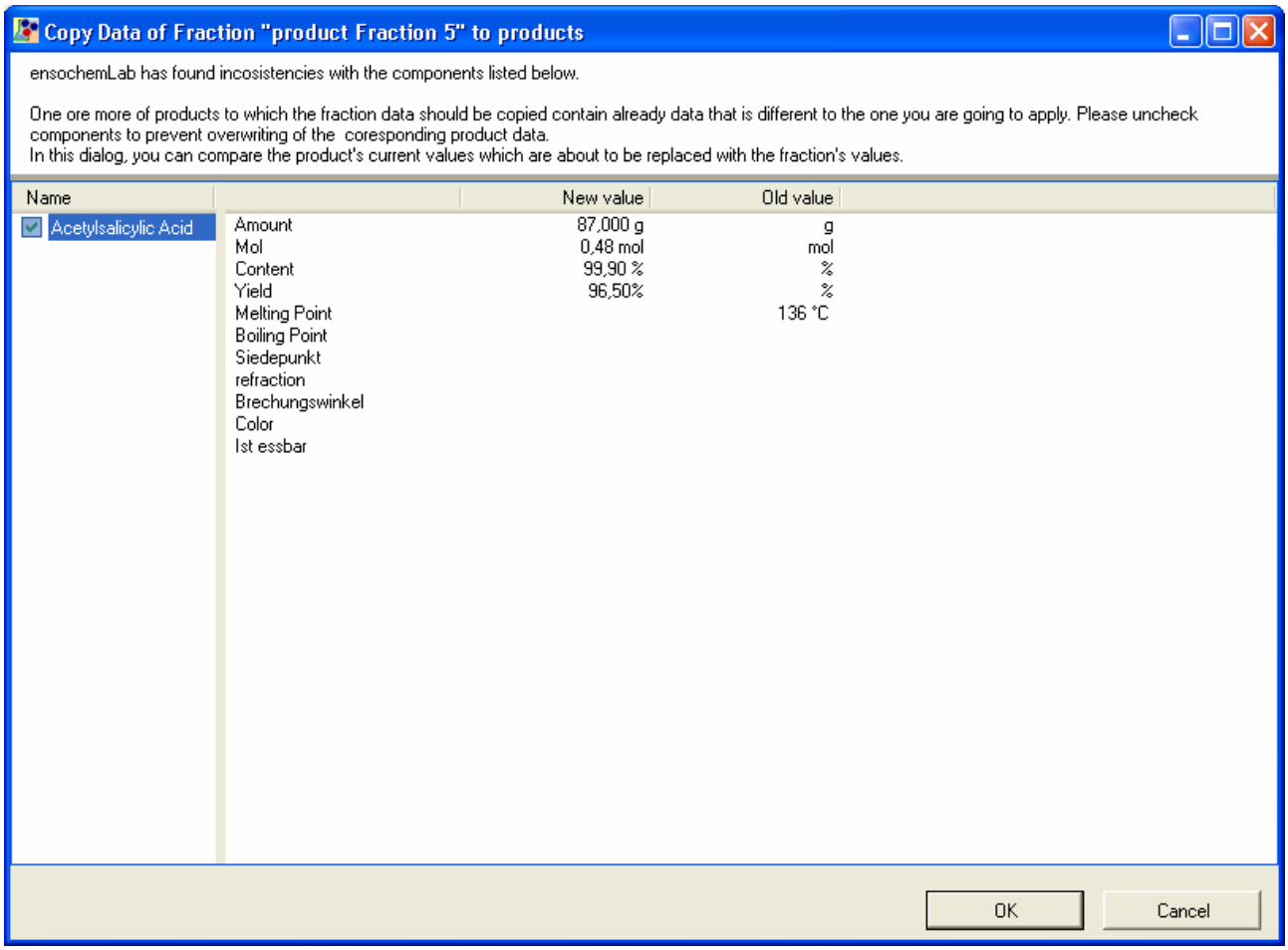
The "Copy fraction data to products" function ( ) is available on almost every page in the fractions dialog. You can use it to apply the current fraction's data as your product data. This defines the fraction to be the "master fraction", the one to be used for synthesis. However, you should only do so when you are sure that the data will not change that often in the future any more. Otherwise, you would have to repeat the progress several times.

When you click on the button, the following window will appear:



This window gives you a short overview of the products that you have selected for usage with fractions on the first page of the fraction dialog. The table shows that most important data fields from the experiment assistant and the physical data. This display is for reference only; you do not have to select or mark anything.
If you click on OK, the current fraction data will be copied into all products listed on this page. By clicking on "Cancel", you can return to the fractions dialog without applying any data.

If one or more products already have data different to that you want to assign, the following dialog will be shown:

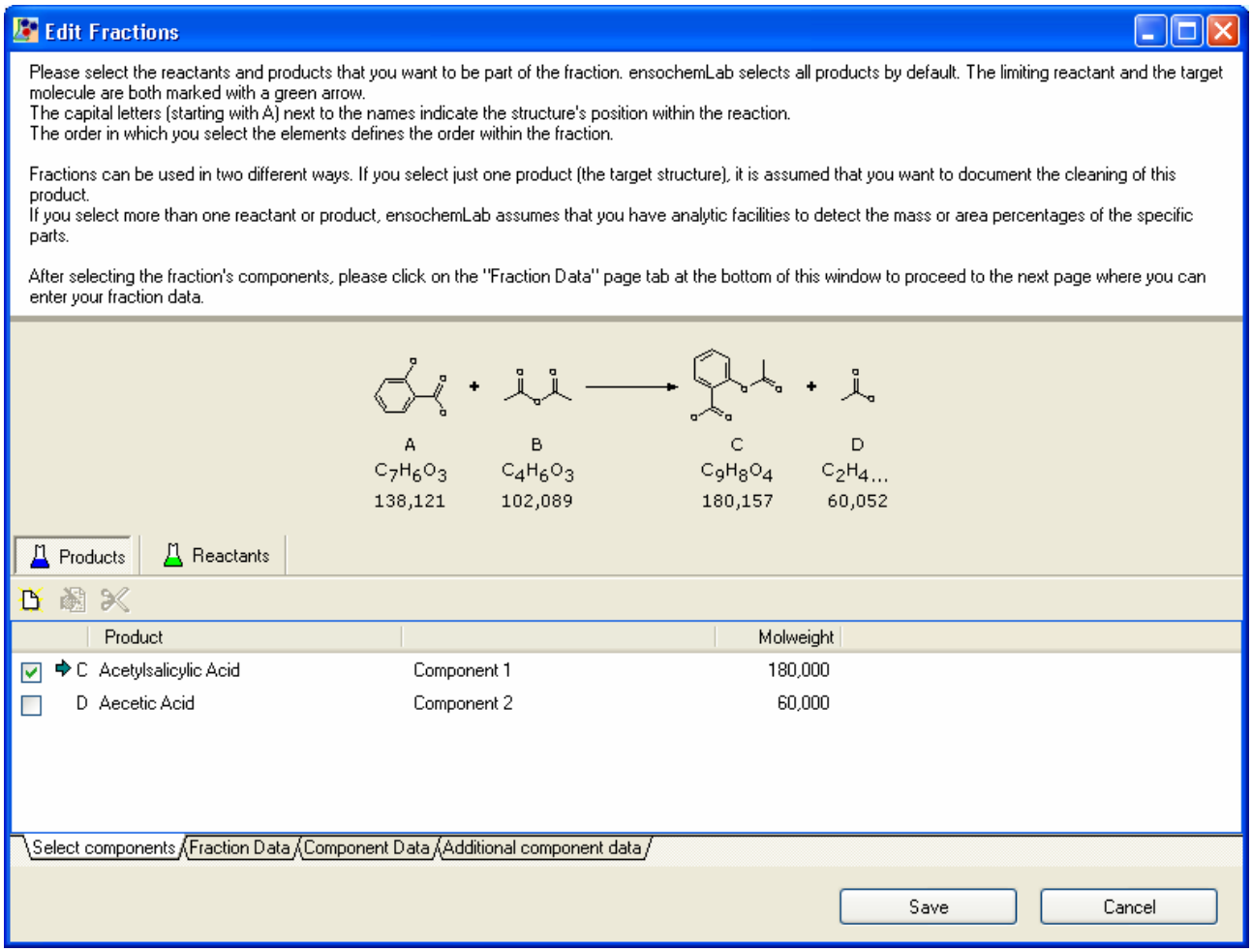


You can now use the list at the right side to mark all the products you want the data to be assigned to. For every selection on the left side, the corresponding old and new data (that is the one to be replaced and the one to be copied) will be shown in a table in the display pane at the right side of the window. It is not possible to modify the data directly on this page.
Please click on “OK” to apply the data to the selected products. By clicking on “Cancel”, you can return to the fractions dialog without applying any product data.

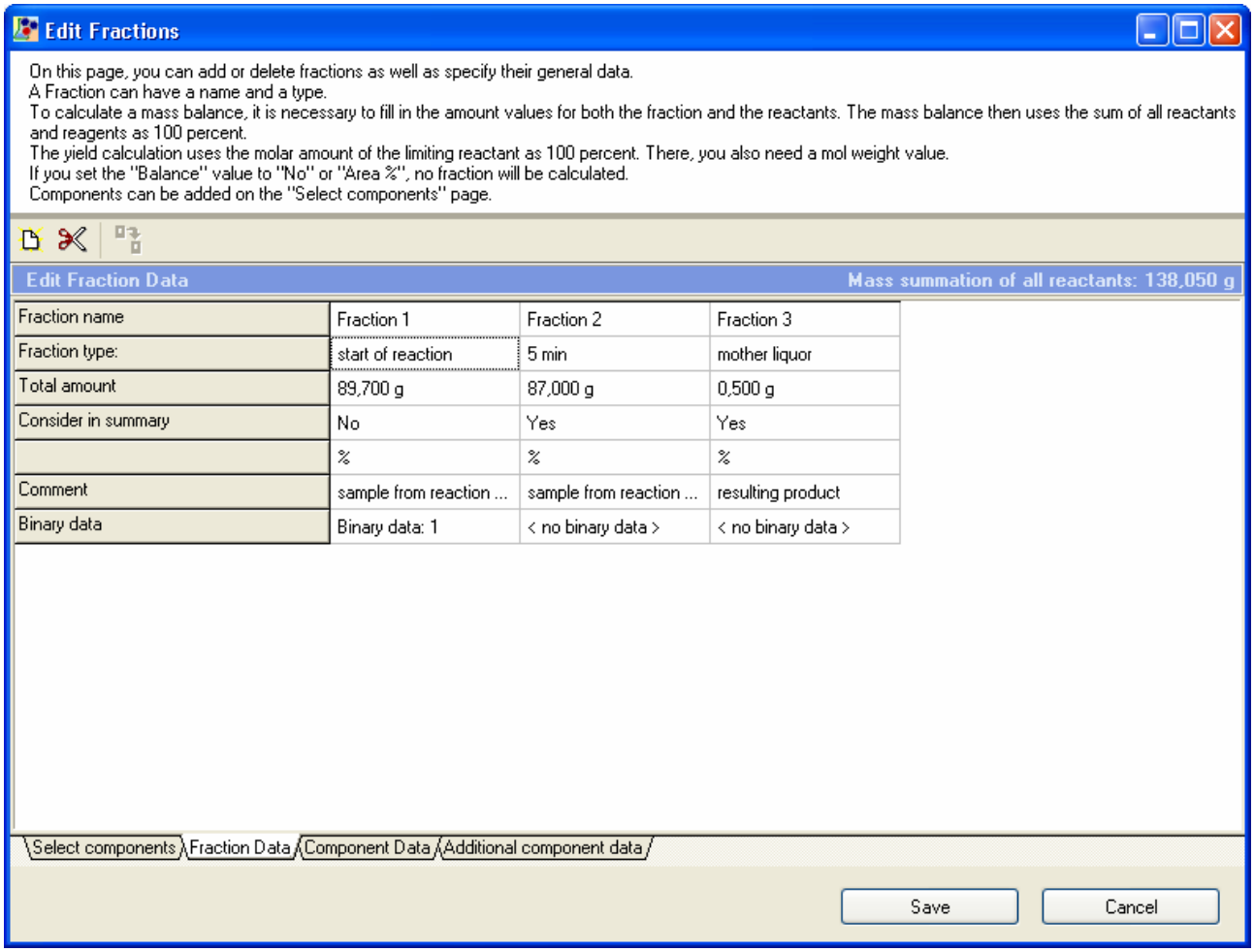
After a successful data transfer, the  symbol will be shown beside the name of the fraction you have copied.

Example B:

We start again with the same reaction and the same data, used in example A. But now we do not use HPLC and we are only interested in the purification procedure of the main product acetylsalicylic acid. Therefore only acetylsalicylic acid is selected on the first page of the fraction dialog:

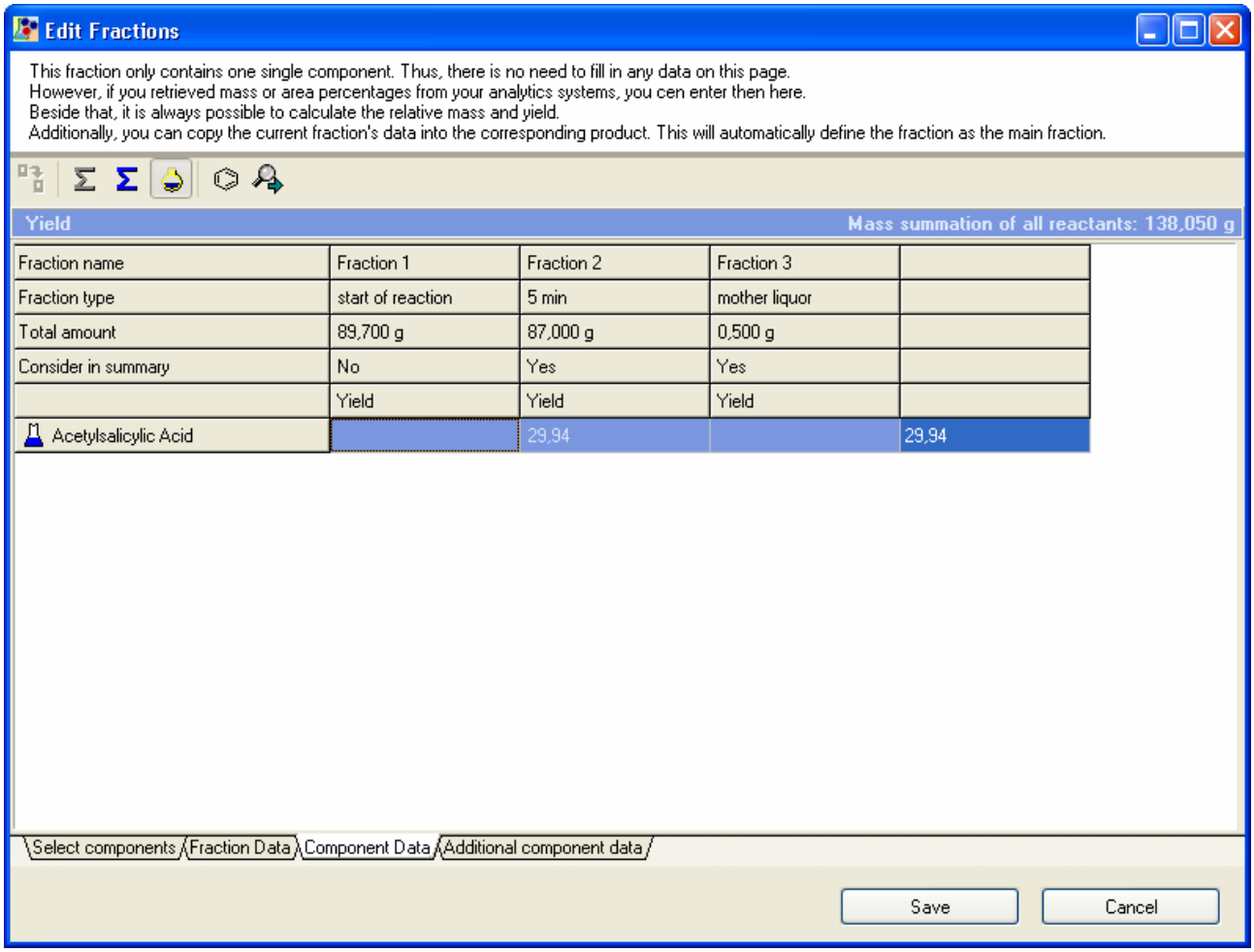


On the “Fraction data” page three fractions for single step purification are assumed:



No input is required on the “Component data” page, because it is considered that 100% of the fraction consists of the product acetylsalicylic acid, because we have no analytical aid to determine the real composition of fractions.

We can directly have a look to the yields of each fraction and the overall yield of the last two fractions.

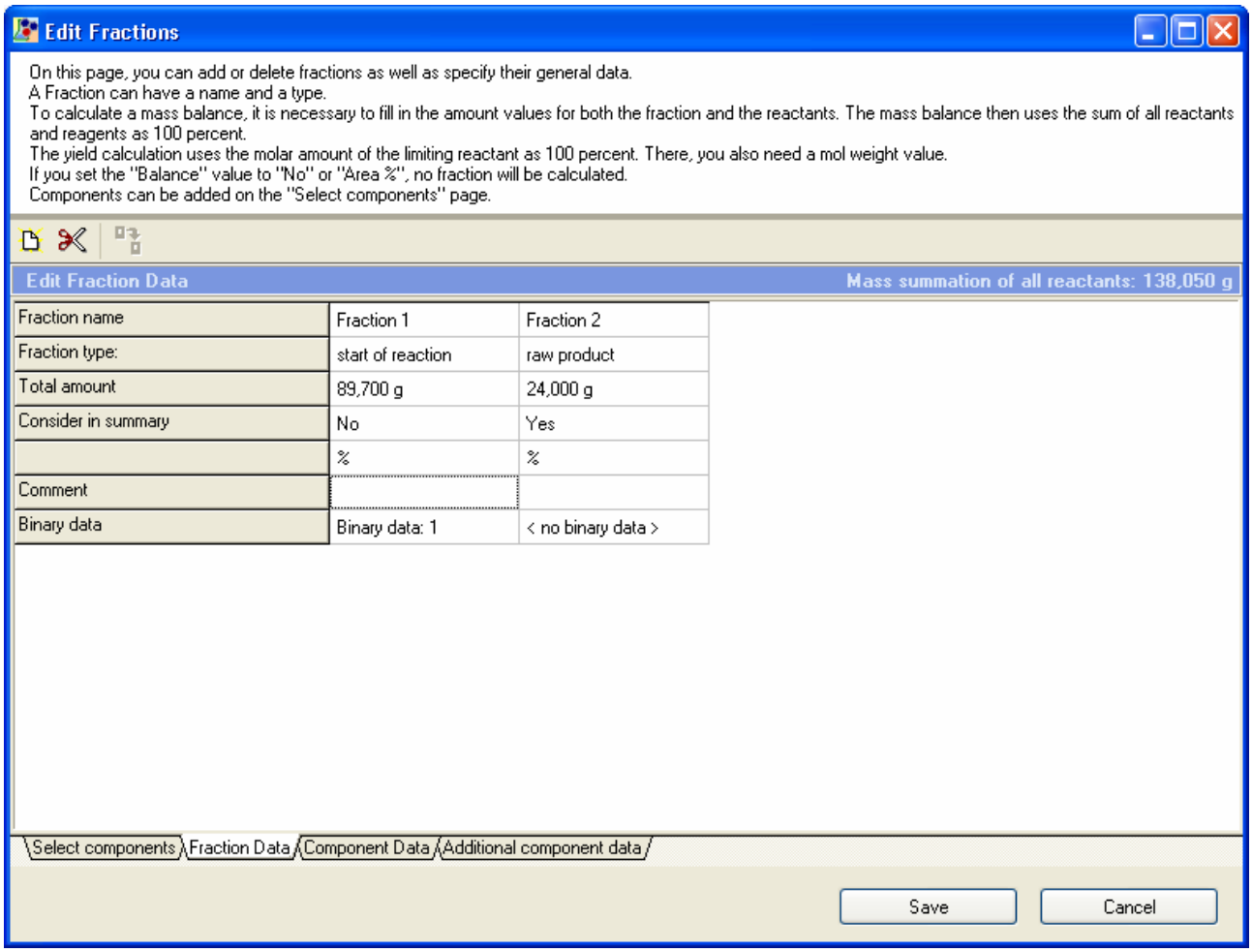


Example C:

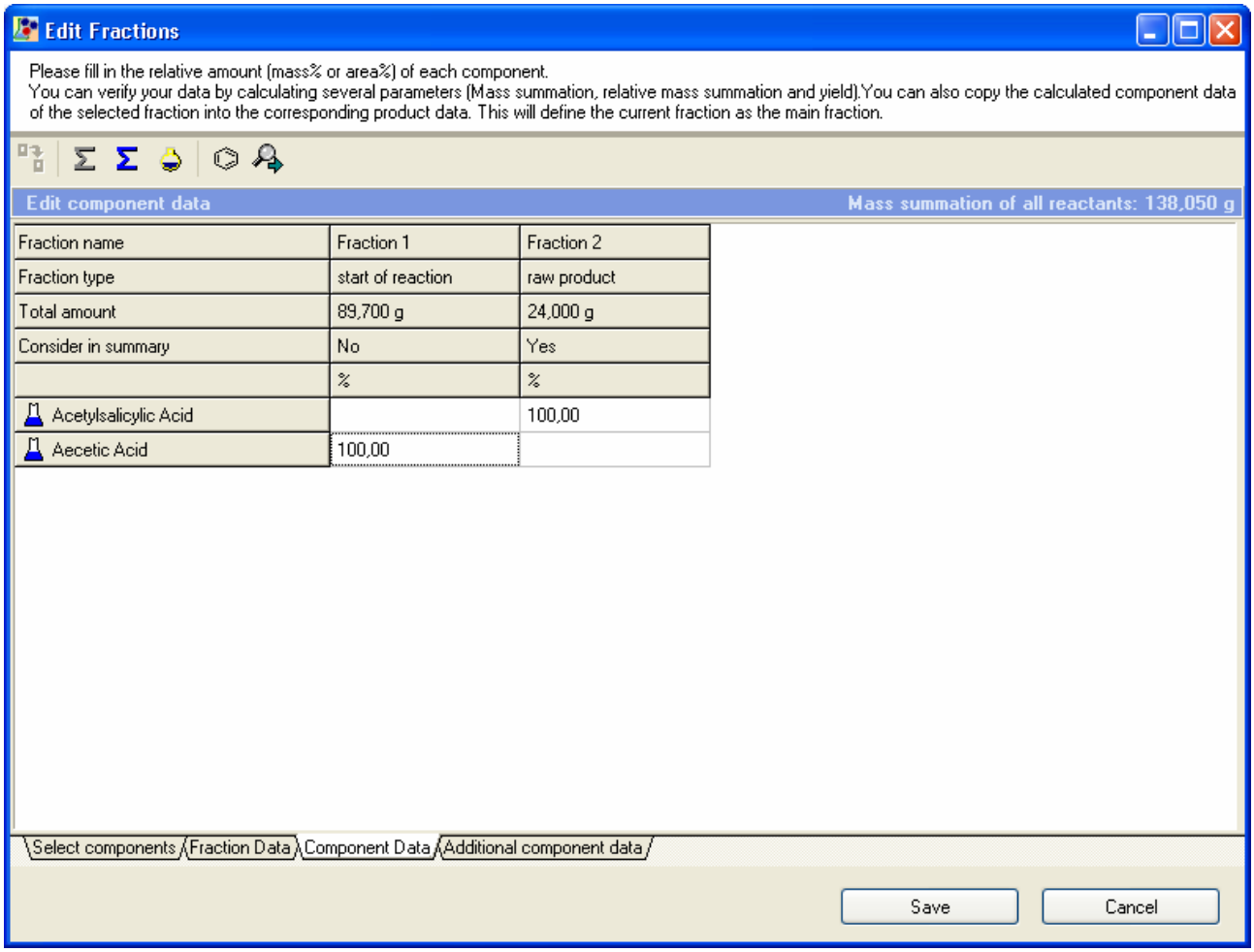
We start again with the same reaction and the same data, used in example B. This time we will document not only the target product acetylsalicylic acid like in example B but also the byproduct Acetic Acid. Therefore we include both products in the fractions.

After suction filtering acetylsalicylic acid is found mainly in the suction filter whereas the Acetic Acid is found in the filtrate.

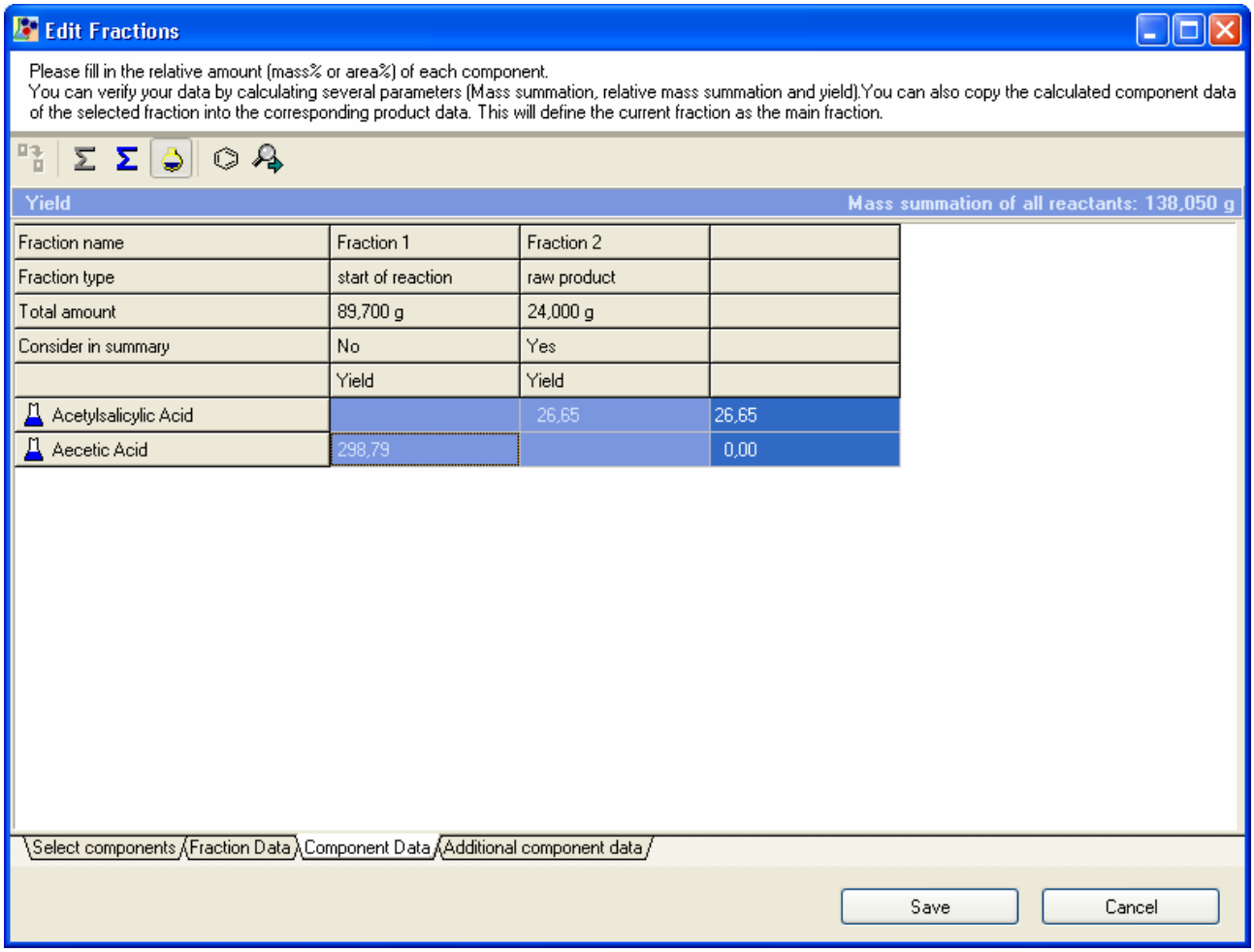
The “Fraction data” page is filled as follows:



And the “Component data” page:



Because the products have been separated both products are considered in the summation of the yield:



Summary:	With the fractions dialog, you can document the reaction processes and purification procedures with or without use of analytical methods like HPLC or GC.

15. Multistage Reactions

In terms of a complete and comprehensible documentation of syntheses, the support of multistage reactions is an important issue. Especially the clearness of context and intuitive handling must be realized properly.

Generally there is a difference between multistage reactions which intermediate products aren't processed and those with worked up, assured steps. Both types are an inherent part of daily laboratory work.

15.1. General Considerations

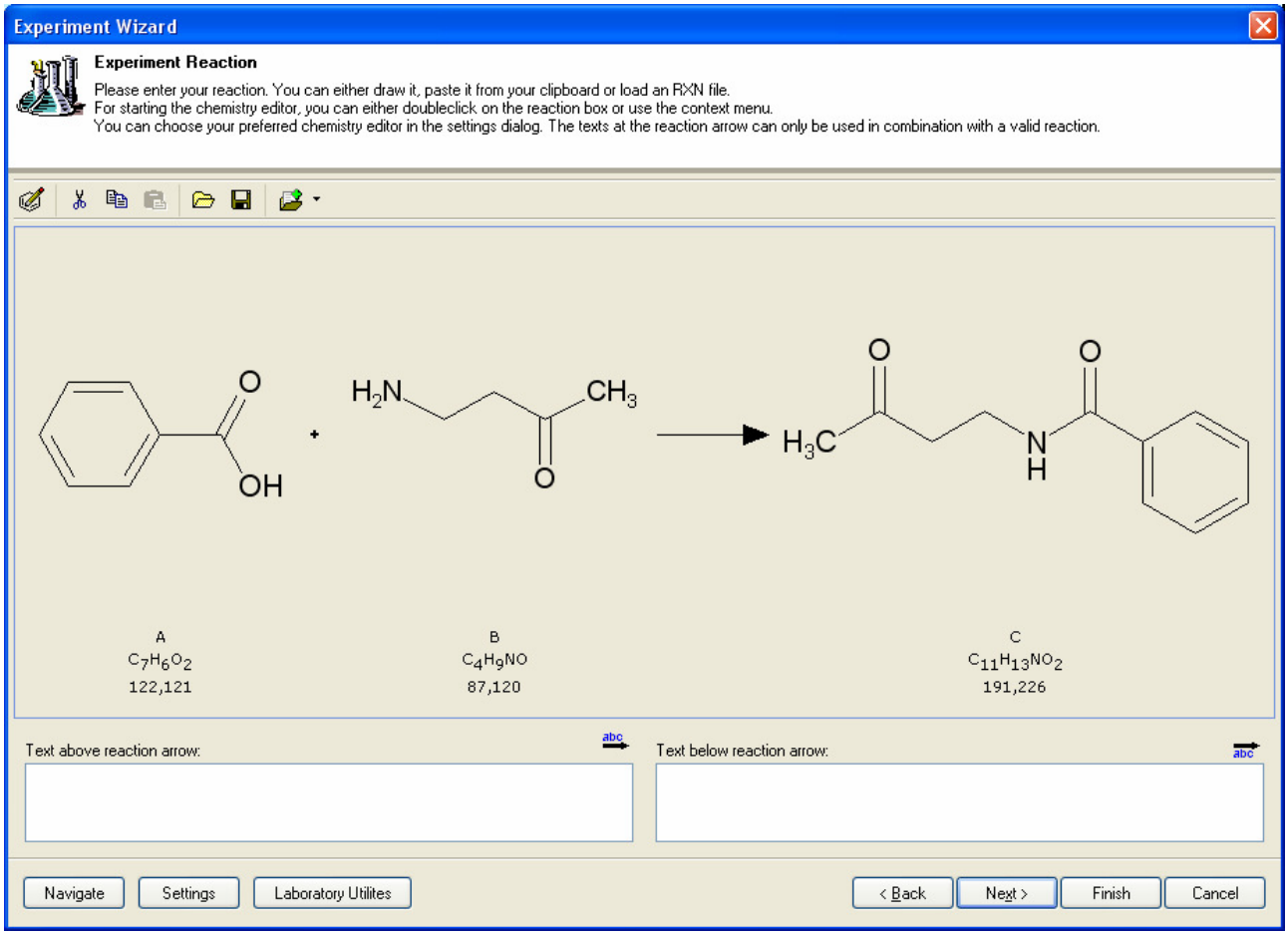
Currently ensochemLab supports the registration of multistage reaction without working up intermediates. The documentation of concrete steps can be done with the function "Create follow up experiment" (Main- or Reaction-context-menu). In a next version, ensochemLab will provide a convenient solution for those too.

15.2. Enter Data

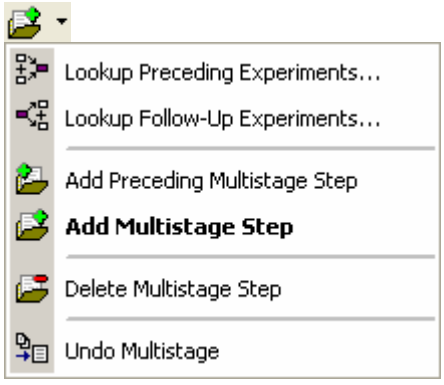
To document a multistage reaction please start the creation of an experiment just as you are used to it. Enter the reaction of the first step and after that, take advantage of the tool  to create a follow-up step or a preceding one. Doing so, results in the first product being taken as limiting reagent of the following step and is converted to an intermediate respectively. The resulting overall reaction won't show these structures.

In the following the process is shown and explained step by step.

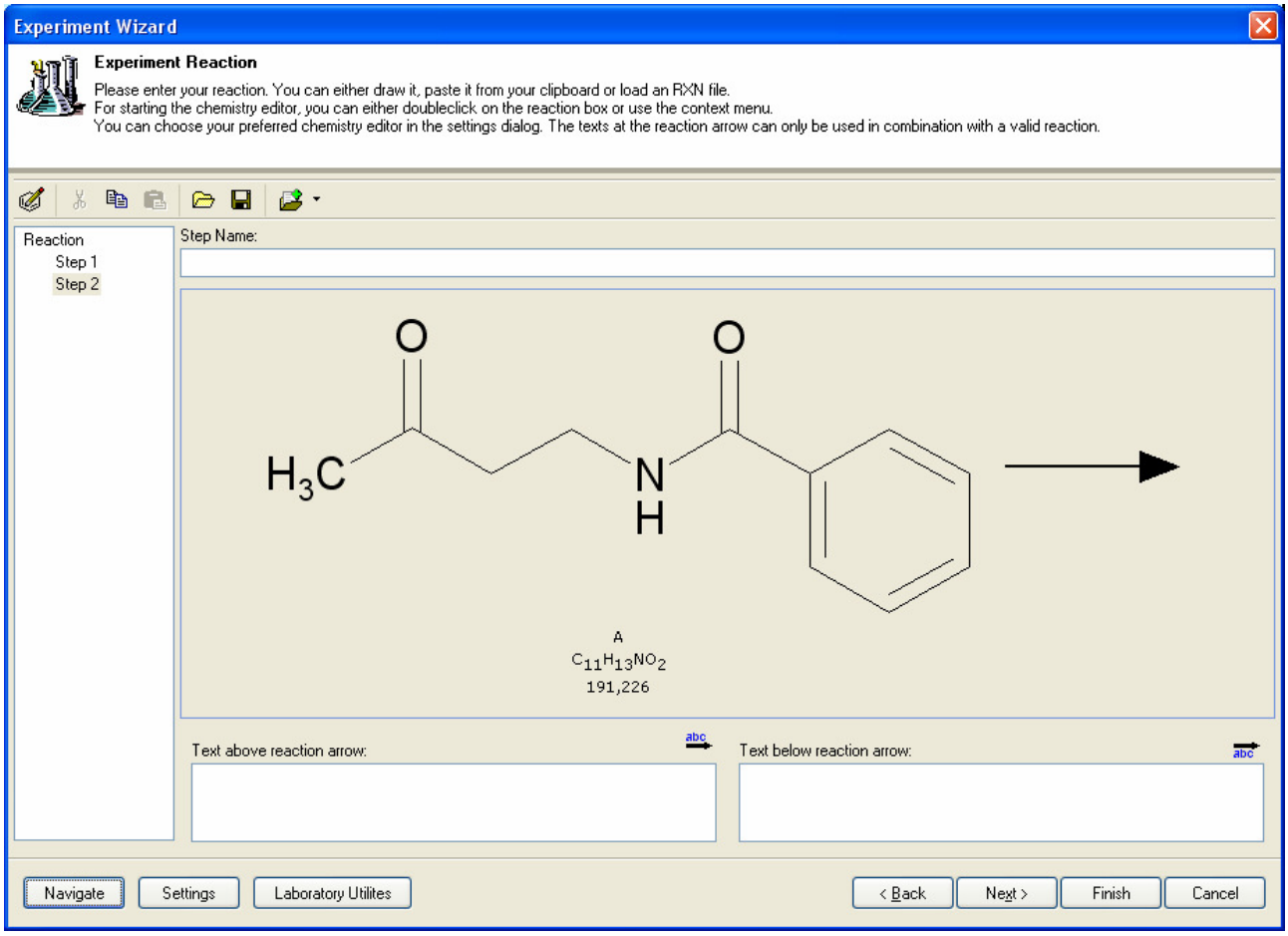
You start with providing the reaction of the first step, which results in this view of the reaction page in the wizard.



Now you are going to create a second step by selecting the appropriate action in the toolbar.

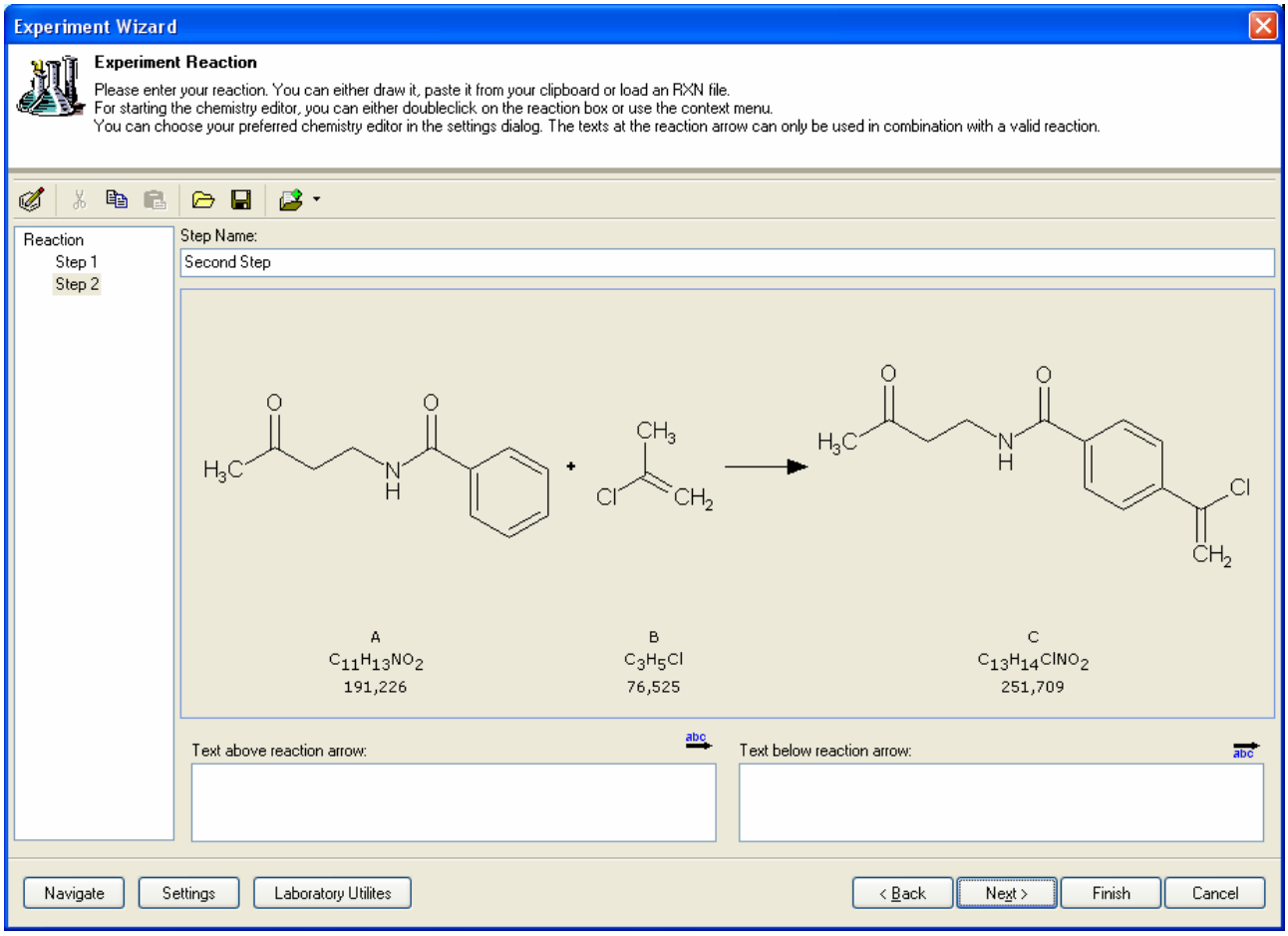


If you want to, it's possible to look-up already existing, matching reactions in ensochemLab (this will be explained later in this chapter) or to create an appropriate step and edit the reaction, as you are used to, directly in the wizard.

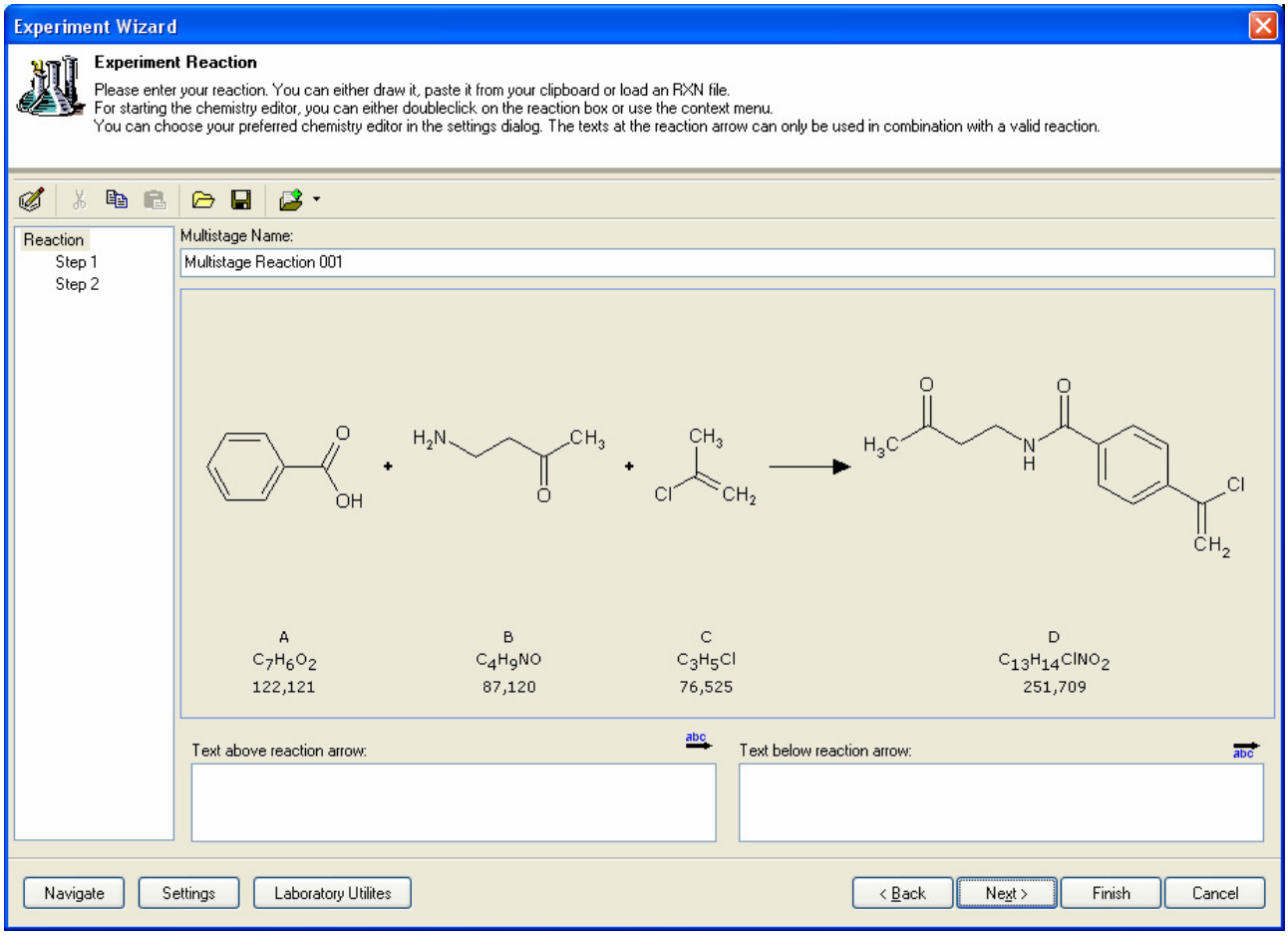


ensochemLab will prepare the follow-up reaction by taking the first product of the currently last step as limiting reagent. You complete the reaction as needed.

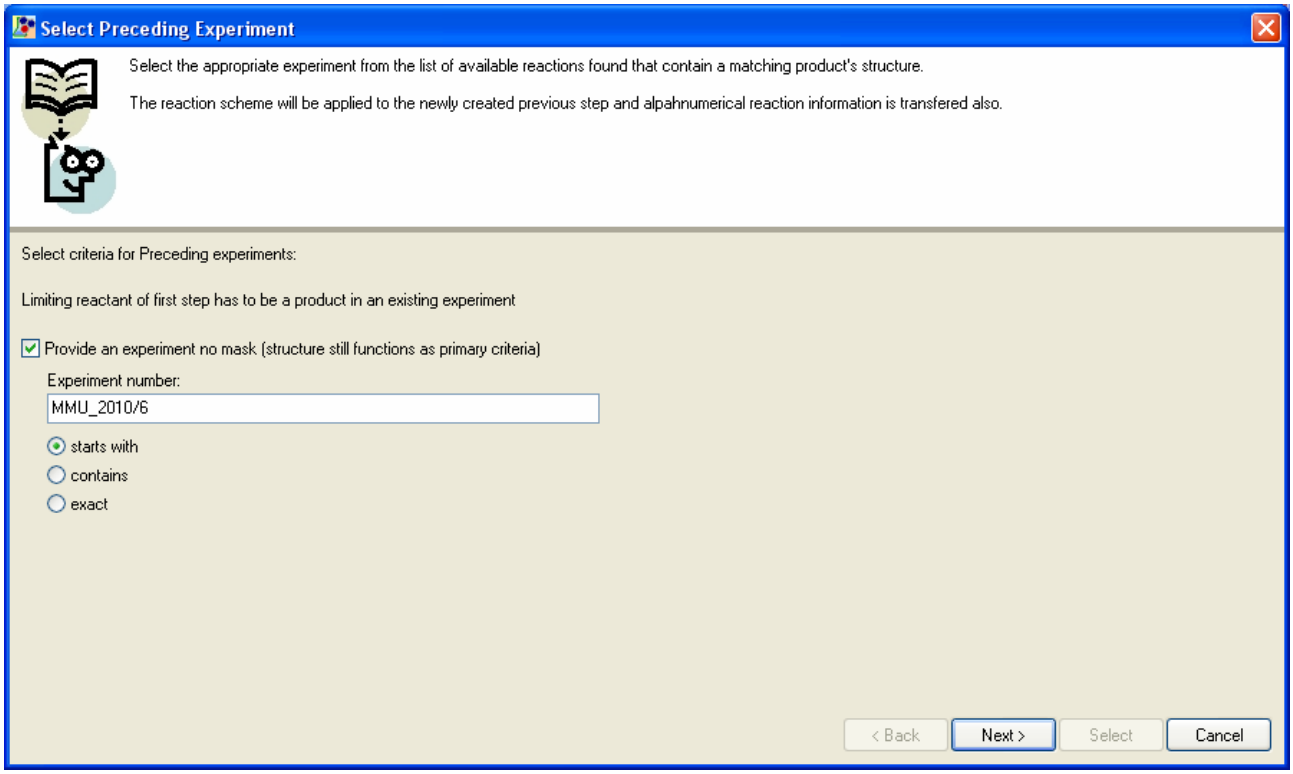
In case a reaction is entered which's reactant doesn't match the product of the preceding step or includes a product that differs from the corresponding reactant of the follow-up step respectively, a warning will be shown. You have the choice of either keeping the already existing structure, replace it with the new one or to cancel the editing.

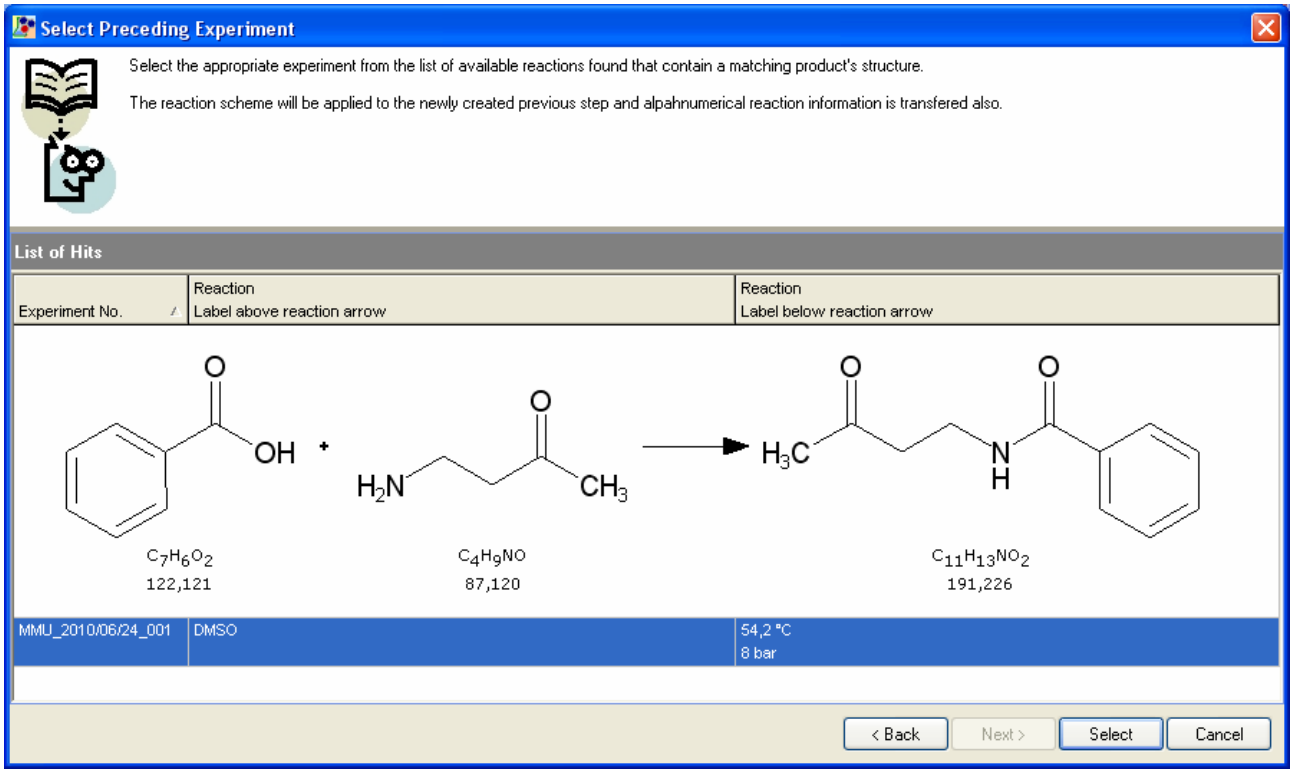


This is an example for a valid follow-up reaction. By clicking the node “Reaction” in the tree, the resulting overall reaction will be shown. The rule, when creating the resulting reaction, is to combine all steps’ reactions but not including the intermediates.



As already mentioned you can use a look-up functionality too. Simply select the appropriate action from the menu and search, assisted by a wizard, for reactions stored in ensochemLab. You may specify a filter, in addition to chemistry, by providing an experiment number mask. Basic rule is that in a follow-up step the reaction must have a matching limiting reagent and a preceding step an identical product respectively.

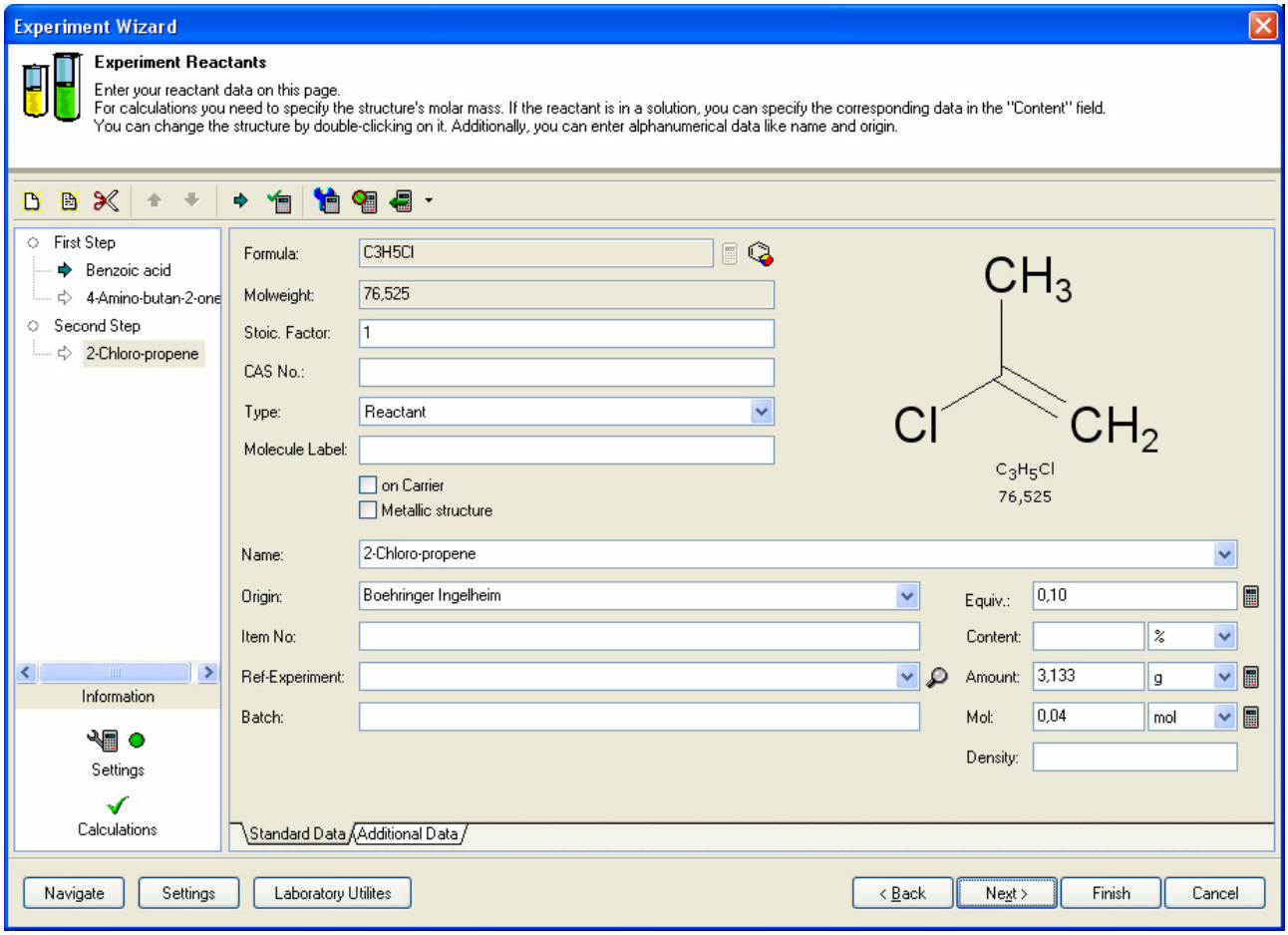




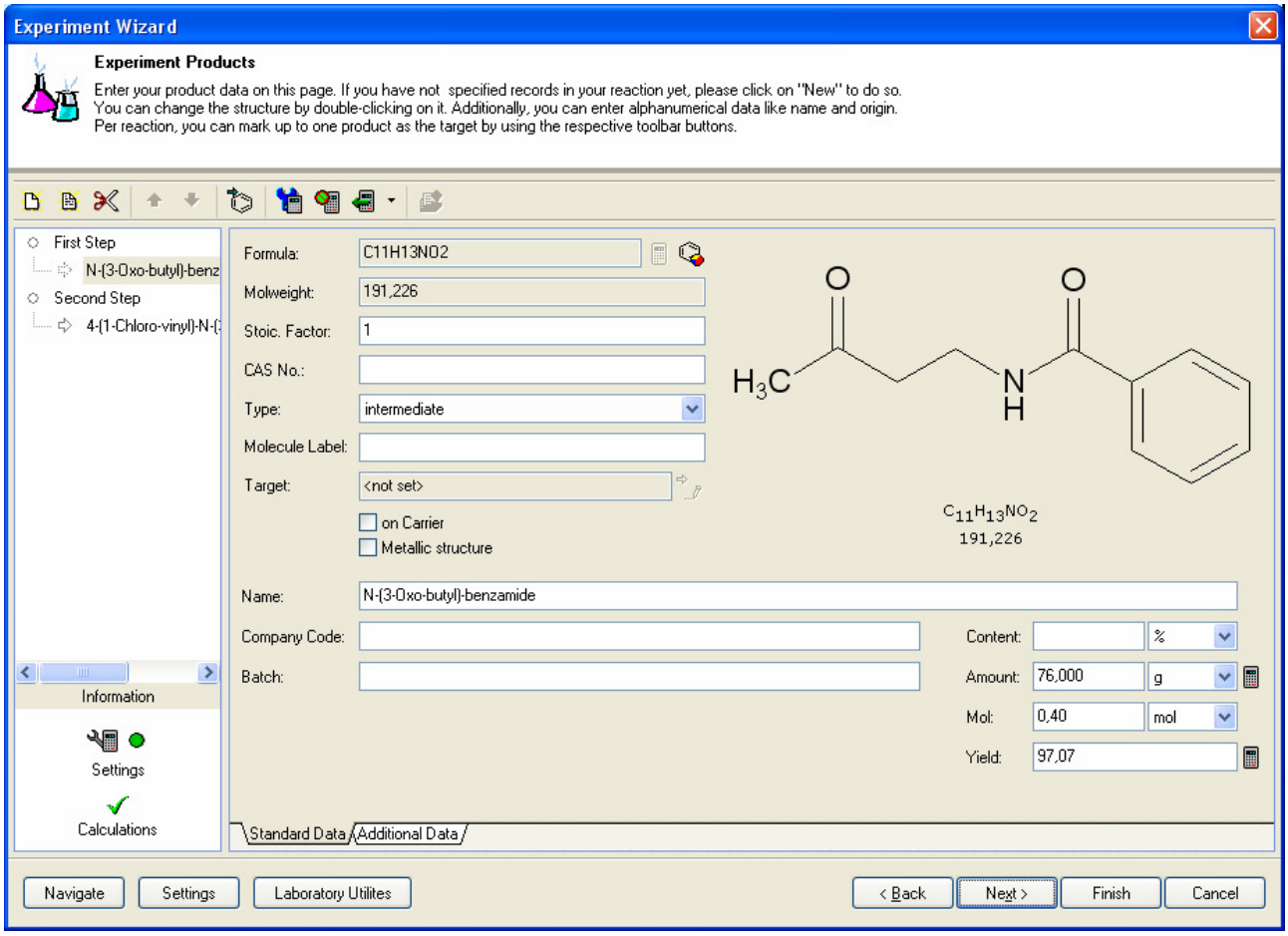
You choose the reaction that fits best from the list of available ones and transfer the reaction plus reaction arrow texts, if there are any, into the new step. Please note that this is only a copy of the data and not a reference as a persistent link yet.

After entering the appropriate step reactions, the corresponding pages for reactants and products in the wizard will show the step information too. This way it's guaranteed that you are supported any time and that the actions are controllable in an understandable manner.

Entering additional data is performed as usual; reactant calculations are done by using the first reactant of the first step as a reference.



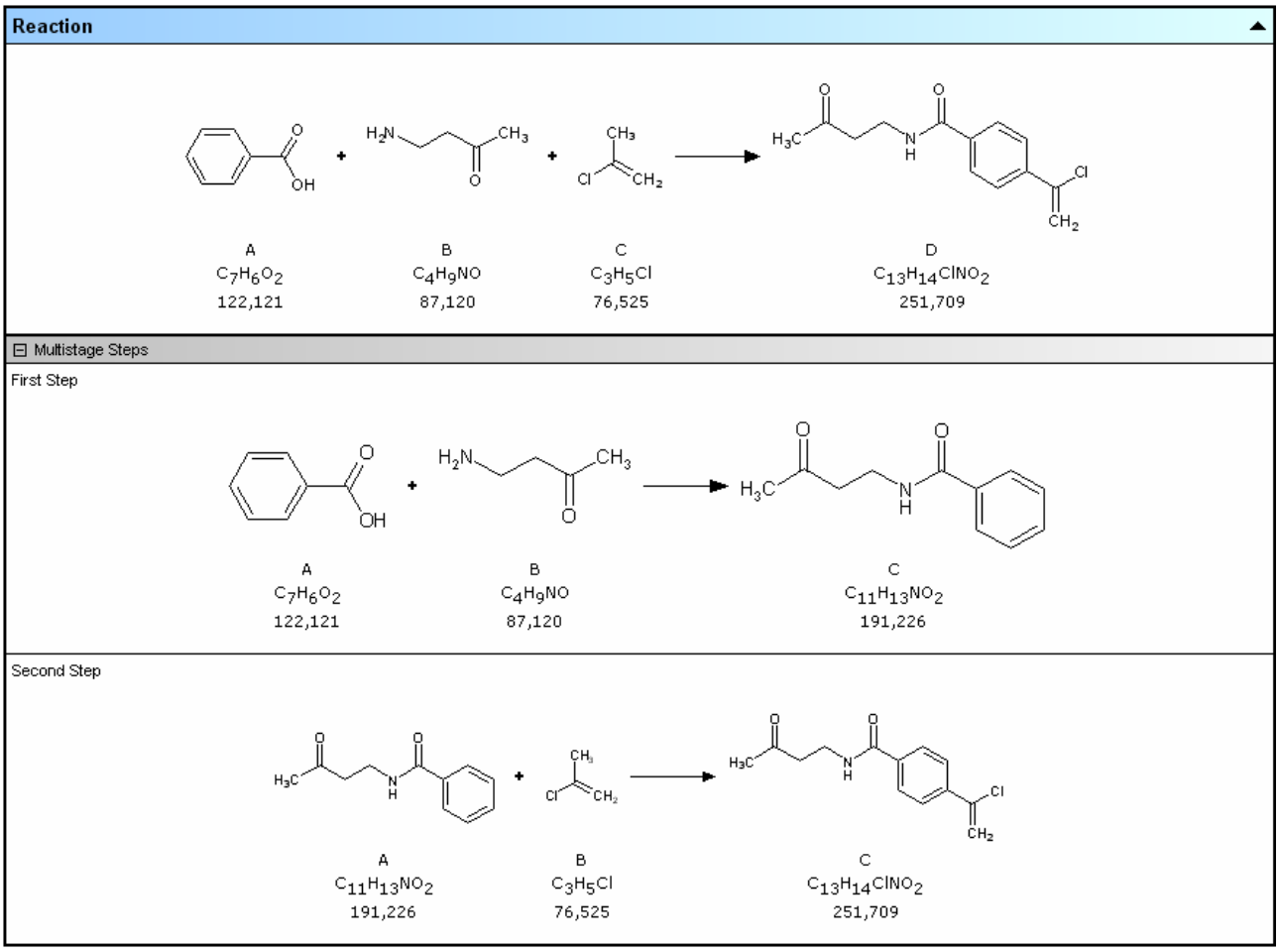
The intermediate products won't be available on the reactant page but can be only edited in the list of products. The information is shown according to your entered data in the tree of the wizard.



Calculations of yield are using the first step's first reactant also. Detail data is entered as usual too.

15.3. Display

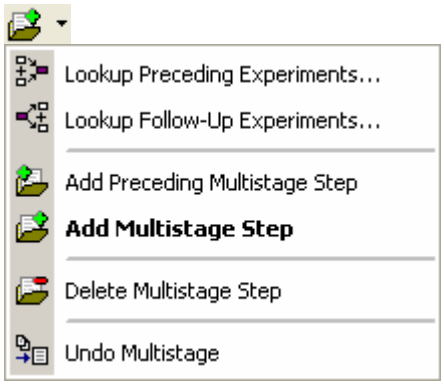
The experiment will show as reaction scheme the resulting reactions build out of the steps. By expanding the steps section all details for the intermediates are shown and might be e.g. included in a printout.



This display is thought to be the first step on the way to provide a complete documentation of multistage processes and in a next version it will be extended to e.g. support syntheses pathes.

15.4. Deletion

If needed you can delete single steps or undo the multistage. To do so please select the appropriate function from the menu.



The action „Undo Multistage“ will result in keeping the overall reaction and deleting all intermediate information, like reaction and product data.

16. CSV Data Exchange

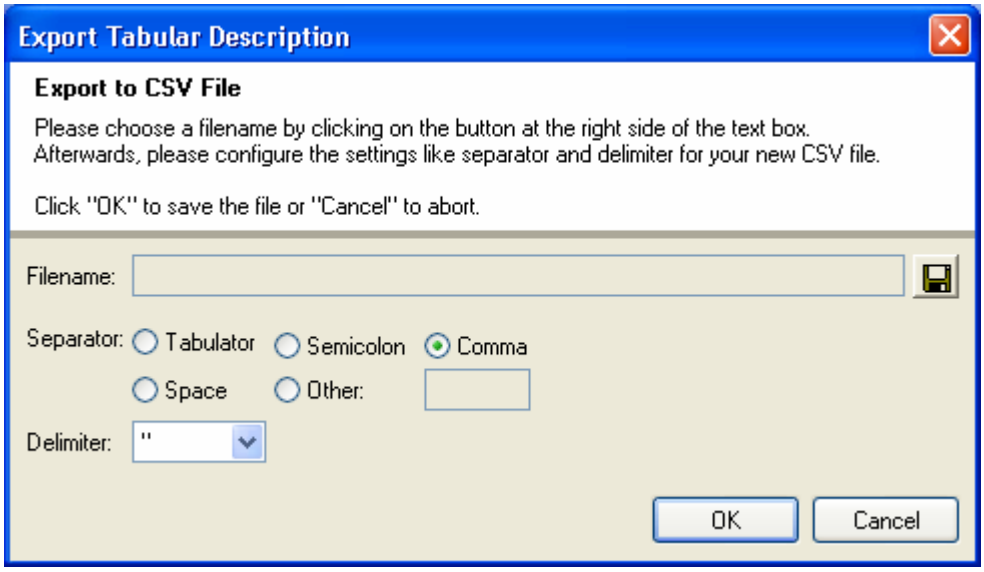
The CSV file format is used for exchanging data between different applications in a standardized way. With the respective functions in ensochemLab, you can, for example, insert your tabular experiment description as a table into a Word document or transfer the experiment results you have collected in an Excel spreadsheet into your emnsochemLab experiment.

16.1. Exporting tabular data to CSV

At the positions within the application where you can work with tabular data, ensochemLab offers you capabilities for exporting the contents into a CSV file. Concretely said, this feature is available for the following modules:

- the tabular description
- the reaction parameters
- the process description

The export function can be launched from the experiment display as well as from the experiment wizard. Inside the display mode, please click on “Export <ELEMENT>” () (<ELEMENT> refers to the experiment part you are currently dealing with) in the context menu. Inside the experiment assistant, there is a toolbar button labeled “Export” (). In both cases, the following window appears:



The first step is specifying the name and path of the file into which you want to export your data by clicking on the “Save As” button (). The application now opens a normal “File Save” dialog that you know from many other windows programs.

In the lower part of the export window, you can configure your desired CSV file options. The “Separator” is the dividing character that is placed between two columns in a file:

```
Amount,Unit
12,g
```

The “Delimiter” encloses the content of a single field at its left and right side. This especially important if the field data already contains the “separator” character:

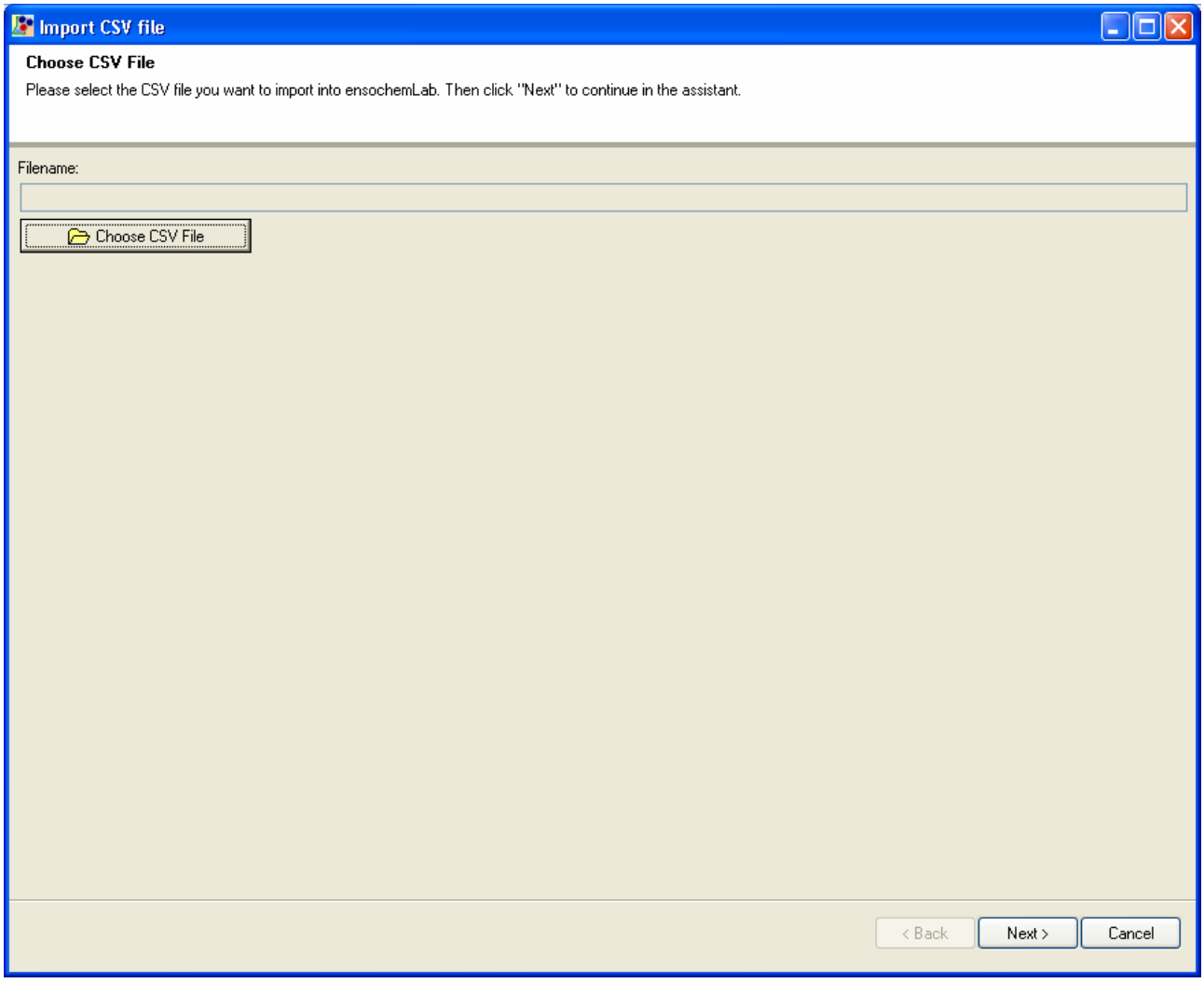
```
Name,Comment
“Smith, John”,”Temperature increased by 5 °C”
```

For starting your export operation, please click on “OK”. With a click on “Cancel, you can return to the previous ensochemLab module without exporting any data.

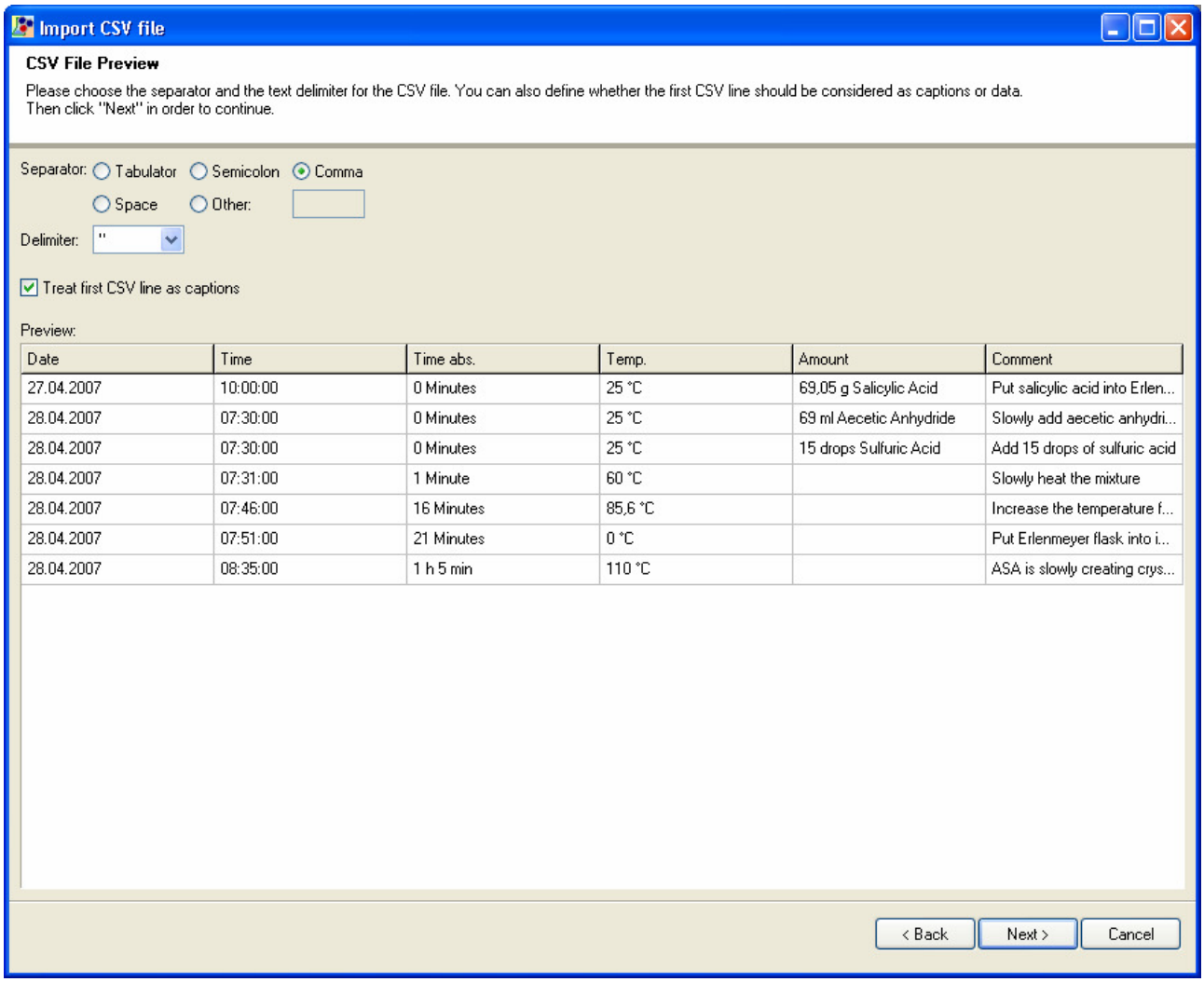
16.2. Importing tabular data from CSV

At every place described in the previous section, there is of course also a function for re-importing your externally modified CSV data. The workflow is the same in all modules and always leads to the same import wizard. However, please note that existing data is always overwritten by the imported values.

For launching the import wizard, please click on the “Import” button () in the respective module’s toolbar. The following dialog appears:



On the assistant's first page, you can select the file you want to import by clicking on the "Choose CSV File" button (). Alternatively, you can also drag a file from the Windows Explorer and drop it onto the window. Afterwards, you can use the "Next" button to proceed to the next wizard page.



On this page, the software displays a preview of the data in the CSV file.

However, at first, this preview may look a bit strange:

Column 1
Date,Time,Time abs.,Temp.,Amount,Comment
27.04.2007,10:00:00,0 Minutes,25 °C,69,05 g Salicylic Acid,Put salicylic acid into Erlenmeyer flask
28.04.2007,07:30:00,0 Minutes,25 °C,69 ml Aecetic Anhydride,Slowly add aecetic anhydride dropwise
28.04.2007,07:30:00,0 Minutes,25 °C,15 drops Sulfuric Acid,Add 15 drops of sulfuric acid

If this happens, you have to change the import settings in the upper part of the window. They define how your CSV data shall be processed. In the example above, you can see that the values for the different fields are separated by commas each. Thus, the "separator" has to be set to "comma" which makes the preview already look slightly better:

Column 1	Column 2	Column 3	Colum...	Column 5	Column 6
Date	Time	Time abs.	Temp.	Amount	Comment
27.04.2007	10:00:00	0 Minutes	25 °C	69,05 g Salicylic Acid	Put salicylic acid into Erlenmeyer flask
28.04.2007	07:30:00	0 Minutes	25 °C	69 ml Aecetic Anhydride	Slowly add aecetic anhydride dropwise
28.04.2007	07:30:00	0 Minutes	25 °C	15 drops Sulfuric Acid	Add 15 drops of sulfuric acid

Still, there is one problem left: The first row contains column headers (titles) instead of real data. You can select the “Treat first CSV line as captions” row for informing the program of this circumstance. After you have done so, the correct result is displayed for this example:

Date	Time	Time abs.	Temp.	Amount	Comment
27.04.2007	10:00:00	0 Minutes	25 °C	69,05 g Salicylic Acid	Put salicylic acid into Erlenmeyer flask
28.04.2007	07:30:00	0 Minutes	25 °C	69 ml Aecetic Anhydride	Slowly add aecetic anhydride dropwise
28.04.2007	07:30:00	0 Minutes	25 °C	15 drops Sulfuric Acid	Add 15 drops of sulfuric acid

Let’s have a look at another example:

Column 1
Date,Time,Time abs.,Temp.,Amount,Comment
27.04.2007,10:00:00,0 Minutes,25 °C,69,05 g Salicylic Acid,A comme, here with a comma

As you already know, the “separator” needs to be set to “comma” here. Furthermore, you have to activate the option for excluding the column headlines from the data. As soon as you have done this, however, the next problem appears:

"Date"	"Time"	"Time abs."	"Temp."	"Amount"	"Comment"	Column 7	Column 8
"27.04.2007"	"10:00:00"	"0 Minutes"	"25 °C"	"69	05 g Salicylic Acid"	"A comme	here with a comma"

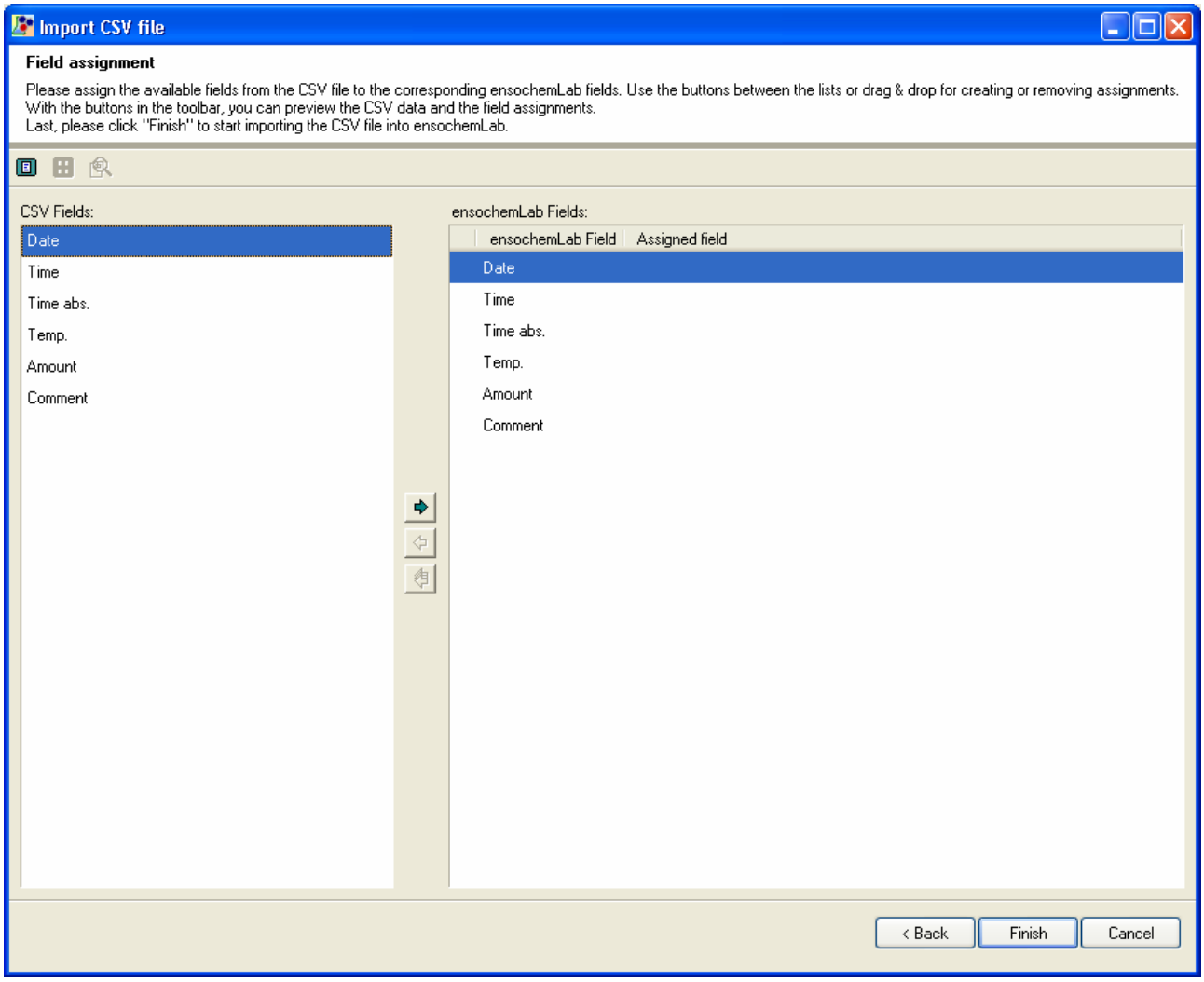
The last two columns contain a text that is normally part of a single cell. But as the text contains a comma and since we have defined the comma to be the column divider, the text is separated into two cells. The solution to this problem can be found by regarding the quotation marks in front of and behind the text as a whole. If we configure them as “delimiters”, the application automatically combines all data between two quotation marks in a single cell:

Date	Time	Time abs.	Temp.	Amount	Comment
27.04.2007	10:00:00	0 Minutes	25 °C	69,05 g Salicylic Acid	A comme, here with a comma

If you have personally exported the CSV file, please just specify the same settings for importing that you have also configured when the export was done. If you do not have this information, you can use the tips above for finding out the correct parameters with only one or two tries in most cases.

After you have correctly configured the import options and verified that the preview pane shows the data correctly, please click on “Next” to proceed in the assistant.

The next page looks like this:



On this page, you have to assign the fields in your CSV file to the correct ensochemLab fields.

The program tries to automatically perform this assignment via the column names. Of course, this method can only work if you have selected the option indicating that the first row in the CSV file contains the column names on the previous page. Otherwise, ensochemLab assigns continuous names following the scheme "Field 1", Field 2" … to the columns without knowing their content.
Another condition for the automatism to function is that the column titles correspond to the ensochemLab field names (those in the application, not in the database itself). This is the case with all data exported with ensochemLab. For self-created CSV files, you can either specify the correct field names or manually perform the assignment on this page.

If you need to see the contents of your CSV file again before you can assign the fields, please click on the "Preview of the CSV File" button ( ) in the toolbar. A separate window containing the same preview grid that you have already seen on the previous assistant page will be opened.

Important: Do not use the import wizard's "Back" button if you just want to see the CSV file preview again. If you do so, all assignments that you have already configured will be lost!

For assigning a field, please select it in the list on the left side. You now have two options: First, you can use drag & drop to move the CSV field over the correct ensochemLab data field in the list on the right side. Alternatively, you can also select the desired target field and then click on the “Assign Field” button (). With both methods, the two assigned fields will then be shown as one row in the table on the right side of the dialog.

For removing an assignment, you can either perform another drag & drop operation for moving the field entry back to the list on the left or you can select the assignment table entry and then click on “Remove assignment of selected ensochemLab field” ().

If you want to remove all field assignments, please click on “Remove all ensochemLab field assignments” ().

The definition of a CSV file allows all fields to contain every kind and every possible representation of data. A field named “Temperature” could thus contain the text “three Degrees”. In ensochemLab however, every field is of a specific type. This means that some fields can only contain numbers while others are limited to date values. This is why the text “three degrees” would lead to an import error when you try to import it into a number field.
You can already see such errors while assigning the data fields without having to run import tests. If one or more records cannot be imported, ensochemLab displays a red X () in the first column of the assignment table. If you move your mouse over such a symbol, a hint window containing the number of records that cannot be imported will be shown. If this number reflects the count of records in your CSV file, the field has probably been assigned incorrectly. Please check your CSV file contents and review the assignments when this happens.

For additional information concerning such a problem, you can use the “Preview of the selected CSV file fields” function (). It displays the preview dialog that you already know, this time, however, only with the field of the currently selected assignment. Cells with import errors are marked with a small symbol in this mode. Thus, the following example shows a date field that has been assigned a temperature in error:

Date
25 °C
25 °C
25 °C

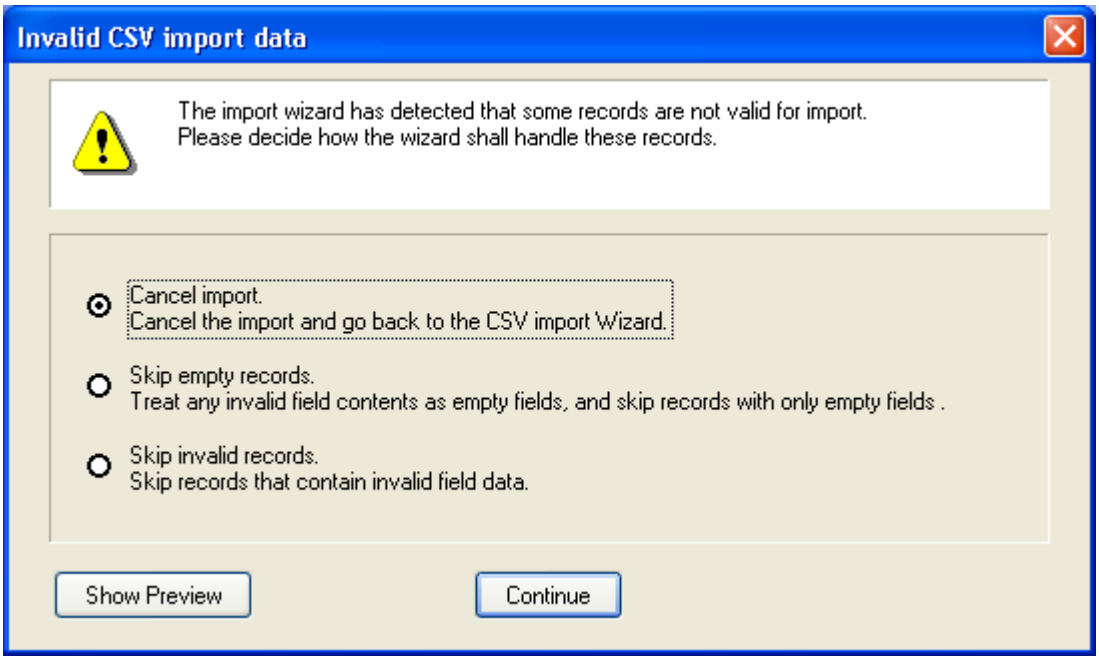
If you want to see all assigned data fields, please click on the “Preview of all assigned fields of the CSV file” button (). The preview dialog appears once again, but does not contain only one column. Instead, all fields of your CSV file that have already been assigned will be visible. Just as in the previously explained mode, all erroneous cells contain the error mark symbol:

Time	Temp.
27.04.2007	25 °C
28.04.2007	25 °C
28.04.2007	25 °C

The exact error message for every single record can be viewed by holding your mouse cursor over the respective error symbol in one of the data views.

An error symbol in the header row indicates that at least one record has an error in the respective column.

If you are satisfied with your assignments, please click on “Finish” for transferring the data into your ensochemLab module. If there are still errors at that time, a dialog will be shown in which you can choose how such records shall be processed:



With the first option in the dialog, you can cancel the import process and return to the import wizard to modify your assignments and then try again.
With the second option, you can have the application skip all erroneous records in your CSV file. These records will then be treated as empty ones and not be imported.
The third option enables you to have ensochemLab skip a whole record if one of its columns contains an error which means that the other cells are not imported either.

At this position, there is also the possibility to show a preview of your CSV file. This mode exactly corresponds to the one containing all assigned ensochemLab data fields.

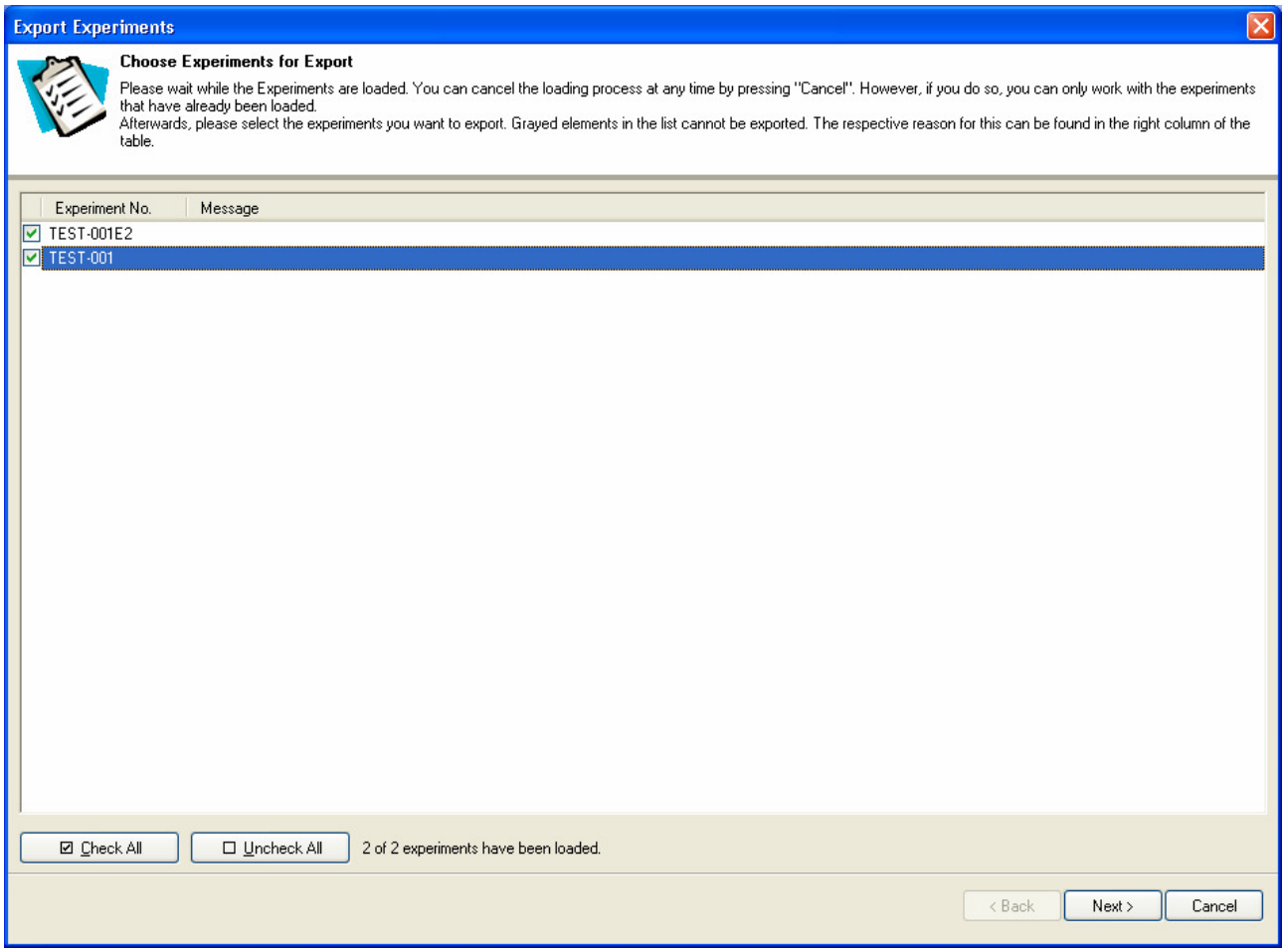
With a click on “Continue”, you confirm your selection and resume the import process.

The import wizard will then be closed and you return to the application module from which you started it. There, you will find the imported data which you can now either directly apply or manually change.

16.3. Exporting experiment data to CSV

With this function, you can export your experiment's reactant and product data into a CSV file. One CSV file can contain only *either* reactant *or* product data, never both at a time. This data can, however, come from an arbitrary number of experiments. The function does not allow exporting other experiment data (like header data).

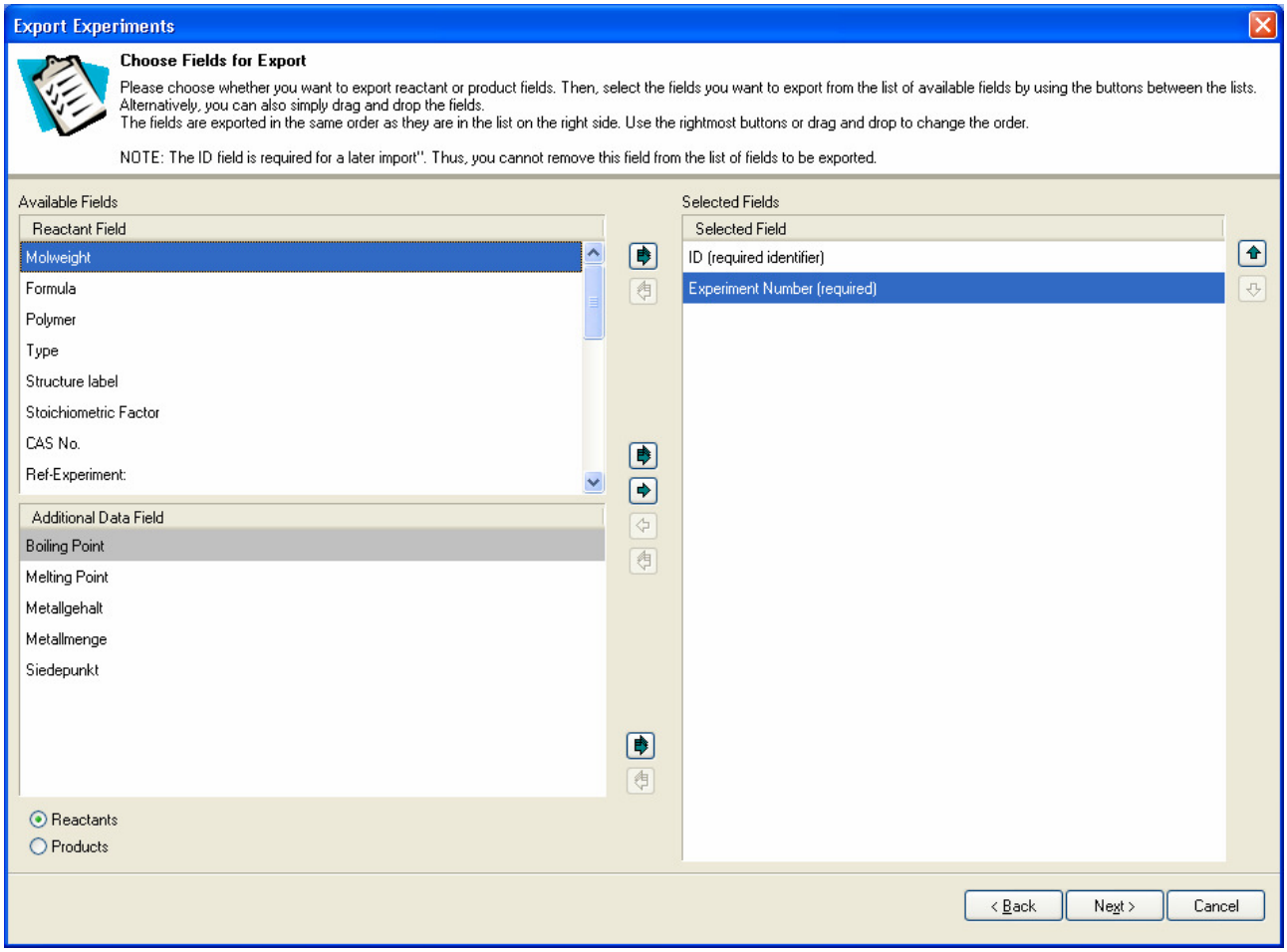
You can start by first selecting the appropriate folder in the main window's navigation pane. Alternatively, you can also just display one of the experiments within it. Afterwards, please click on the "Export Experiments" entry in the "List" menu. The following dialog appears:



In the list, you will find all of the current folder's experiments. Experiments that cannot be exported are displayed in gray and cannot be selected. In such a case, the second table column gives you the corresponding reason.

Please check the experiments that you want to export. With the "Check all" and "Uncheck all" buttons, you can set or remove the marks at all entries in the list.

After you have made your decision, please click on "Next".



On this page, you can select the fields you want to export. Please decide first whether you want to export reactant or product data and choose the appropriate radio button on the left lower side beneath the two lists. You should do this as your first action on this page since if you change your selection afterwards, all already selected export fields will be lost. As already said in the introduction to this chapter, exporting reactant and product data at the same time (that is into the same file) is not possible.

The pictures in this manual show the export of reactant data.

The upper left list shows all data fields of the selected category (reactants or products). Beneath it, you can find all additional data fields defined by the administrator. On the right side, there is the list of fields that shall be exported.
In order to add a data field to the export list, you can either use drag & drop to move it from one of the lists on the left into the list on the right, or you can select it on the left and then click on the “Add selected field” button (). The same command is also available via the context menu.
For removing a field from the export list, there are again multiple possibilities: You can drag it out of the list on the right and let it drop on the left, you can select it and then click on “Remove selected field” () or you can use the context menu after the selection.

For adding all reactant or product data fields, please click on the “Add all reactant fields” / “Add all product fields” button (). The other way round (that is removing the fields) is available via the “Remove all reactant data fields” / “Remove all product data fields” button (). Both functions can be found at the top between the lists on the two sides.

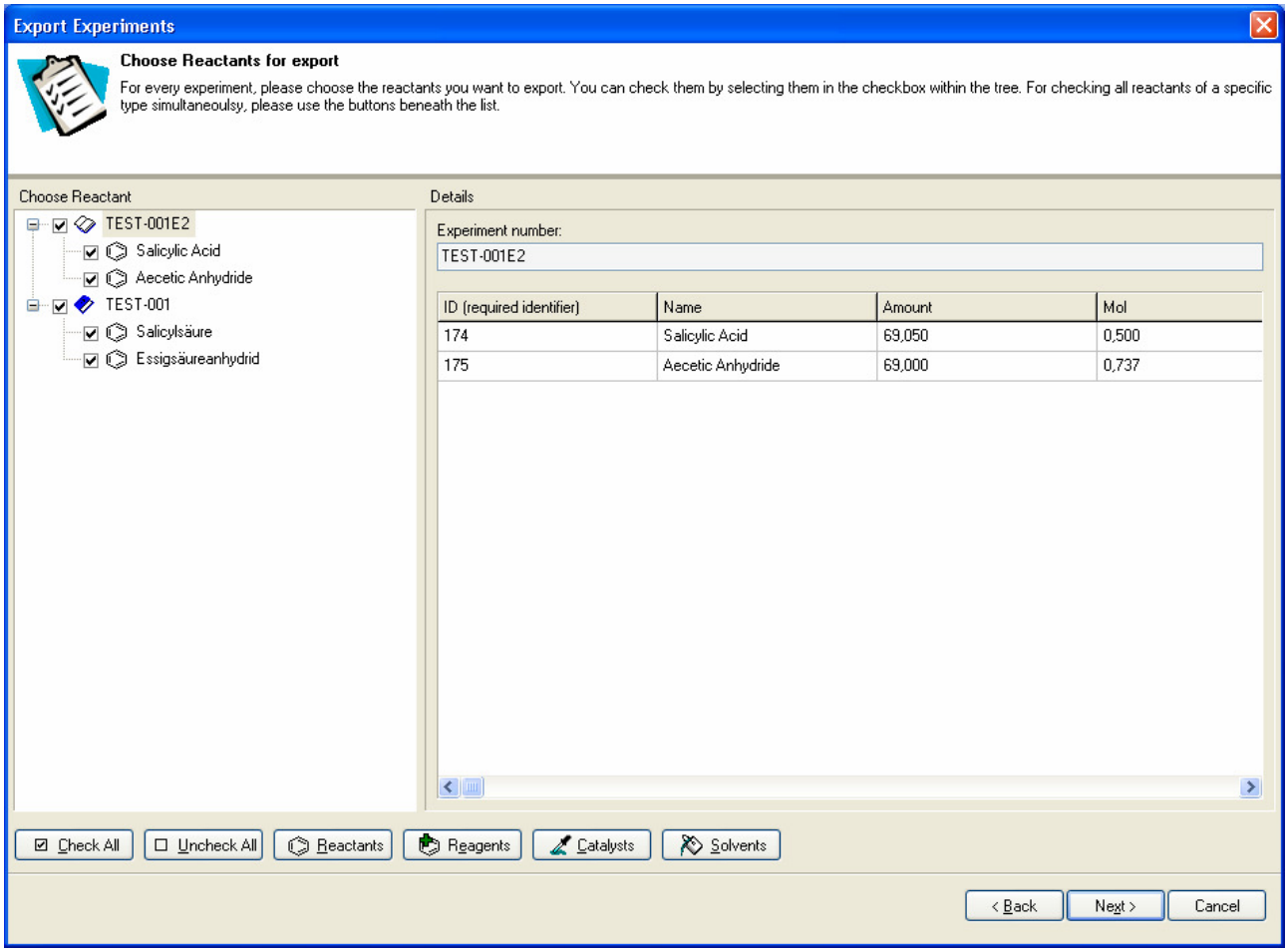
As you can see, buttons with the same symbol are also located in the middle and at the lower end between the lists. The reason for this is that the buttons which are located at the side of the reactant / product field list only apply to these fields. Correspondingly, the buttons beside the list of additional data fields only handle additional data.

If you want to export really all data fields independently of their category, please use the “Add all data fields” or “Remove all data fields” buttons in the middle of the window.

You can also change the order in which the data fields will be present in the later file. This can be done via drag & drop. Just drag a field onto the desired position and let it drop there. Of course, you can also use the “Move up” (⬆) and “Move down” (⬇) buttons at the right side of the list.

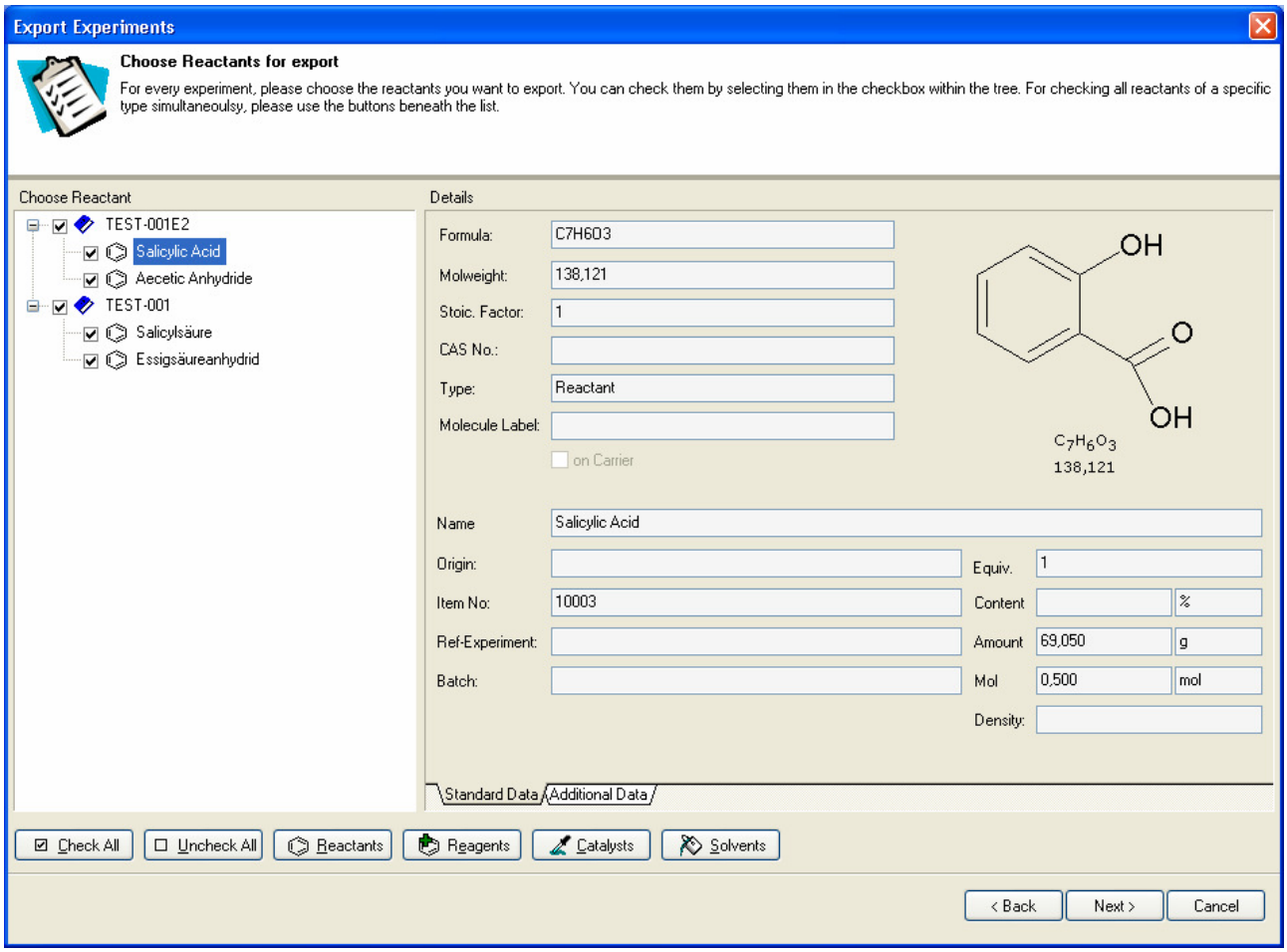
ensochemLab always exports two data fields that you cannot remove either: The “Experiment number” and the “ID”. The latter is a unique identification number representing the respective reactant or product. This data is needed if you want to re-import your data back into ensochemLab after external modification.

With a click on “Next”, you can continue to the wizard’s next page:



On this page, you can choose which reactants or products you want to export. The data is grouped by their corresponding experiment and is displayed in a corresponding structure that you can see in the list on the left side. If you select a whole experiment branch there rather than a single reactant or product, you can see its experiment number and a table containing a preview of your experiment data in the preview pane on the right side. The table contains the data fields that you have specified along with the mandatory “ID” field required by ensochemLab.

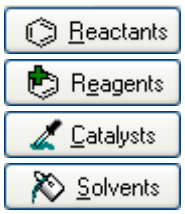
If you select a reactant or a product, you can see a preview of all data contained in the respective record in a display mode that much resembles the experiment wizard. Just as there, you can use the tab control to switch between standard and additional data. This preview is for information purposes only and is intended to simplify your decision on which records you want to export. This is why there is nop possibility of changing individual data.



If you want to export just single reactants or products, please select them in the list by setting their respective check marks. If you check an experiment, all its reactants or products are checked. Deselecting an experiment automatically deselects all its child elements.

In order to select all entries, please click on “Check all”. With a click on “Uncheck all”, you can remove the selection marks from all records.
Additionally, ensochemLab offers you a couple of functions for selecting just the items of a specific type:

Reactants



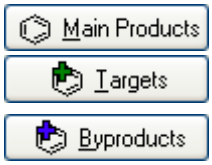
Selects all normal reactants

Selects all reactants that have been marked as reagents

Selects all reactants that have been marked as catalysts

Selects all reactants that have been marked as solvents

Products

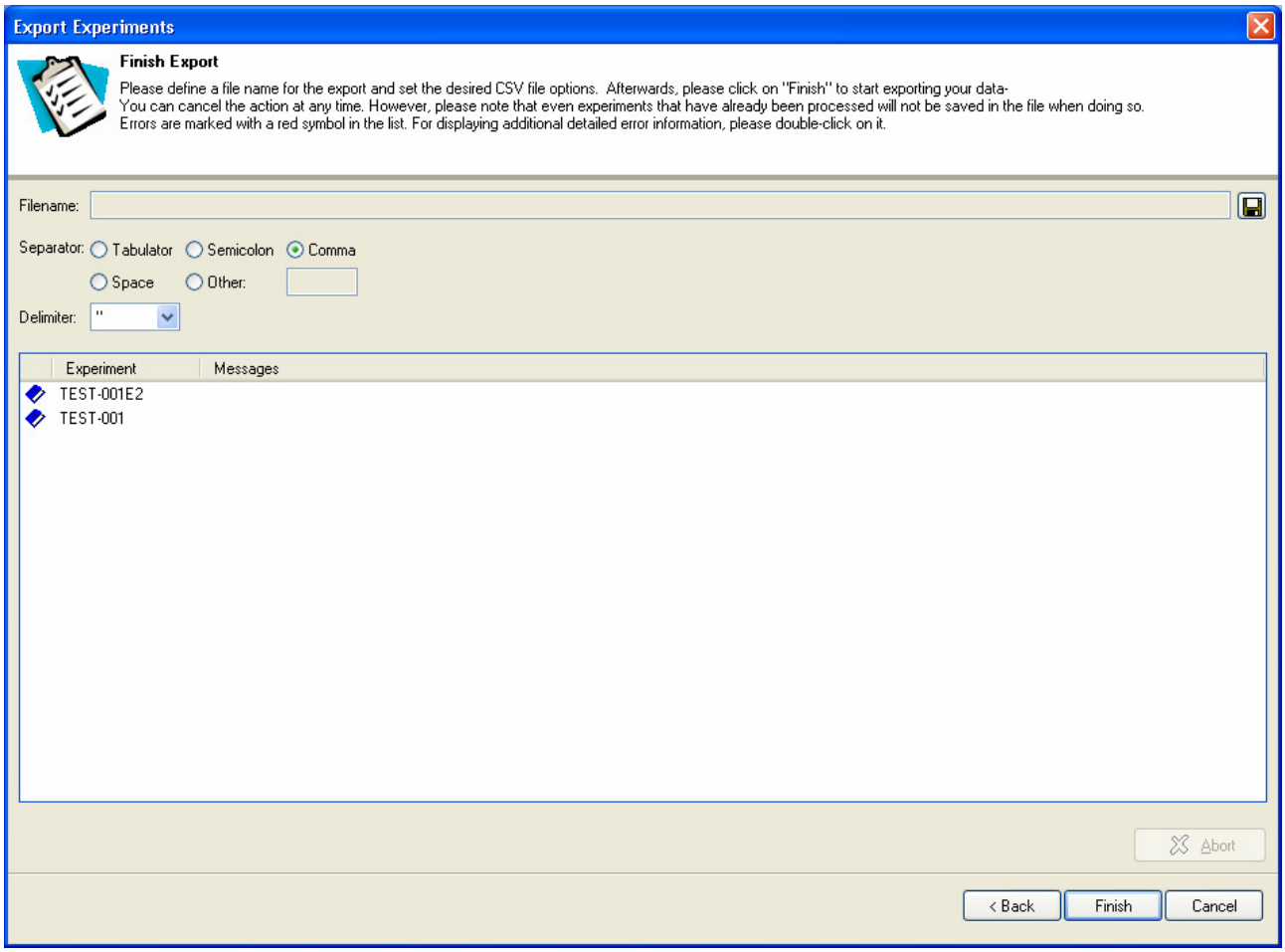


Selects all main products

Selects all products marked as targets

Selects all byproducts

After you have selected the items you want to export, please click on “Next”.



On this last page of the export assistant, you can specify the name and path of the file into which you want to export your data by clicking on “Choose file name” ( ). A normal “save as” dialog will appear that you already know from a host of other Windows applications.

Additionally, you can configure some options for your CSV file. The possibilities and impacts have already been thoroughly discussed in a previous chapter about the export of tabular data.

Finally, please click on “Finish” to start exporting your reactants or products and creating the file. You can abort this process at any time by clicking on the “Abort” button. However, please note that this will cancel the operation as a whole which means that no file will be created and even the data that has already been processed will not be exported.

During the import, the list of experiments displays the current status. If the export of data belonging to an experiment has failed, the respective reason(s) or error message(s) can be found in the “Messages” column.

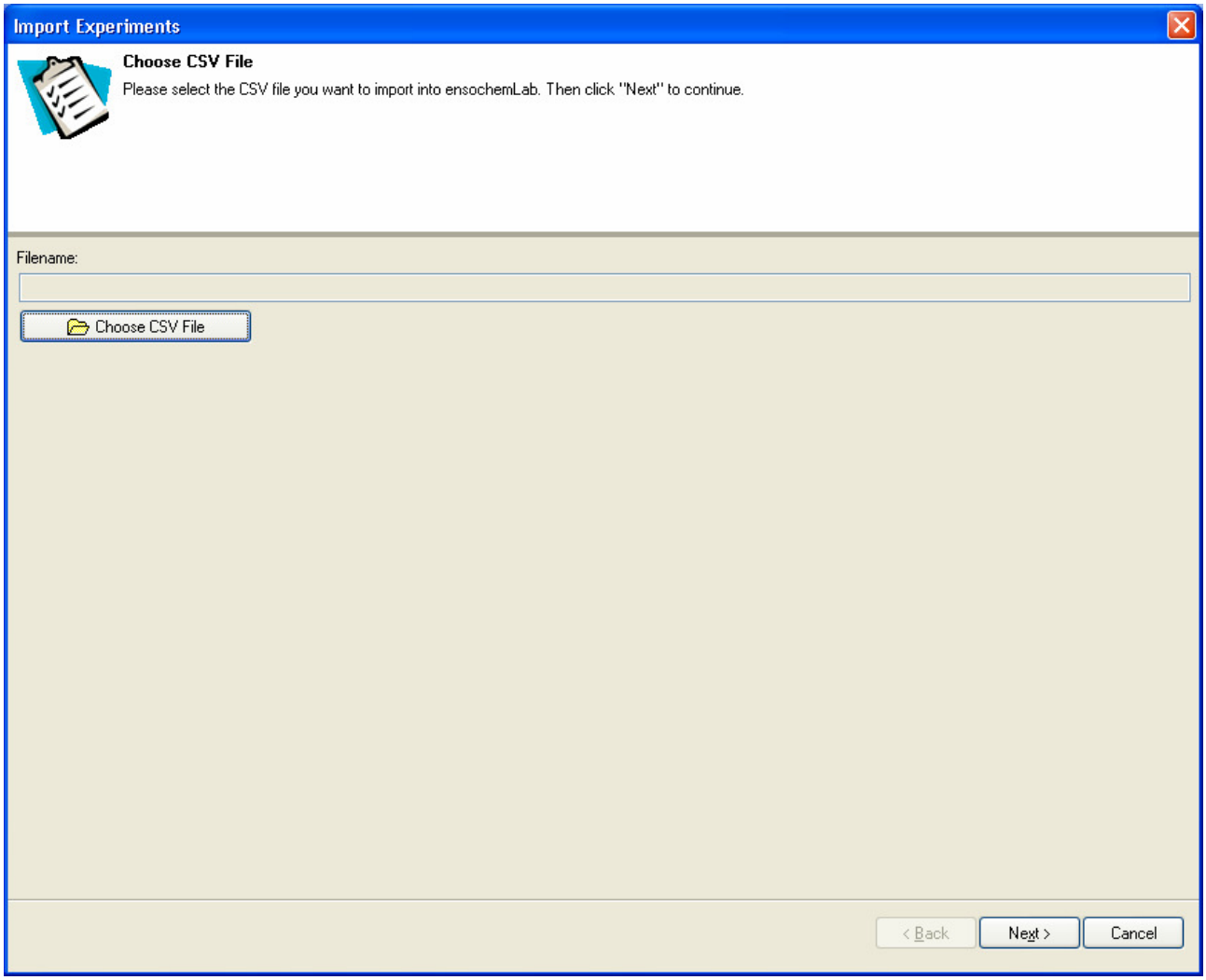
After the process has finished and you have reviewed the result table, please click on “Close” in order to return to the ensochemLab main window.

16.4. Importing experiment data from CSV

The CSV file import function built into ensochemLab mainly serves as a means of re-importing data that has been exported by the software and then modified in an external application back into the database. Please note that the “Experiment number” and “ID” fields may not be lost during editing. There is support of reconstructing them or manually assigning the data.
When creating records fully externally, you have to fill both columns with valid values.

This feature has not been designed to create new experiments. It can only import data into existing experiments and their reactants or products. During the process, the imported data always replaces the existing records in your database without further confirmation. This is why you should always make sure that you are importing the correct data. Restoring the previous data is only possible with optionally purchasable versioning module.

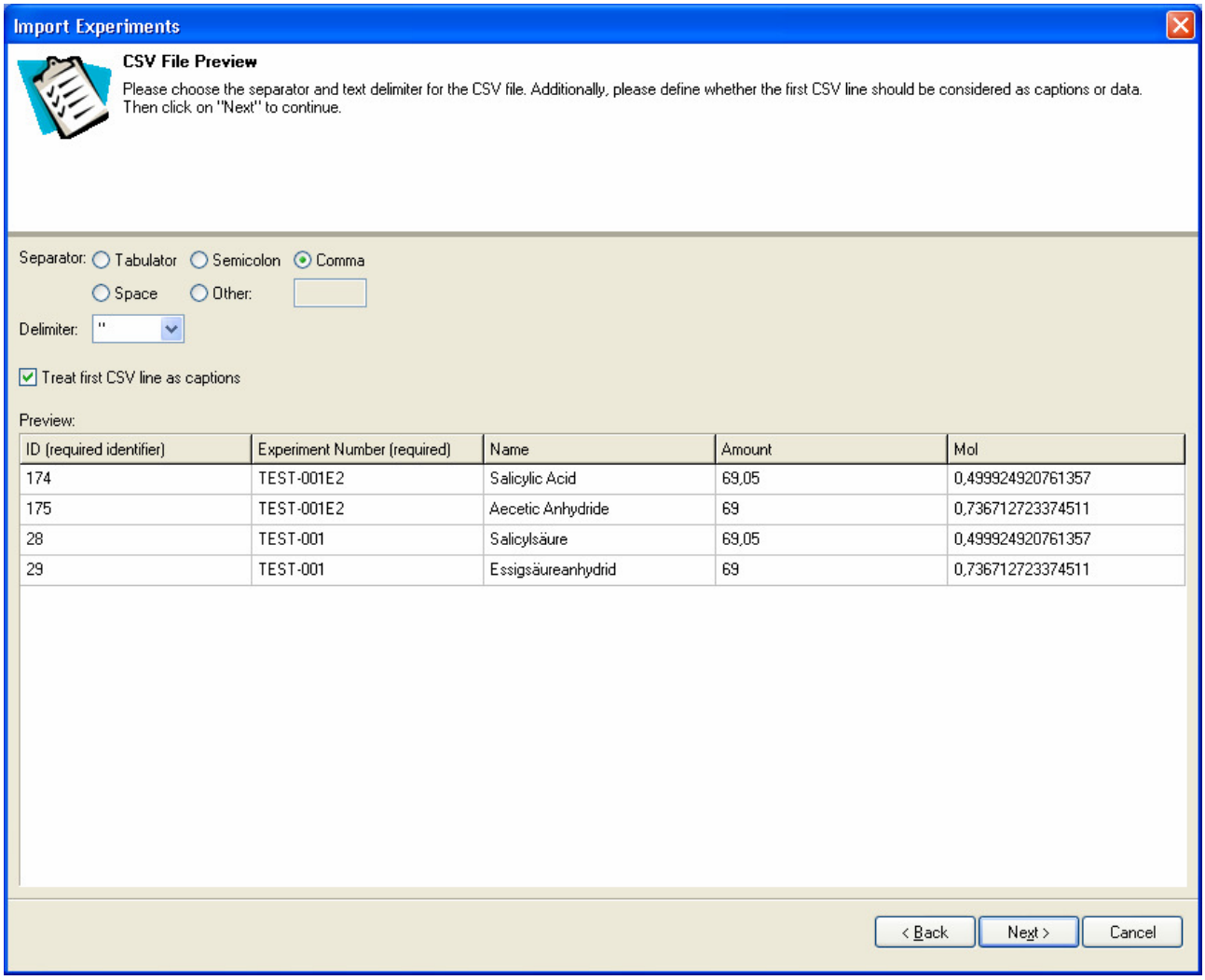
For starting the import assistant, please click on “Import experiments” in the “List” menu of the application’s main window. The current selection in your navigator has no impact here. The following dialog will appear:



As a first step, you have to select the CSV file you want to import. Please click on the “Choose CSV file” button () for launching a normal “file open” dialog that you already know from many other common Windows applications. As an alternative, you can also drag a file from the Windows Explorer and drop it on the window.

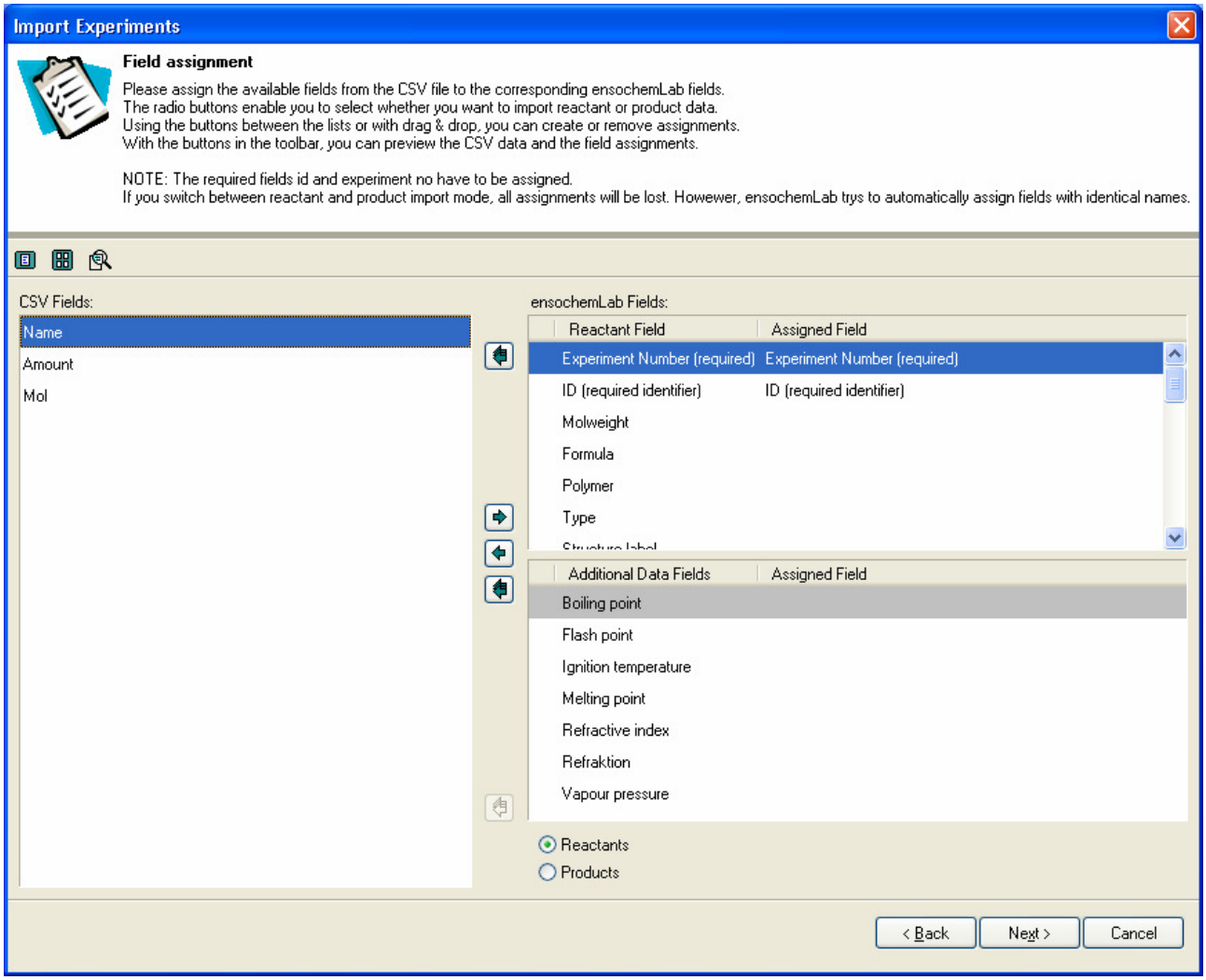
After you have selected your CSV file, it will be shown with its full path and file name in the “File name” field. Please click on ”Next” to proceed to the next import wizard page.

On the now following page, you can configure your CSV file’s formatting options. Just as explained in a previous chapter about importing tabular data from CSV files, the application provides you a preview table where you can see the impacts of the available CSV file options on the processing and detection of the content.
If you have exported the file via ensochemLab, you should use exactly the same options that you have also used with the export function. General recommendations and tricks on finding the correct options with third-party provided or otherwise unknown files are described in the already mentioned previous chapter in this manual.



You can basically check your import options with the “ID” field. This field has to contain a valid, positive integer value for all records. It may not be empty with any record. If there are errors, you should check your CSV file options.

If you are satisfied with the data preview, please click on “Next” to proceed.



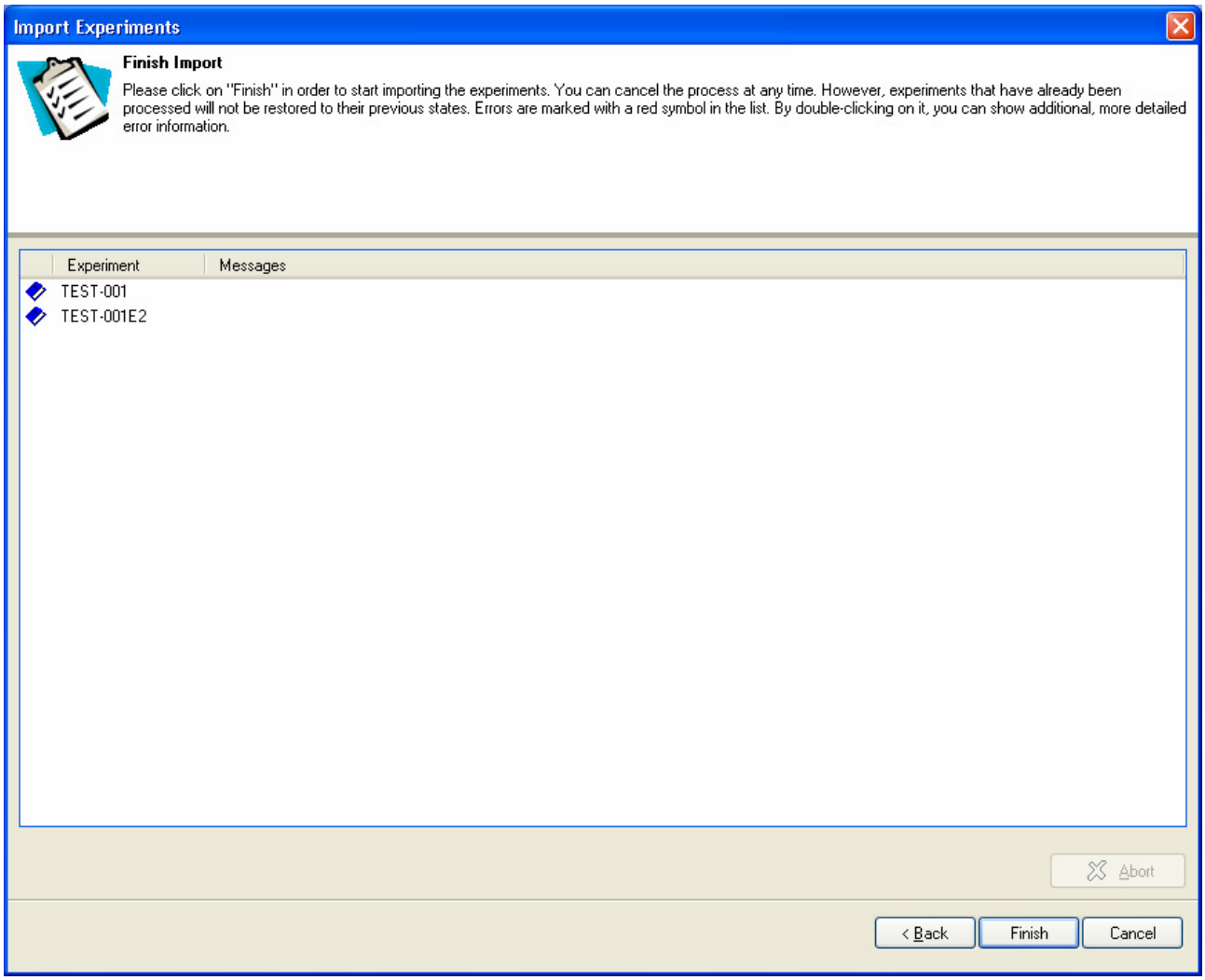
On this page, you can assign the fields in your CSV file to the ensochemLab data fields. However, please note that you should first select whether you want to import reactant or product data. If you change this selection later, all field assignments that you have already made will be lost.

In its main principle, this assignment page works just like the one described in the previous chapter about importing tabular data. The only difference is that, on this page, there are not only the normal data fields, but also the additional ones defined by the administrator. Still, for them too, the assignment of import fields works as just usual.
In comparison to the familiar field assignment tool, you will find a couple more buttons for the removal of field assignments (): The button at the very top (beside the list of standard fields) removes all standard data fields; the one at the bottom (beside the list of additional data fields) deletes all additional fields. With the “Remove” button the middle of the window, you can remove all assignments independently of their category.

In this module, ensochemLab also tries to automatically assign known fields via their name. Manual assignments are only necessary if the field names do not correspond to the field identifiers used in ensochemLab.

The “Experiment number” and “ID” field always have to be assigned as they are necessary for distinctly identifying the single records in the database. Additionally, you have to assign at least one field containing “real” (that is to say user-defined) data.

After you have assigned all necessary fields, please click on “Next” to continue:



This is the import assistant’s last page. Here you can see a list of all the experiments for which you are about to import data. The image in the table’s first column identifies the respective record’s current state (not started yet, in process, finished, failed). If the import of a record belonging to an experiment fails, you can see the respective error message(s) in the third column.

For starting the import process, please click on “Finish”. ensochemLab now processes all experiments in the list one after another. You can stop the import at any time by clicking on the “Abort” button. However, please note that already processed experiments will not be restored.

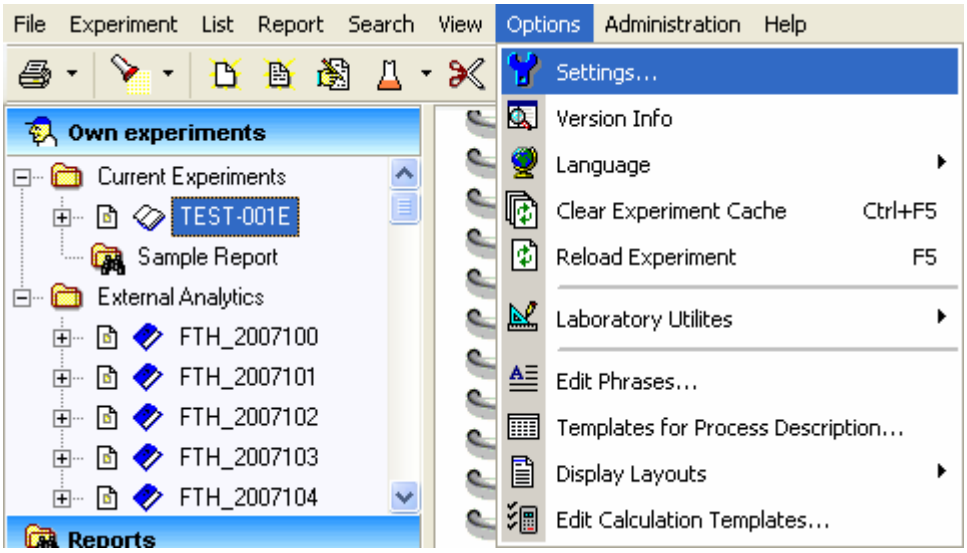
After the whole process has been finished and you have reviewed the result table, please click on “Cancel” in order to return to the application’s main window.

Summary:	ensochemLab enables you to import the contents of a CSV file in all modules

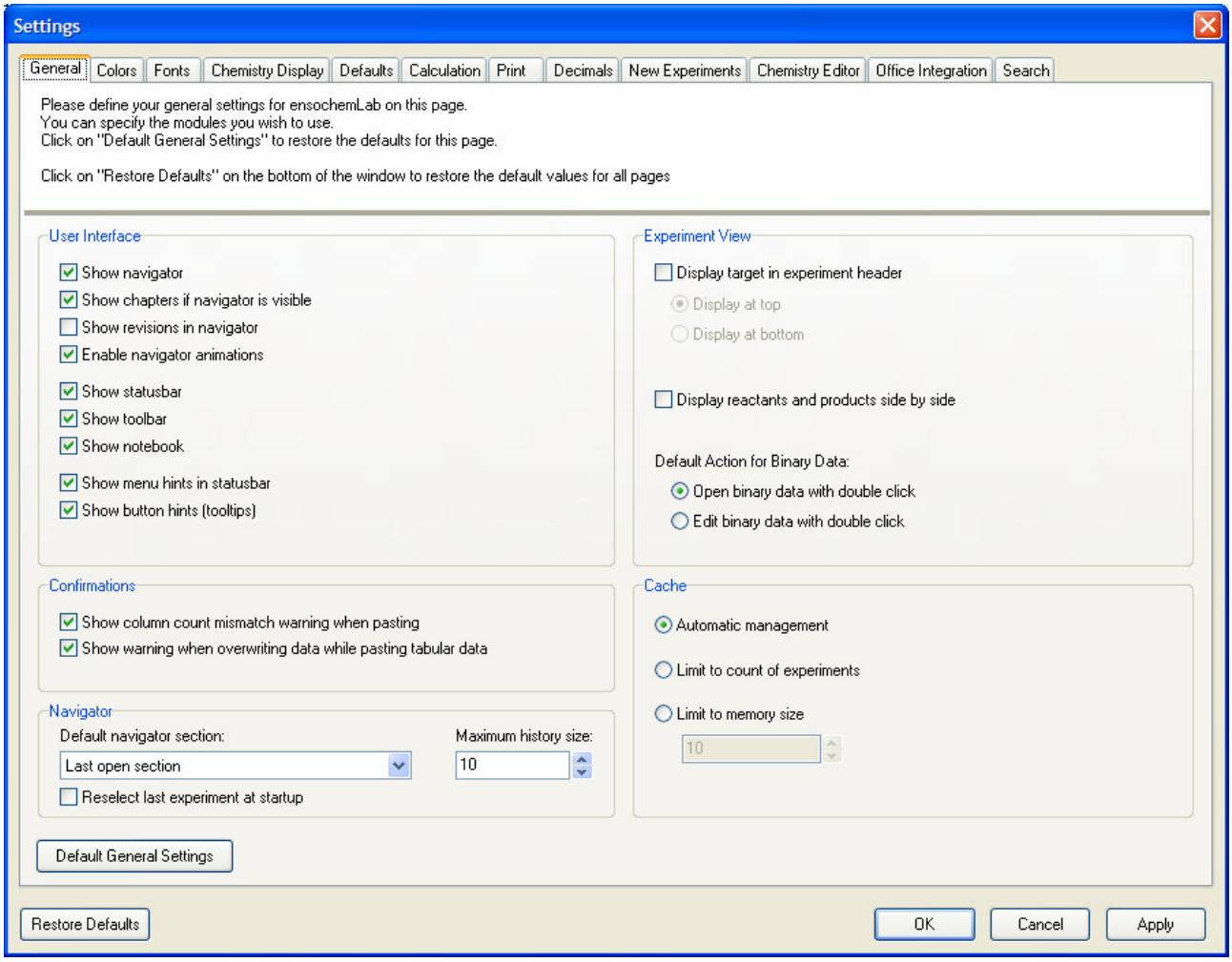
	where you can work with tabular content. A comfortable wizard guides you through the necessary steps. With the various preview options, you can try out the different import options before actually importing your data. Additionally, you can also exchange reactant and product data with other applications using the CSV file format.

17. Customize your settings

Until now, you have used ensochemLab with the default settings. These settings are appropriate for most users and work areas. However, every user can customize the software according to his personal regards. The settings that he defines are for his account only. This means that he cannot affect the accounts of other users.
To do so click on the “Options” entry in the main menu and then on “Settings”:



The settings dialog will appear:



This chapter will introduce all the settings that are available on the several pages.
If you are not sure what a function does, just try it! With the “Default … settings” buttons on the bottom of the page, you can go back to the default settings at any time. If you want to restore all settings on all pages, then click on the “Restore defaults” button in the lower left corner of the window.

With the “Apply” button, you can save your new settings without leaving the dialog. This can, for example, be extremely useful when setting display properties like colors as the changes are applied to the main window right at once. However, please note that you cannot undo your changes with the “Cancel” button anymore after you have clicked on “Apply”.

17.1. General

This page is used to set general layout parameters for ensochemLab.

User Interface:

Show navigator	Indicates whether the navigation bar shall be visible in the application’s main window.
Show chapters if navigator is visible	Indicates whether the chapter selection pane beneath the navigator shall be visible. If the navigator is invisible, the chapter selection

	pane is also automatically removed.
Show revisions in navigator	Indicates whether the different revisions of an experiment shall be displayed as sub-entries to the respective experiment nodes in the navigator.
Enable navigator animations	Indicates whether the navigator chapters shall smoothly move into their new positions when the current chapter is changed. When dealing with slow systems or terminal servers, we recommend disabling this option.
Show status bar	Indicates whether the status bar shall be visible in the application's main window.
Show toolbar	Indicates whether the toolbar in the application's main window shall be visible.
Show notebook	Indicates whether a notebook graphic shall be displayed left to the experiment data in the default display mode.
Show menu hints in status bar	Indicates whether additional information about the current menu item shall be displayed in the status bar.
Show button hints (tool tips)	Indicates whether description windows (tool tips) containing short explanations shall be shown for the functions in the toolbars.

Confirmations:

Show column count mismatch warning when pasting	Indicates whether a warning shall be displayed when a table with a different column count than the one defined in the application is pasted (for example as a process description).
Show warning when overwriting data while pasting tabular data	Indicates whether a warning message shall be displayed when you insert tabular data from the clipboard and thereby override existing data.

Navigator:

Default navigator section	Specifies the default navigator section that will be expanded after login.
Reselect last experiment at startup	If this option is checked the last selected experiment will be automatically reselected when ensochemLab is started and the appropriate experiment data will be shown.
Maximum history size	Indicates the number of experiments that are saved in the "History" folder until the oldest of them is automatically overridden.

Experiment View:

Display target in experiment header	Indicates whether the name of the target molecule shall be displayed along with an experiment's header data. You can choose it to be displayed either above or below the other header items.
Display reactants and products side by side	If this option is checked, the reactant and product tables in the experiment display are shown side by side, otherwise they are shown beneath each other. (see chapter "The main window").
Default action for binary data	Indicates which operation is to be executed by default when you double-click on a binary record in the experiment display.

Cache:

Automatic management	With this option, ensochemLab automatically defines the experiment cache settings. This is the recommended configuration.
Limit to count of experiments	With this option, you can define the maximum number of experiments. If this number is reached and a new experiment is loaded, the oldest entry is removed from the cache.

Limit to memory size	With this option, you can define the maximum memory size of the experiment cache. If this size is reached and a new experiment is loaded, the oldest entry is removed from the cache.

17.2. Colors

On this page, you can choose the colors that ensochemLab should use in the experiment display and when printing. To change a color, just click on the arrow beside it and select a new one from the list.
If your system supports more than 256, you can use gradients. ensochemLab will then use the colors you define on this page as start colors and makes them slowly lighter until the end value oft the specific color scheme is reached.

17.3. Fonts

To change a font, please click on the button beside the preview box. A dialog will appear where you can select the desired font. The sample text boxes also use the colors you have chosen for the corresponding items on the “Colors” page. Thus, you can use it as a nearly complete preview for the resulting design.

Hyperlinks:

With this option you can decide how "Link Fields" are to be displayed within ensochemLab. The setup is valid for references in analytic, literature or the additional data of type Link specified by your Administrator.

17.4. Chemistry Display

On this page, you can define how reactions and molecules are to be displayed in ensochemLab. These settings are applied for all application modules (experiment wizard, display, print preview …).

Highlighting Reactants and Products:

With this option, you can mark certain types of reactants and products so that they become obvious at the first view. If another option than “None” (no highlighting) is selected, you can choose a different color for every available type. ensochemLab offers the following highlighting modes:

None	Reactants and products are not highlighted in any way.
Colored structure	The structure is drawn with the configured color.
Colored frame	A colored rectangle is drawn around the respective structure.
Colored background	The respective structure’s background is filled with the selected color.

Highlighting Targets:

Separate to the reactants and “normal” products”, you can also configure the same set of highlighting options for target molecules. This enables you, for example, to only frame reagents and catalysts, but fill the background of target molecules.

With the “Use highlight settings while printing” option, you can choose whether to also include the configured highlighting options in experiment printouts.

Chemistry:

The “Show molecule position symbol” option indicates whether a continuous position indicator (A, B, C …) is to be shown under the single molecules within a reaction.

Show formula and molweight” not only refers to single structures, but also to whole reactions where these values are displayed for every single contained molecule under the respective structure.

The hydrogen display options have already been fully discussed in the “Create your first experiment” chapter.

Additionally, you can choose whether and how reacting centers should be displayed. ensochemLab offers the following possibilities:

No display	The reacting centers are not displayed at all
Color	The reacting centers are displayed in color
Hash	The reacting centers are displayed as dashed bonds

ensochemLab can also display atom mapping. In order to activate it, just select the appropriate checkbox!

With “Show reaction labels”, you can define if you want to include the texts above / below the reaction arrow that are defined in the experiment data in the normal view mode.

“Show molecule labels” is the same option for molecules and refers to the description texts saved along with reactants and products. They are only displayed below the molecule in normal display mode if this option is selected.

The “Reaction view options” block can be used to show / hide solvents, catalysts, reagents and byproducts in the experiment display within the main window. Deselect the checkboxes to hide these parts of the reaction in order to increase the clarity when dealing with huge reactions, for example.

17.5. Defaults

On the defaults page, you can configure some default values for the application.

Experiment Wizard Pages:

If you want to work in another order when creating new experiments, you can change the sheet order on this page. Just select the page you want to move and then click on the arrow buttons ( ) at the right side of the list to specify the direction. Pages higher in the list are displayed earlier.
Please note that this does not affect the order of the data blocks in the main window.

Experiment Wizard Settings:

In this section, there are the following options you can configure:

Use equivalents	Indicates whether the assistant shall automatically activate the equivalent fields for calculations.
Analytic results as text	Indicates whether you prefer entering your analytic results as text. If the box in not checked, the default is numeric.
Check calculation of reactants and products	Specifies whether ensochemLab shall check the values you have entered for the reactants and products before saving the experiment. When doing so, it uses the results of the automatic calculation functions as a comparison basis. If not all values are equal to the automatically calculates ones, it will show a warning. The check is done whenever you try to save an experiment, no

	matter if it new or just modified. Additionally, an extra check is done when leaving the reactants and products page in the wizard.
Check calculation result ranges	Specifies whether the range of (automatic) calculation results shall be checked according to a set of fixed criteria. If the calculation has resulted in values which are too large, a warning will be displayed.

Viewing Binary Data:

In this section, you can configure the way binary data is displayed within an experiment. ensochemLab offers the following options:

Thumbnails only	Only displays a preview image of the configured size.
Thumbnails and names	Displays the preview image along with the respective file name.
Icons and names	Displays a small icon representing the file type along with respective file name.

Please note that displaying a preview image is only possible for certain binary file types supported by ensochemLab.

Additionally, you can define how large the preview pictures in the experiment display shall be. The size is defined in pixels. Possibly are all integer values between 16 and 128.

For the file names, you can define whether the names are allowed to break into the next row if they are too long to be wholly displayed. Otherwise, they are truncated with three dots at the end (Example: “A very long file na…”).

Loading Binary Data:

Binary attachments can either always be downloaded or only on request or on request if they are larger than a certain value. In most cases, this depends on your connection to the ensochemLab server. If you are linked to the server over a slow or dialup connection, you should download binary files larger than a certain size only if you really need them. For this configuration, please select the appropriate option and then enter the maximal size.

Never download binary files	All binary files have to be manually loaded from the server.
Always download binary files	All binary files are always automatically downloaded from the server regardless of their size.
Download binary files up to a size of	Binary files are only automatically downloaded if they are smaller than a configured size. Larger files have to be loaded manually.

Fraction Dialog:

This section is used for defining the fraction editor that is to be launched by default. The default editor is used when you click on the “Edit Fractions” symbol in the main window’s toolbar without explicitly specifying an editor from the drop-down menu.

17.6. Calculation

On this page, you can change a number of settings concerning automatic and manual calculations of reactants and products. At the very top, you can use the two checkboxes to decide whether calculations should be automatically performed whenever possible. If you do not enable them, you can still manually calculate by clicking on the calculator symbols in the experiment wizard.
This rest of the page deals with how calculations shall be done. You can set which values should be adapted when others are changed. To modify a setting, just click the respective link and select another option from the context menu that appears. Then, the text instantly changes to reflect the new setting.

All calculation options and their respective meanings are explained in a separate chapter: “Automatic Calculations”.

17.7. Print

The settings on this page depend on the technical data of your printer and the paper you want to print on.

Page Margins (mm):

In this area, you can configure page margins that should be left empty when printing data from ensochemLab. Please make sure to set the correct values for the paper you use. Borders and header bars with company logos have to be excluded with the page margins function as well as areas in which your printer does not support printing.

Footer Section:

Here you can configure whether a footer bar shall be printed. If the option is enabled, the following possibilities are available:

Print signature field on every page	Signature fields are printed in the footer of every page of your experiment.
Print signature field only on last page	A footer bar containing signature fields is only printed on the last page of your experiment.
Do not print signature field	No signature fields are printed at all.

Overview List Printing:

Here you can choose how many experiments should be visible on a physical page of a folder overview list. When dealing with a default installation, ensochemLab prints the experiment number, the reaction and some other header data for every experiment in the list.
If you increase the number of experiments per page, the reaction is drawn smaller in order to free up more space.

The additional list printing options are:

Print list overview as cover sheet	Specifies whether a list overview page shall be printed as a cover sheet when printing experiment lists.
Print invalid experiment notice	Specifies whether a notice page shall be printed for every invalid experiment contained in an experiment list that is printed. If this options is not selected, such experiments will be ignored without further notice.

Print Layout:

In case you want to use a special print layout, this is where you can make a selection:

Layout	List of all layouts available. The one selected will be preset in dialog "Page Setup".
Use active layout	With this choice the standard print out won't show the "Page Setup" dialog.

Printing of Colors and Binaires:

If your printer is a color printer, you can choose whether you want to print in color or not. To do so, please select the checkbox “Enable printing of colors”. If you are using a monochrome printer, all colors will be rendered to grey scales. This can affect the quality of your printout very negatively, so you should not use color printouts in this case.

Additionally, you can select for every kind of binary data whether the respective records shall be printed or not.

With the “Automatically rotate PDF pages” option, you can define how PDF documents attached to experiments shall be printed. Automatic rotation is a feature for documents that contain pages in a different orientation than the one of the experiment printing process. For example, if you print your experiment in portrait mode and it contains a PDF file with pages in landscape mode, this feature can be useful. It automatically rotates such pages by 90° for best fit on the page and thus minimizes the necessity for downscaling with can lead to measurable quality loss. Your experiment contents are of course never changed.

17.8. Decimals

Here you can enter how much decimals ensochemLab should display. You can enter a value in the range of 0 to 8 for every supported category.

17.9. New Experiments

This page is only available if you have the rights to create experiments.

These settings are applied to the assistant when creating new experiments. In the fields “Department, “Project” and “Laboratory”, you can only select entries from a list predefined by the administrator. A free text entry is not possible for these fields.

Using the field “Experiment number starts with”, you can enter a prefix for your experiment numbers. When opening the assistant in order to create a new experiment, ensochemLab automatically inserts this prefix into the “Experiment” number box, so that you only have to enter a unique suffix instead of typing the whole string again.

You can also customize the default visibility for new experiment. The value you select here will be the already selected default when creating new experiments. This data field is only available if your company has enabled ensochemLab’s integrated default user administration module.

Depending on the settings configured by your administrator, you may not be able to change the values of some of these fields. In such a case, the respective fields are marked with a gray background. If you are not allowed to change any of these values, the whole page is hidden.

17.10. Chemistry Editor

On this page, you can choose which chemistry editor you want to use for entering chemical structures and reactions.

Please note that only ensochemEditor is included with ensochemLab. All other editors have to retrieved, licensed and installed separately. Additional license and installation information can be found in the respective editor's manual.

If you select an editor that is not available on all computers that you use for ensochemLab, a corresponding notification message will be displayed when you log in whenever such a problem is detected. The software then automatically switches to ensochemEditor Web Edition as the default editor.

17.11. Office Integration

This page is used to configure how ensochemLab should interact with certain Microsoft Office Products. If the features are enabled, you can create Word documents and Excel spreadsheets directly when entering your experiment description. These items can be viewed and printed as parts of your experiments. Modifications are also directly possible. (See chapter "Create your first experiment").

Displaying these documents as thumbnails can reduce performance when viewing experiments. If performance is unbearably slow, you can disable the feature.

You can also choose how you want the application to print your data. If you use the operating system for printing, the documents are not included into the page counting and layout.

The layout options define the size and location of Office documents on printed pages.

17.12. Search

On this page, you can select your default search mode. The default search is always started when you click on the search button in the main window's toolbar without explicitly selecting a search mode from the drop down menu.

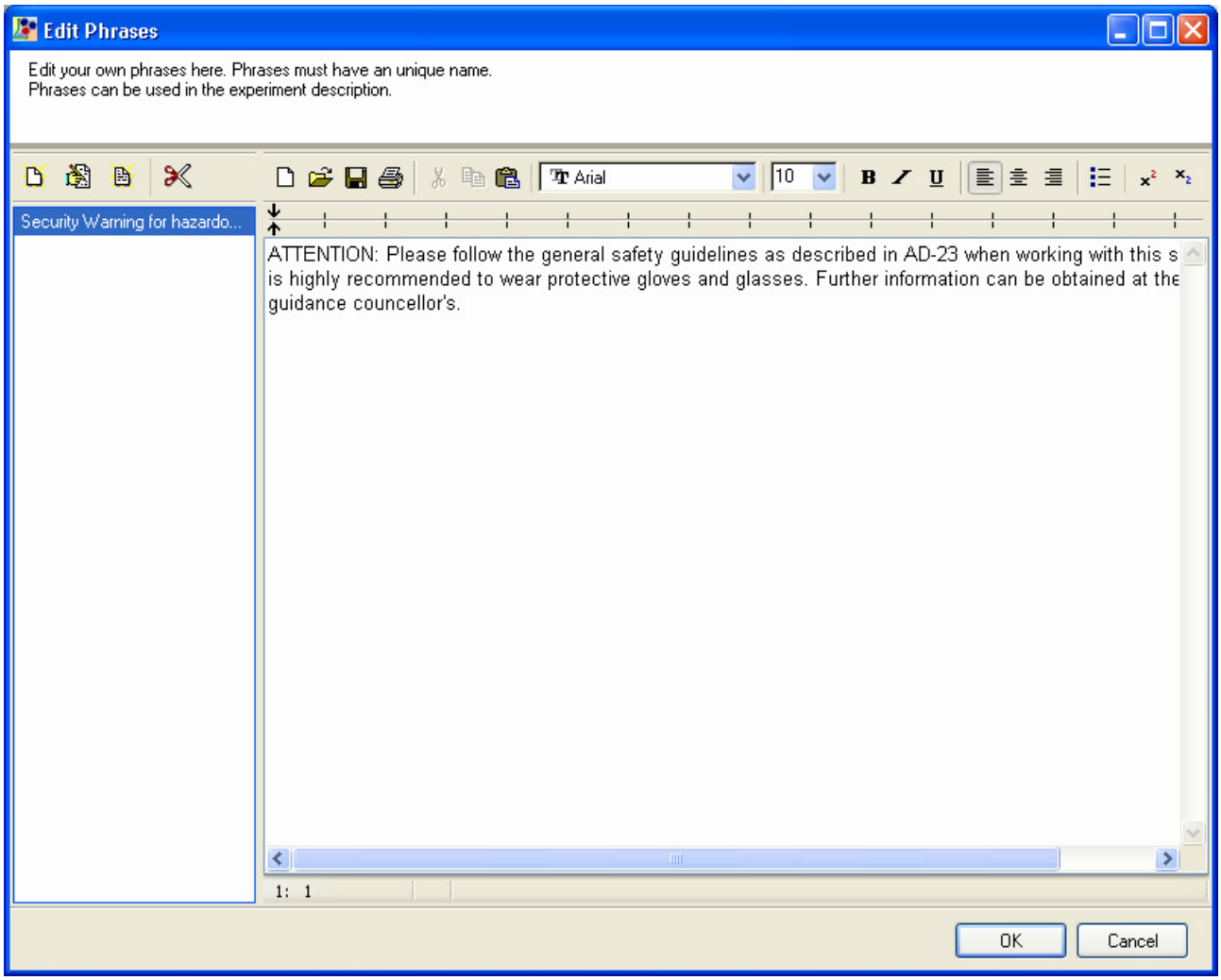
Furthermore you can specify if the default sort order for search results is ascending or descending.

Click on "OK" to save your settings or choose "Cancel" to abandon all changes. The "Apply" button activates the new settings without closing the dialog.

Summary:	The settings dialog can be used to customize your personal settings for ensochemLab. It includes colors, fonts, default values and other useful options.

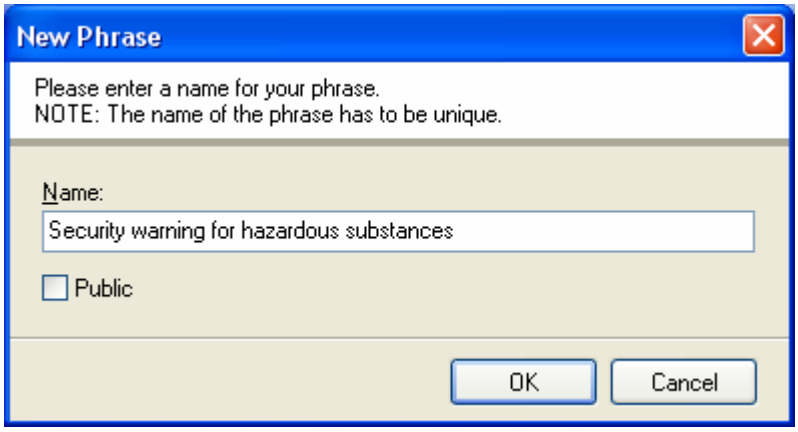
18. User defined phrases

In the “Create your first experiment” chapter, there was already a hint that you cannot only use phrases predefined by your administrator for all users, but that you can also create your own, personal ones. In order to do so, please open the respective management dialog which can be found in the main menu at “Options” / “Edit Phrases”: The following dialog will appear:



In the list on the left side, you can see the phrases that you have already created. If you have just started your work with ensochemLab, it is presumably empty.

In order to create a new phrase, please click on the “New Phrase” button () in the toolbar. ensochemLab will now prompt your for a name for your new phrase. If your administrator has enabled the respective function, you can also mark your phrase as public which will make it available to all ensochemLab users. Please note that the name has to be unique in such a case. However, there are no further restrictions concerning usable characters or others.



After you have clicked on “OK” the new phrase will be added to the list on the left side of the dialog. On the right side, you find a text field where you can enter the text for your new phrase. All phrases must contain text, empty ones cannot be saved to the database.

Just like with the experiment description, ensochemLab offers you a rich variety of formatting options for your phrase text. Besides, you can also import files in the RTF or TXT format from your local hard disk.

You do not have to explicitly save changes to single phrases. Just do your changes and when you are finished, click on “OK”. All changes will then be stored in the database at a time.

If you want to change an existing phrase, just select it in the list and then edit its text on the right side.

It is also possible to rename a phrase. For doing so, please select it and click on the “Edit Phrase” button () in the toolbar. The naming window that you already know by now will appear and let you change the current name.

Deleting the currently selected phrase is likewise easy: Just click on the “Delete Phrase” button ().

If you need a phrase that just slightly differs from an existing one, if you just have to change a single word or have to add a remark, you don’t have to type it all again. Instead, ensochemLab allows your to copy the respective record with its “Copy Phrase” button (). After you have clicked it, you are prompted to enter a name for the new phrase which will then be initialized with the text from the old one.

In order to save your changes, just click on the “OK” button. With a click on “Cancel”, you return to ensochemLab without saving anything.

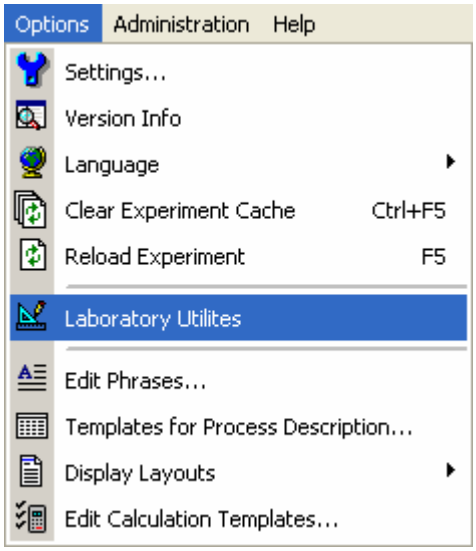
Summary:	With the phrases feature, you can save certain often used text phrases under a short name so that you can later insert them into experiment description data for example with just a few clicks and without having to enter them again every time.

19. Laboratory Utilities

ensochemLab offers a number of tools for some of the most common calculation duties in a chemical laboratory. These functions are not combined with an experiment. You can:

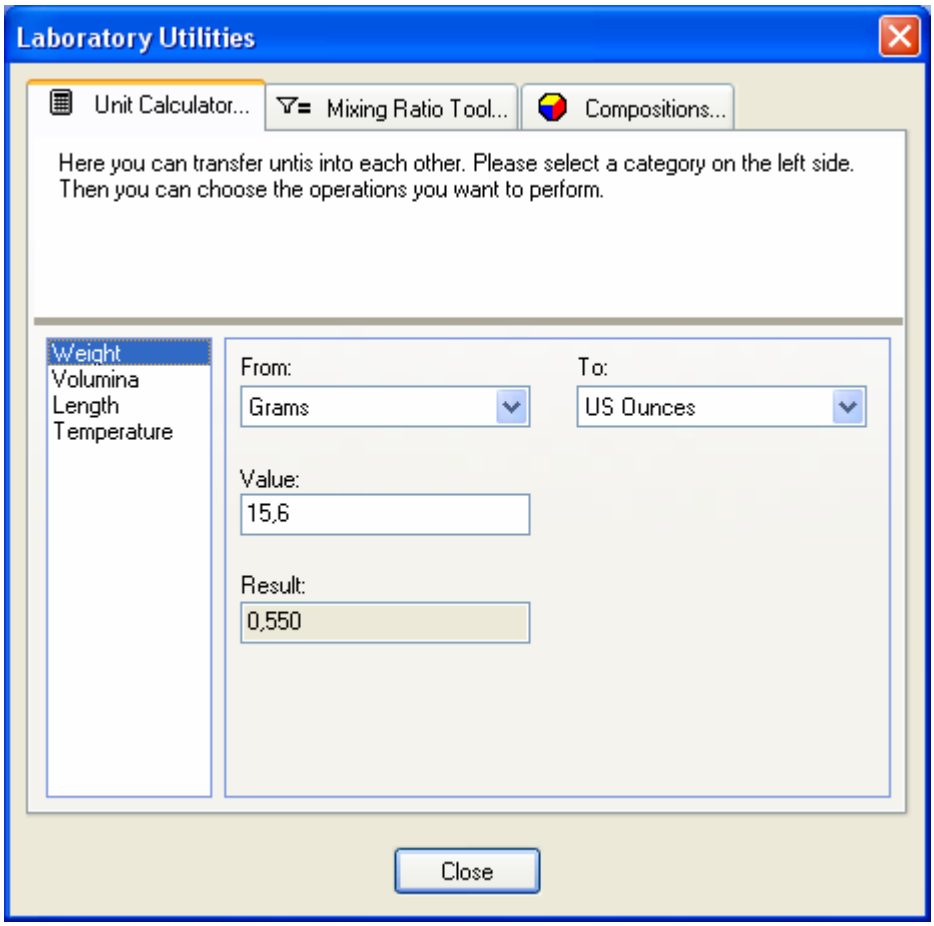
- Convert units
- Calculate mixing ratios
- Calculate the composition of a formula

To start the appropriate program, click on the “Laboratory Utilities” entry in the “Options” menu.



19.1. Unit calculation

At first, please select the unit calculator. The following window appears:

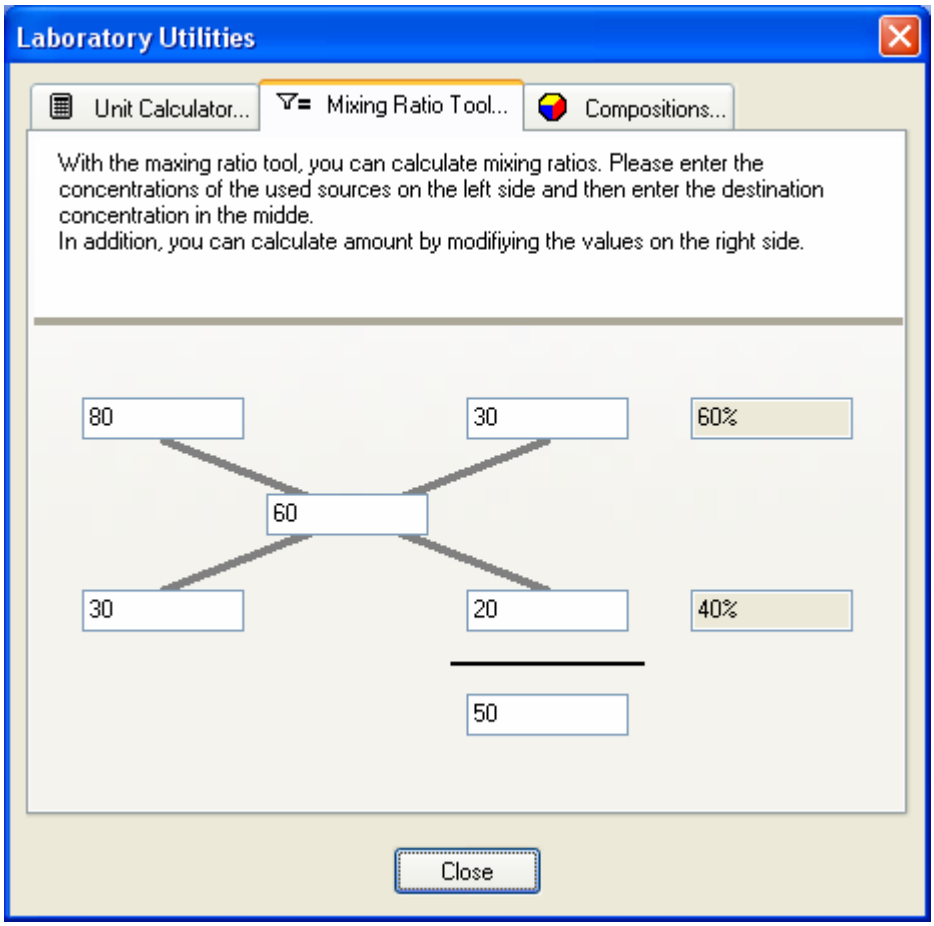


Please select the desired category from the list at the left side at fist. Then you can use the two dropdown boxes at the right side to specify which unit shall be used as source unit. Afterwards, please select the destination unit. Now please enter a value. This may be any floating point value of your choice. After you have done so, ensochemLab will automatically calculate the result and display it in the lower field. Thus, our sample calculation (see screenshot above) is:

15.6 Grams = 0.550 US Ounces

19.2. Mixing ratio calculation

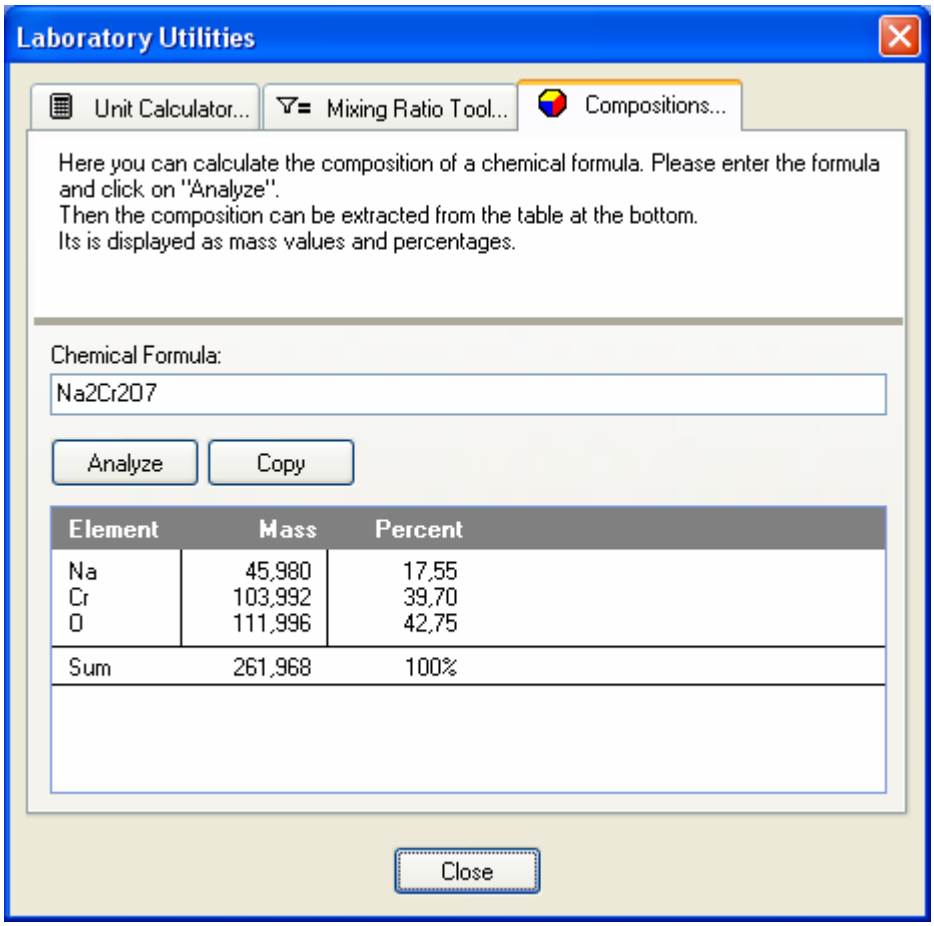
Next, we will take a look at the Mixing Ratio Tool by selecting the appropriate page:



As soon as you change one of the values in the cross, ensochemLab automatically calculates all the other values so that they match accordingly.
The percent relatives cannot be changed directly, only the absolute numbers.

19.3. Composition tool

Last but not least, there is the Compositions tool:



Please enter an arbitrary formula into the “Chemical Formula” field and then click on “Analyze”. The program will display a table similar to this one:

Element	Mass	Percent
Na	45,980	17,55
Cr	103,992	39,70
O	111,996	42,75
Sum	261,968	100%

The application shows the absolute mass and the corresponding percent value for each element contained in the formula. The last row shows the mass of the whole molecule and, for control purposes, the addition of the percent values.

The process of analyzing the formula is done on the basis of a number of rules:
All upper case letters are elements. All lower case letters belong to the last element the application has processed. Separators override this decision, so that the next letter after a blank is always an element. Numbers are multiplied with the last previous element or bracket. The parts of a salt are separated by *.

The following examples clarify how ensochemLab processes formulas:

Examples:

HCl	H + Cl
NaCl2	Na + (Cl * 2)
Na(OH)2	Na + (O * 2) + (H * 2)
NaCl * H2O	Na + Cl compound with (H * 2) + O
K Br	Spaces are separators between two elements

Invalid formula entries:

NaCL	L is regarded to be element
NAOH2	Only the H atom is multiplied with 2
2H2O	The formula always has to start with an element
OH-	Charges are not supported
Ds	Darmstadtium is not yet implemented as an element

Please note that ensochemLab does not perform a semantic check. Thus, it is possible to enter constructions like “CH13Cl” and others to let ensochemLab “calculate” them…

Summary:	The laboratory utilities can automate some of the daily calculations in a chemical laboratory. You can find the programs in the “Options“ menu (main window).

20. End of tutorial

Congratulations! You have successfully created your first experiment and learned about the most important functions in the software. Our short tour through ensochemLab is now over.

Nevertheless, this does not mean that there is nothing more in ensochemLab! There are even more useful functions that simplify your work and, in some cases, even fully automate it. Just try it!

enso Software GmbH also offers other solutions to simplify the daily work in a laboratory. Our product portfolio includes fully customer-dependent solutions especially for your needs as well as standard products that can be customized. Please check out our homepage at www.enso-Software.com for further information.

If there are new ensochemLab versions or version announcements, you can also refer to our homepage for a list of major new features.

We wish you an easy and productive work with ensochemLab

The ensochemLab product team

21. Appendix A: Glossary

In this manual, there were a lot of technical expressions related either to computer technology in general to electronic laboratory notebooks in particular. The chapter shall offer some help as well as a reference for these terms. It is sorted in an alphabetical order.

Account
An account is user access information that is identified by a unique user name and the corresponding password. Each account can have personal data assigned to it. That is, for example, your folder list and color scheme.

Administrator
One or more users can be defined as administrators. This special privilege enables them to change settings that are valid for all users. Examples are the predefined lists for origins, solvents and others.

Binary data
This kind of data is like an attachment to an E-Mail: It can be every kind of external file, for example a word document, an image or files from a third-party analysis system. Inside ensochemLab, you can save binary records for your experiment descriptions and analytics.

Block
A block is the same as a chapter. The experiment display is divided into chapters. The reaction, for example, is such a chapter and the description is another one.

Client
The client is the local part of your ensochemLab installation. It is the application you can see and use to enter your data. All data is sent to / received from a server.

Component
A component is a part (reactant or product) within a fraction.

Database
The database is the place where ensochemLab stores all data (experiments, settings…). Beside the pure data storage, the database also creates links between the particular records. (Experiment <> Reference experiment, User <> his or her settings…)

Display layout
A display layout is a set of experiment display settings like currently visible chapters, their order, column widths and others.

EC_LAB_ADMIN
This Oracle role combines the EC_LAB_REG role with the permission to specify general settings for all ensochemLab users in the administration dialog.
This privilege is only available when using Oracle as your database system.

EC_LAB_READ
Users who are assigned this Oracle role have the permission to read all experiments in the database.
This privilege is only available when using Oracle as your database system.

EC_LAB_REG

This Oracle role contains the EC_LAB_READ role extended by the permission to create, modify and delete own experiments.
This privilege is only available when using Oracle as your database system.

Edition

ensochemLab can be customized according to the special requirements of your company by developing a special editing. However, this means that some of the pictures or explanations in this manual might be a bit different depending on your special edition.

There are two ensochemLab applications that are also called editions: One application for Windows and one that is running on a web server. This manual deals solely with the Windows edition.

ensochemEditor

This module is the chemistry editor included in ensochemLab that can be used to draw chemical structures and reactions. Within your personal settings, you can configure the application to use a different editor.

Exact fragment search

With this search mode, at least one fragment of the molecule in the database has to chemically exactly match your search structure for the record to be a hit. This search mode is not available with all chemistry databases.

Exact search

When performing an exact search, the molecule in the database has to exactly equal to the search molecule you have drawn.

Experiment cache

To minimize the time it takes to load an experiment, ensochemLab saves all experiments you have already viewed in that session in your computer's memory. This procedure is called "Caching" and the memory reserved for it "Cache".
If an experiment is changed by another user and you want to see the new version with his changes, you have to manually clear the experiment cache by clicking on "Clear Experiment" Cache in the "Options" menu.
Such a clearing is done every time you log out from ensochemLab.

Experiment link

An experiment link is information that just defines which experiment is assigned to where it is located in the database. This enables ensochemLab to add one experiment to multiple folders without having to actually store it multiple times.

Experiment protocol

See "Protocol"

Finalized

"Finalized" is a status description. Such an experiment cannot be modified any more unless it is reset to the "in work" status.

Floating Point Value

A floating point value is a decimal value like 0.5.

Fraction

A fraction contains the percentages assigned to reactants and products in relation to the whole reaction mixture as well as corresponding additional data. It is always a record taken at a specific time during the reaction.

ID

An ID is a unique identifier for a particular record. You experiment numbers, for example, are IDs.

In work

"In work" is a status description. It defines that an experiment can be edited or processed further. Such experiments are mostly still in progress and likewise current.

Password

A password is a secret character string that is, in connection with your user name, necessary to authenticate you against the database system.

Laboratory utilities

The category „Laboratory Utilities" includes a number of useful tools to automate certain everyday calculation tasks in a chemical laboratory.

Login

By logging in, you authenticate yourself against the database system. This guarantees data security and protection against unauthorized access. It enables all users to have their personally customized settings.
You have to log in every time you start ensochemLab. However, this process can also be done automatically (see chapter "Login").

Logout

If you terminate the program or use the "Logout" function in the "File" menu, you will return to the login window. This means, that ensochemLab disconnects you from the database and makes it possible for another user to login and work with the program.

List

In general, a list is a collection of records. The type of the data that is stored depends on the kind of list you working with. ensochemLab always works with lists. If you want to modify or delete an experiment, you have to put it into a list by searching or having it in your personal experiment folder.

Lookup list

A lookup list contains elements predefined by the administrator. For the record you are currently working with, you can select one of them as a value. In most cases, you can also enter a free text instead. However, this entry will not be saved for new records or other users.
The project list, for example, is a lookup list.

Multi language

ensochemLab supports multiple languages. You can use the program in German, English and French. To change your language, go to the login dialog and click on the flag. A window will appear where you can select the desired language. Before logging on, ensochemLab always uses the language you have selected at your last login.

Module

A module is a part of an application like ensochemLab. Each module has specific tasks that it performs. One module, for example, is used to edit chemistry data and another one for printing experiments.

MOL File

While a word document is used save text, a MOL file contains a chemical molecule.

Mol percent

See chapter 3 („Create your first experiment"). It starts on page 3.

MSDE

Microsoft **S**QL Server **D**esktop **E**ngine: The free desktop version of the well-known database server which is used for ensochemLab Workgroup Edition.

MSXML

MSXML stands for a number of operating system libraries that ensochemLab uses to access the server. If you receive an error message that tells you about these DLL files, please contact your administrator.

Ownership

An experiment can only be changed by one user. If you create an experiment, you automatically own it.
If your administrator has activated overtaking experiment, you can take the ownership of a colleague's experiment by clicking on "Take Ownership" in the "Experiment" menu (main window)

Phrase

A phrase is a commonly used text block which has been saved into the database for allowing a quick insert into text fields like the experiment description. Further information is available in the "User defined phrases" chapter.

Pixel

A pixel is the logical measure unit for displaying and calculating computer graphics. Normally, a pixel on the screen is about 0.28 mm large. However, this depends on your screen resolution, so you should not rely exactly on this size.

Privileges

When creating your user account, your (database) administrator has granted you a number of rights. This permits you to perform certain operations within the application. For example, you may have been granted the right to create and modify experiments or to manage global administrative parameters.

Protocol

Some actions like taking over an experiment or resetting its state to "in work" are logged in the database. This means that an administrator can find out who has done the action when and why. If he has activated the corresponding function, this display is also available to normal users by pointing at the protocol symbol in the status bar with your mouse.

Record

ensochemLab saves all data within records. All data that belongs together is one record. Analytic data, reactants and products are all records, even the experiment itself.

Rights

See "Privileges"

Limiting reactant

The limiting reactant is the basis for all calculations that affect the resulting substance amounts and yields. It is always assigned an equivalent of 1. Example: The yield of a product is the amount of the product in comparison to the amount of the limiting reactant.

Rich Text

See "RTF Format"

RSS

RSS stands for "**R**eaction **S**ubstructure Search" and means that a reaction only has to contain the query to be a result. If you search query contains two reactants and one product, for example, you will find all experiments that contain these two reactants and the product, even if they are only parts of bigger molecules.

RTF Format

RTF stands for "**R**ich **T**ext **F**ormat" and enables you to use complex formatting information like bold face letters, italic characters, different fonts and much more in your text.

RXN File
Just as a Word document is used to store text, a RXN file contains a reaction.

Server
The server is the remote part of your ensochemLab installation. All data is sent there for storage and processing. Afterwards, it is transferred back to your client and the results are displayed.

Service
See “Server“

Subsequent experiment
When creating a subsequent experiment, ensochemLab uses one of the current experiment’s products as the default reactant for the new experiment.

Visibility
In ensochemLab, en experiment is visible for all users that are authenticated successfully. No exceptions are possible at this point.

Session
A session is the time between login and logout as well as all actions performed in this time.

SSS
SSS stands for “**S**ub**S**tructure **S**earch“. This means that the search molecule just has to be part of the structure in the database to be a result.

Status
ensochemLab supports two different status types for experiments: “in work” and “Finalized”. Experiments in the “Finalized” state cannot be modified any more.

Substructure search
See “SSS“

Target molecule
A target molecule is a product that you wanted to synthesize with your experiment or row of experiments. You can define an arbitrary number of special names for a target molecule, as you might want to have both trade name and synonym.
Reactions that contain a target molecule cannot be modified at their whole. Additionally, the chemistry information of the product that is registered as the target cannot be modified.
Please note that there may be only one target per experiment.

Undo
If you are in dialog, you can undo most changes by clicking on the “Cancel” buttons. However, there are some exceptions for that: One example is the dialog for target molecule management. All those dialogs are marked with a special hint in their description, so that you can see whether you can undo your changes or not.

User account
See “Account“

User administration
The ensochemLab default user administration enables you to manage users, sites, departments and laboratories as well as the respective connections (User A belongs to laboratory B …).

User name
This name has been assigned by your administrator and authenticates you against the database system. ensochemLab uses it to identify the creator of an experiment, for example.

A login is only possible with the corresponding password.

User rights

See “Privileges“

Version

The module version specifies how current the module. The higher the first part of the version number is, the newer is the module. Example: Version “1.1.0.3” is newer than “1.0.2.5”.

Visibility

If you do not have any user administration module enabled, everyone is allowed to display every experiment in the database. If you activate the default user administration module, you can specify for each experiment who is allowed to see it.

22. Appendix B: Fields and search modes

The following list describes all fields that are available in the Query Builder and defined which search mode is appropriate for them.

Experiment header:

Field	Search mode
Assessment	Text search with the possibility to select a value from the list of assessments predefined by the administrator
Comment	Text search
Date closed	Date search
Date experiment	Date search
Department	Text search with the possibility to select a value from the list of departments predefined by the administrator
Experiment number	Text search
Project	Text search with the possibility to select a value from the list of projects predefined by the administrator
Purpose	Text search
State	Selection of status records – no free text possible
Step	Text search
Test series	Text search
User ID	Text search
User name	Text search

Reaction:

Field	Search mode
Label above reaction arrow	Text search
Label below reaction arrow	Text search

Reactants:

Field	Search mode
Amount	Numerical search
Amount / unit	Numerical search for the amount combined with a search for the appropriate unit as a selection field
Amount unit	Text search with the possibility to select a value from the list of amount units predefined by the administrator
Batch	Text search
CAS No	Text search
Chemical carrier	Text search with the possibility to select a value from the list of carriers predefined by the administrator
Content	Numerical search

Content / unit	Numerical search for the content combined with a search for the appropriate unit as a selection field
Content unit	Text search with the possibility to select a value from the list of content units predefined by the administrator
Density	Numerical search
Item number	Text search
Load	Numerical search
Mol	Numerical search
Mol / unit	Numerical search for the mol amount combined with a search for the appropriate unit as a selection field
Mol unit	Text search with the possibility to select a value from the list of mol units predefined by the administrator
Molecule label	Text search
Molpercent	Numerical search
Molweight	Numerical search
Name	Text search
On chemical carrier	Yes / No query
Origin	Text search with the possibility to select a value from the list of origins predefined by the administrator
Reference experiment	Text search
Type	Selection of supported types – no free text possible

Additional reactant data:

This group contains additional data fields defined by the administrators. Their type thus depends on the configured field definition. If you have questions, please contact your administrator or support personnel.

Products:

Field	Search mode
Amount	Numerical search
Amount / unit	Numerical search for the amount combined with a search for the appropriate unit as a selection field
Amount unit	Text search with the possibility to select a value from the list of amount units predefined by the administrator
Batch	Text search
CAS No	Text search
Chemical carrier	Text search with the possibility to select a value from the list of carriers predefined by the administrator
Content	Numerical search
Content / unit	Numerical search for the content combined with a search for the appropriate unit as a selection field
Content unit	Text search with the possibility to select a value from the list of content units predefined by the administrator
Load	Numerical search
Mol	Numerical search
Mol / unit	Numerical search for the mol amount combined with a search for the appropriate unit as a selection field
Mol unit	Text search with the possibility to select a value from the list of mol units

	predefined by the administrator
Molecule label	Text search
Molweight	Numerical search
Name	Text search
On chemical carrier	Yes / No search
Substance code	Text search
Target molecule	Text search with the possibility to select from a list of all target molecules registered
Type	Selection of supported types – no free text possible
Yield	Numerical search

Additional product data:

This group contains additional data fields defined by the administrators. Their type thus depends on the configured field definition. If you have questions, please contact your administrator or support personnel.

Description:

Field	Search mode
Binary data abstracts	Text search
Binary data file name	Text search
Binary data title	Text search
Text (case sensitive)	Text search

Reaction parameters:

Field	Search mode
Alphanumeric value	Text search
Comment	Text search
Name	Text search
Numeric value	Numerical search
Unit	Text search

Tabular description:

Field	Search mode
Amount	Text search
Comment	Text search
Date	Date search
Temperature	Text search
Time	Text search

Literature:

Field	Search mode
Article	Text search
Authors	Text search
Comments	Text search

End page	Text search
Issue	Text search
Journal	Text search with the possibility to select a value from the list of literature entries predefined by the administrator
Patent no.	Text search
Start page	Text search
URL	Text search
Year	Numerical search

Analytics:

Field	Search mode
Binary data abstracts	Text search
Binary data file name	Text search
Binary data title	Text search
Comment	Text search
Condition	Text search
Link	Text search
Method	Text search with the possibility to select a value from the list of methods predefined by the administrator
Result value max.	Numerical search
Result value min.	Numerical search
Result value text	Text search
Result value unit	Text search
Sample no	Text search
Solvent	Text search

23. Appendix C: Keyboard Shortcuts

For making commonly used product features available more quickly and conveniently, ensochemLab offers you a number of keyboard shortcuts. This chapter lists the available keyboard shortcuts for all different program modules.
These pages are designed in a way that enables you to print them and keep them within reach during your first work days with ensochemLab.

For likewise functions (new product, new template, new row…), the same keyboard shortcuts have been chosen in order to simplify the learning process.

Main window:

Function	Keyboard Shortcut
New Experiment	CTRL+N
Copy Experiment	CTRL+O
Modify Experiment	CTRL+F2
Delete Experiment	CTRL+DEL
Reload Experiment	F5
Clear Experiment Cache	CTRL+F5
Edit Fractions	CTRL+R
Print Current Display	CTRL+P
Launch Default Search	CTRL+F
Display User's Guide	F1

Navigator Section:

Function	Keyboard Shortcut
Copy Element	CTRL+C
Cut Element	CTRL+X
Paste Element	CTRL+V
Rename Element	F2
Delete Element	CTRL+DEL
Move Up	CTRL+UP
Move Down	CTRL+DOWN
Sort Descending	CTRL+PLUS (Numpad)
Sort Ascending	CTRL+MINUS (Numpad)

Experiment display:

Function	Keyboard Shortcut

Start of Experiment	CTRL+HOME
End of Experiment	CTRL+END
Scroll Up	CTRL+PG UP
Scroll Down	CTRL+ PG DOWN

Experiment Wizard, Page "Reaction":

Function	Keyboard Shortcut
Launch Chemistry Editor	F12

Experiment Wizard, Page "Reactants":

Function	Keyboard Shortcut
New Reactant	CTRL+N
Copy Reactant	CTRL+D
Delete Reactant	CTRL+DEL
Move Up	CTRL+UP
Move Down	CTRL+DOWN
Launch Chemistry Editor	F12

Experiment Wizard, Page "Products":

Function	Keyboard Shortcut
New Product	CTRL+N
Copy Product	CTRL+D
Delete Product	CTRL+DEL
Move Up	CTRL+UP
Move Down	CTRL+DOWN
Launch Chemistry Editor	F12

Experiment Wizard, Page "Description, Binary Data":

Function	Keyboard Shortcut
Save Binary File	CTRL+S
Open Binary File	CTRL+O

Experiment Wizard, Page "Description, Tabular Description":

Function	Keyboard Shortcut
New Row	CTRL+N
Delete Row	CTRL+DEL
Move Up	CTRL+UP
Move Down	CTRL+DOWN
Copy Table	CTRL+C

Paste Table	CTRL+V
Undo Paste Table	CTRL+Z

Experiment Wizard, Page "Description, Reaction Variables":

Function	Keyboard Shortcut
New Row	CTRL+N
Delete Row	CTRL+DEL
Move Up	CTRL+UP
Move Down	CTRL+DOWN
Copy Table	CTRL+C
Paste Table	CTRL+V
Undo Paste Table	CTRL+Z

Experiment Wizard, Page "Analytics":

Function	Keyboard Shortcut
New Analytic Record	CTRL+N
Copy Analytic Record	CTRL+D
Delete Analytic Record	CTRL+DEL
Move Up	CTRL+UP
Move Down	CTRL+DOWN

Experiment Wizard, Page "Literature":

Function	Keyboard Shortcut
New Literature Record	CTRL+N
Copy Literature Record	CTRL+D
Delete Literature Record	CTRL+DEL
Move Up	CTRL+UP
Move Down	CTRL+DOWN

Creation of Target Molecules:

Function	Keyboard Shortcut
New Structure	CTRL+N
Delete Structure	CTRL+ENTF
New Target Molecule Name	CTRL+T
Edit Target Molecule Name	F2
Launch Chemistry Editor	F12

Modification of Attached Excel Worksheets:

Function	Keyboard Shortcut

Save as a File	CTRL+S
Modify Worksheet	F2

Modification of Attached Word Documents:

Function	Keyboard Shortcut
Save as a File	CTRL+S
Modify Document	F2

Fractions Dialog, Page "Select Components":

Function	Keyboard Shortcuts
New Product	CTRL+N
Modify Product	F2
Delete Product	CTRL+DEL

Fractions Dialog, Page "Fraction Data":

Function	Keyboard Shortcut
New Fraction	CTRL+N
Delete Fraction	CTRL+DEL

Fractions Dialog, Page "Component Data":

Function	Keyboard Shortcut
Move Up	CTRL+UP
Move Down	CTRL+DOWN

Fraction Dialog, Binary Data:

Function	Keyboard Shortcut
New Binary Record	CTRL+N
Modify Binary Record	F2
Delete Binary Record	CTRL+DEL
Save Binary File	CTRL+S

Tabular Fractions Dialog:

Function	Keyboard Shortcuts
Add Fraction	CTRL+N
Delete Fraction	CTRL+DEL
Copy Fraction	CTRL+D

Editing Experiments in Display Mode, Reactants:

Function	Keyboard Shortcut

New Reactant	CTRL+N
Delete Reactant	CTRL+DEL
Launch Chemistry Editor	F12

Editing Experiments in Display Mode, Products:

Function	Keyboard Shortcut
New Product	CTRL+N
Delete Product	CTRL+DEL
Launch Chemistry Editor	F12

Process Description, Templates:

Function	Keyboard Shortcut
New Template	CTRL+N
Save Template As	CTRL+S

Process Description, Template Field List

Function	Keyboard Shortcut
New Row	CTRL+N
Move Up	CTRL+UP
Move Down	CTRL+DOWN

Process Description, Data Entry:

Function	Keyboard Shortcut
New Row	CTRL+N
Move Up	CTRL+UP
Move Down	CTRL+DOWN
Copy Table	CTRL+C
Paste Table	CTRL+V
Undo Paste Table	CTRL+Z

Search, Search Chemistry:

Function	Keyboard Shortcut
Launch Chemistry Editor	F12

Search, Query Builder:

Function	Keyboard Shortcut
Launch Chemistry Editor	F12

Report Wizard, page “Define”:

Function	Keyboard Shortcut
New Alphanumerical Search Element	CTRL+I
New Chemical Search Element	CTRL+H

Report Wizard, page “Display”:

Function	Keyboard Shortcut
Move Up	CTRL+UP
Move Down	CTRL+DOWN

Report Manager:

Function	Keyboard Shortcut
New Report	CTRL+N
Modify Report	F2
Delete Report	CTRL+DEL

List & Label Report Manager:

Function	Keyboard Shortcut
New List & Label Report	CTRL+N
Modify List & Label Report	F2
Delete List & Label Report	CTRL+DEL
Design List & Label Report	CTRL+D
Preview List & Label Report	CTRL+P

Report Display:

Function	Keyboard Shortcut
New Report	CTRL+N
Modify Report	F2
Delete Report	CTRL+DEL
Refresh Report	F5

Export of Experiments into CSV Files:

Function	Keyboard Shortcut
Move Up	CTRL+UP
Move Down	CTRL+DOWN

Display of Changes in an Experiment Revision:

Function	Keyboard Shortcut
Display First Changes	CTRL+HOME

Display Previous Changes	CTRL+LEFT
Display Next Changes	CTRL+RIGHT
Display Last Changes	CTRL+END
Copy Changes	CTRL+C
Save Changes Into File	CTRL+S

Display Layout Manager:

Function	Keyboard Shortcut
Modify Layout Description	F2
Delete Display Layout	CTRL+DEL

Manage Calculation Templates:

Function	Keyboard Shortcuts
New Calculation Template	CTRL+N
Copy Calculation Template	CTRL+D
Modify Calculation Template	F2
Delete Calculation Template	CTRL+DEL

Insert Phrases:

Function	Keyboard Shortcut
Insert Current Phrase	RETURN
Modify Current Phrase	F2

Manage Phrases:

Function	Keyboard Shortcut
New Phrase	CTRL+N
Modify Phrase	F2
Copy Phrase	CTRL+D
Delete Phrase	CTRL+DEL

The predefined phrases administration dialog provides the same keyboard shortcuts.

Reagent List:

Function	Keyboard Shortcut
New Reagent	CTRL+N
Delete Reagent	CTRL+DEL
New Synonym	CTRL+S
Modify Synonym	F2
Import SD File	CTRL+I
Launch Chemistry Editor	F12

Administration Dialog, Page "Users":

Function	Keyboard Shortcut
New User	CTRL+N
Modify User	F2
Delete User	CTRL+DEL

Administration Dialog, Page "Lookup Lists":

Function	Keyboard Shortcut
New List Element	CTRL+N
Modify List Element	F2
Delete List Element	CTRL+DEL
Sort List	CTRL+MINUS (Numpad)

Administration Dialog, Page "Units":

Function	Keyboard Shortcut
New Unit	CTRL+N
Modify Unit	F2
Delete Unit	CTRL+DEL
Move Up	CTRL+UP
Move Down	CTRL+DOWN

Default User Administration:

Function	Keyboard Shortcuts
New Site	CTRL+S
New Department	CTRL+D
New Laboratory	CTRL+L
New User	CTRL+U
Delete Element	CTRL+DEL

Additional Data Definition Management:

Function	Keyboard Shortcut
New Data Field	CTRL+N
Delete Data Field	CTRL+DEL
New Synonym	CTRL+S
Modify Synonym	F2

User Object Management:

Function	Keyboard Shortcut

Reload Data	F5
Select All	CTRL+A
Delete Selected Elements	CTRL+DEL

24. Appendix D: Extensions

ensochemLab offers certain functionality that however is not part of the standard version. With these features, there are two different categories:

- Additionally available extensions
  These extensions can be obtained via our sales partners and have to be separately installed on the ensochemLab server before they can be used (for example: Revision management module).

- Functions that can be optionally activated
  These functions can be activated after a consultation of enso Software GmbH or one our sales partners. A separate installation is not necessary in this case.

These extensions can contain additional functions, more data fields and workflows. Elements of the first category are described in this manual just as normal; still there is a note that they might not be available in your installation.
Extensions of the second category are designed for special scenarios that do no occur with most users and are thus excluded from the standard documentation. If you have activated such an extension, you may have received a separate short documentation or manual. Available extensions of this kind are:

- Extensions for metal chemistry
  The reactant data fields are extended by:
  - Is metallic structure
  - Metal content

  The product data fields are extended by:
  - Is metallic structure
  - Metal content
  - Metal yield