IUCLID 5
INTERNATIONAL UNIFORM CHEMICAL INFORMATION DATABASE

IUCLID 5
Guidance and support

Getting Started

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Getting started - Sample session for beginners

This Getting Started manual is an excerpt from the IUCLID 5 End User Manual, chapter C. To review any references to chapters other than chapter C, see the full manual.

1. Introduction to sample session

The guidance given in this Getting Started manual aims at assisting the novice IUCLID user to set up the application and use it immediately without having to read the details provided with the full version of the IUCLID 5 End User Manual first. The references to specific chapters of the full version are intended as hints for where to find more details. This session is based on the following parts:

- The First steps wizard which guides you through the different steps involved to setting up your application so that you can use it immediately: see chapter 2 Starting IUCLID 5: First steps wizard.
- A self-tutorial sample session which guides you through the most common features needed for handling a Substance dataset, which is the central core of information in IUCLID. This session is subdivided into the following chapters:
  - 3 Creating a dataset for a Substance and assigning a Reference substance
  - 4 Completing a Substance dataset
    - 4.1 Entering/editing data in sections 1 to 3
    - 4.2 Entering/editing data in sections 4 to 13
  - 5 Printing the Substance dataset
  - 6 Creating a Dossier
  - 7 Exporting the Substance dataset
  - 8 Importing the Substance dataset

A number of real examples are presented in this hands-on session. These examples were taken from different published datasets, but are not necessarily related to the sample substances used. In this respect, all examples should be considered as fictitious.

Note

The hands-on examples may not be relevant for your particular submission. Nonetheless, it can be helpful to carry out these self-tutorial exercises to get acquainted with the IUCLID functionality in general.

2. Starting IUCLID 5: First steps wizard

When you start IUCLID for the first time, after installing it on your computer, a First steps wizard will come up, which guides you through the different steps involved to setting up your application so that you can use it immediately. If the IUCLID application and your user account have been set up by your administrator, you can skip this chapter. Any user-related settings can also be made using the features described in the IUCLID 5 End User Manual chapter D.16 Manage Users, Role, Preferences etc., although for some of them SuperUser rights are required (see the IUCLID 5 End User Manual chapter D.16.2.1 Difference between SuperUser and "SuperUser" attribute).

Important

This wizard helps to define a user account, which is a prerequisite to work with the application. This is not possible when logging in with the SuperUser account that is provided as administrator account by default.

Before running this wizard, make sure that at least the Legal entity information of your Company/organisation is stored on your computer in

the form of a IUCLID export file (for more information, see the IUCLID 5 End User Manual chapter D.9.2.1 Creating an "official" Legal entity).

Following information can also be uploaded at a later stage, but it is strongly recommended to have the following files stored on your PC already when you run this wizard:

- EC Inventory (for details, see the IUCLID 5 End User Manual chapter D.12 Inventory (View EC Inventory related information)
- Inventory of Reference substances (for details, see the IUCLID 5 End User Manual chapter D.11 Reference substance (Create and update Reference substance related information))

Note

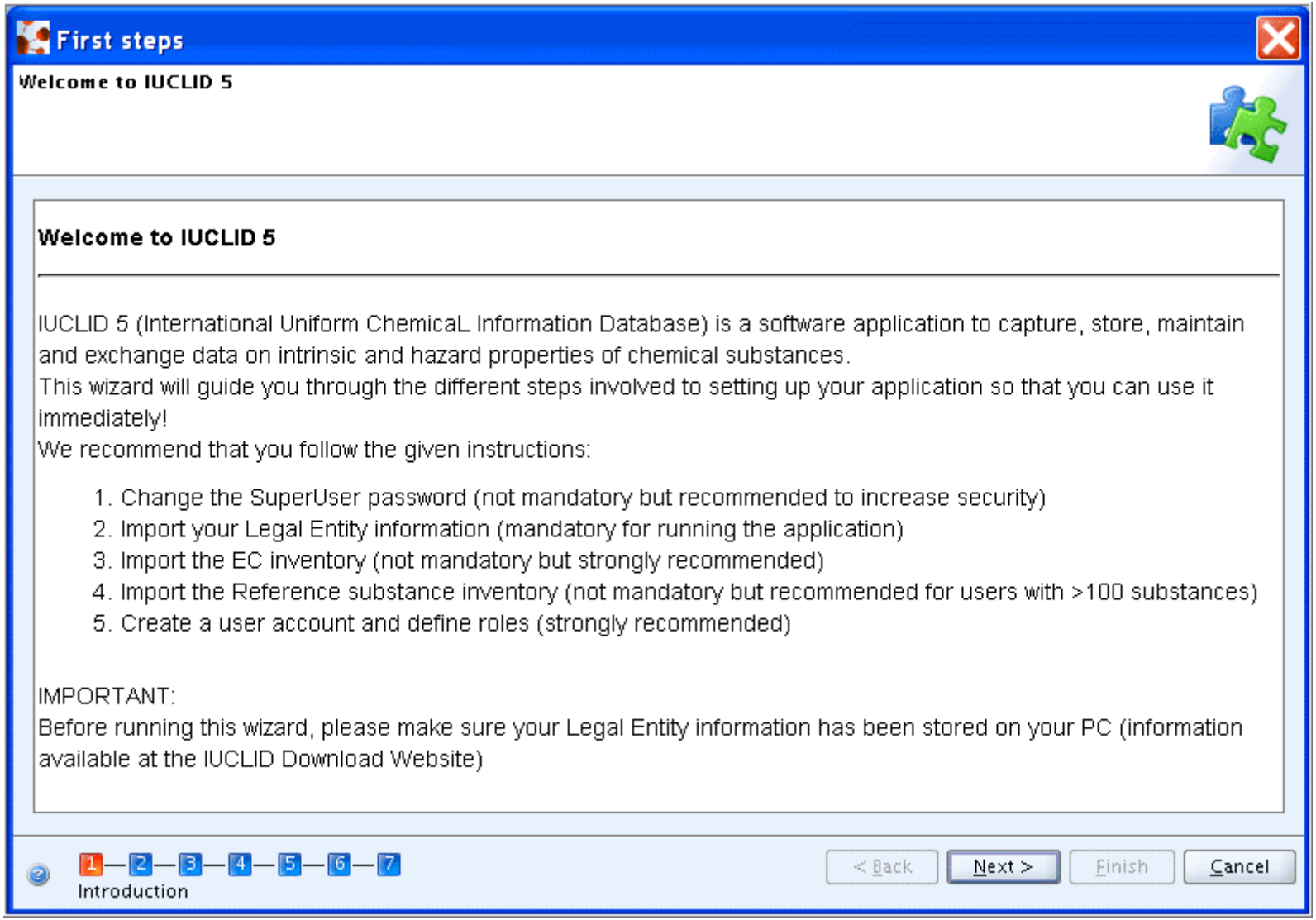
If you want to launch the wizard manually, log in as "SuperUser" and from the File menu select the **Administrative tools** and **Initialise** commands.

To set up your IUCLID application for the first time and create a user account suitable for every day work and to assure that the installation was performed correctly, follow these steps:

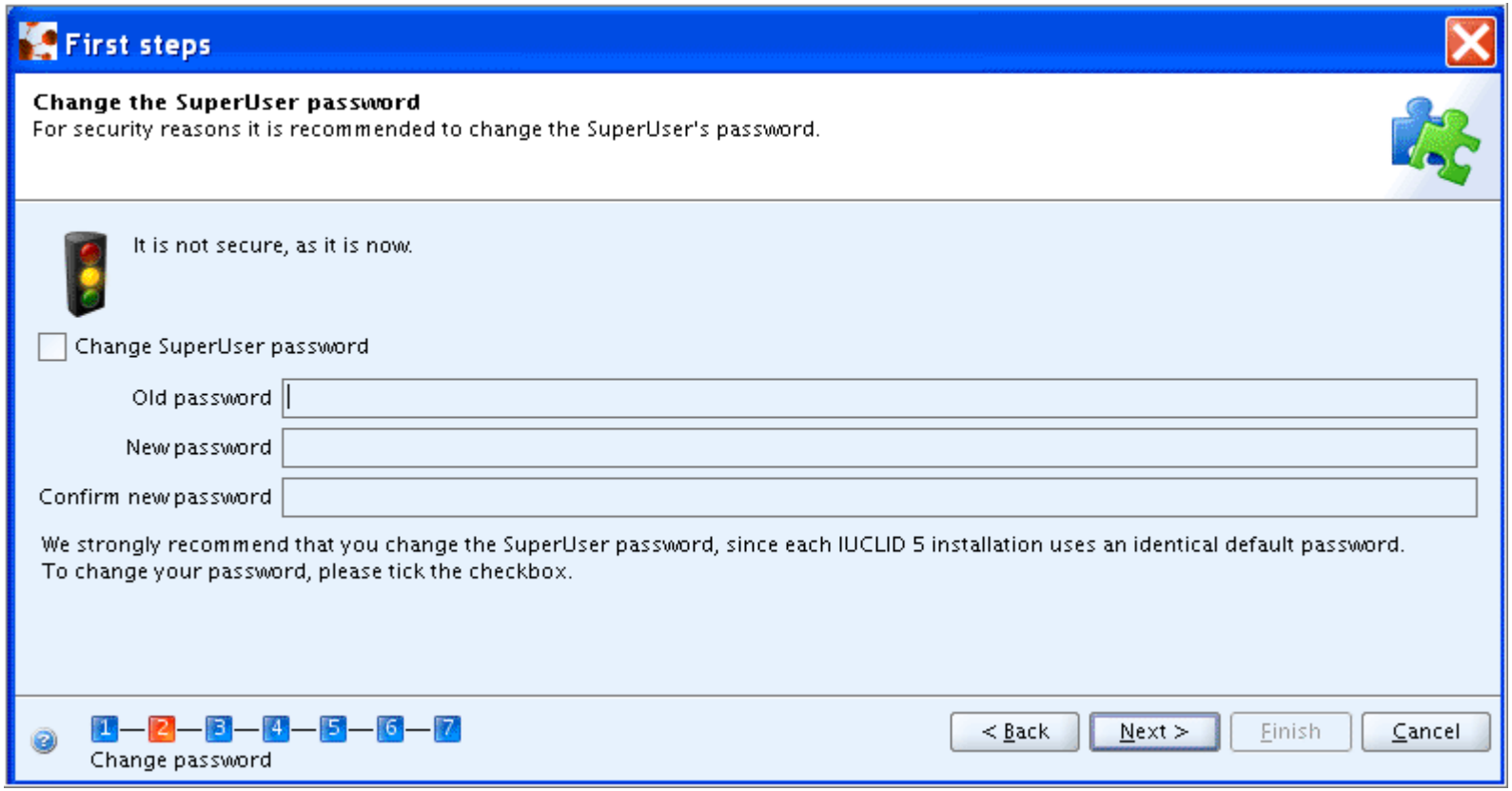
1. Start IUCLID by clicking the respective icon on your desktop

2. When starting the application for the first time, the only user available is the administrator, named "SuperUser". Log in as administrator by entering the following (case-sensitive!) names:
   - Username: SuperUser
   - Password: root

3. The First steps wizard comes up with general information in Step 1. Click the **Next** button



4. Step 2: If you have not changed the default password of the SuperUser to a more secure password, the traffic light in the wizard screen will be yellow. Select the `Change SuperUser password` checkbox, type the old password "root" and then type the new password. Click the **Next** button.

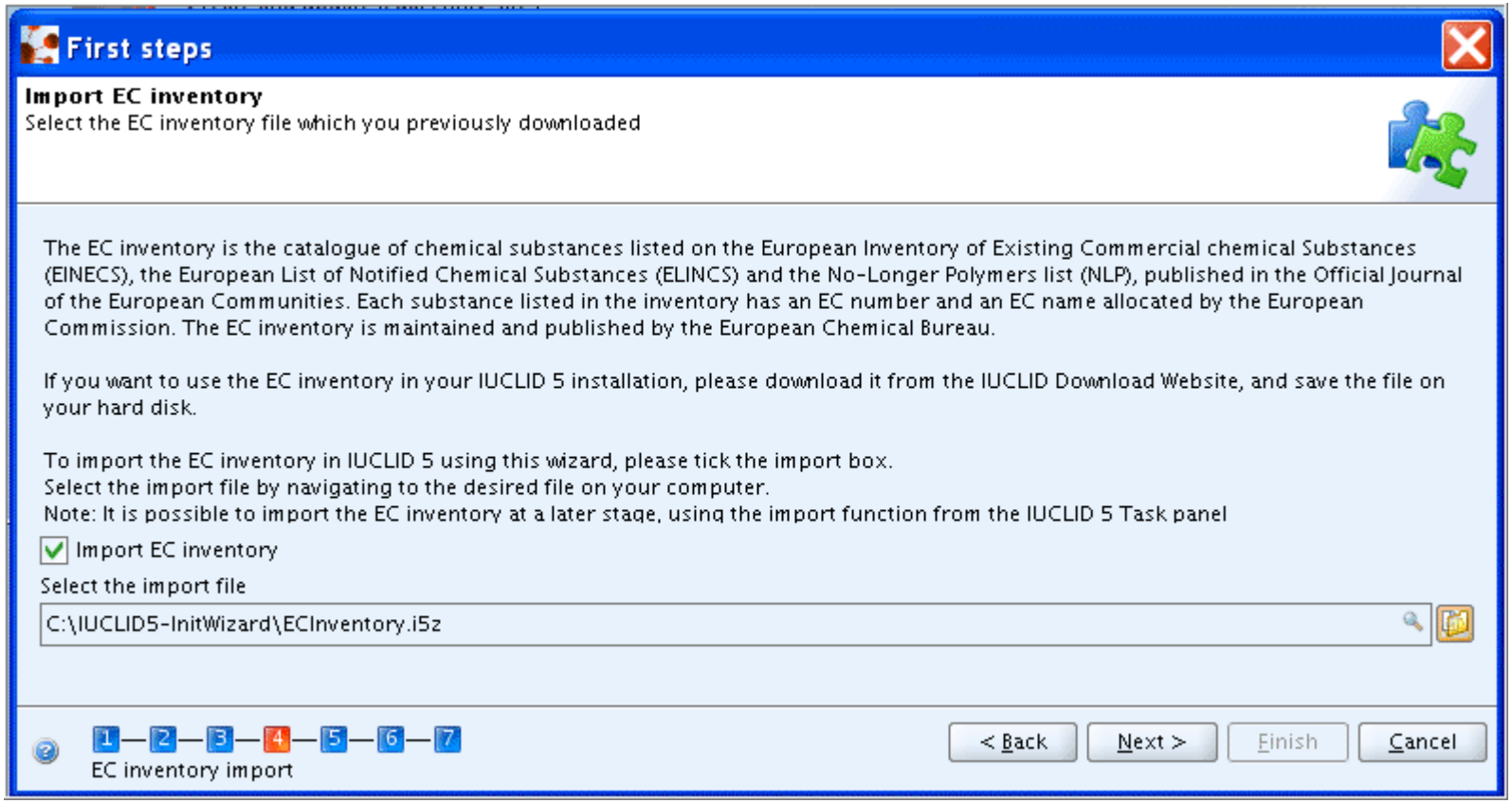


5. Step 3: Select the import file for the Legal entity (see introductory remarks above) and then click the **Next** button. The Legal entity will be imported immediately.

Important

Note that you have to import at least one Legal entity in order to succeed with this wizard. If you have no Legal entity in the IUCLID system, the traffic light in the wizard screen will be red. The First steps wizard will be automatically launched when you log in IUCLID, until a Legal entity has been successfully imported.

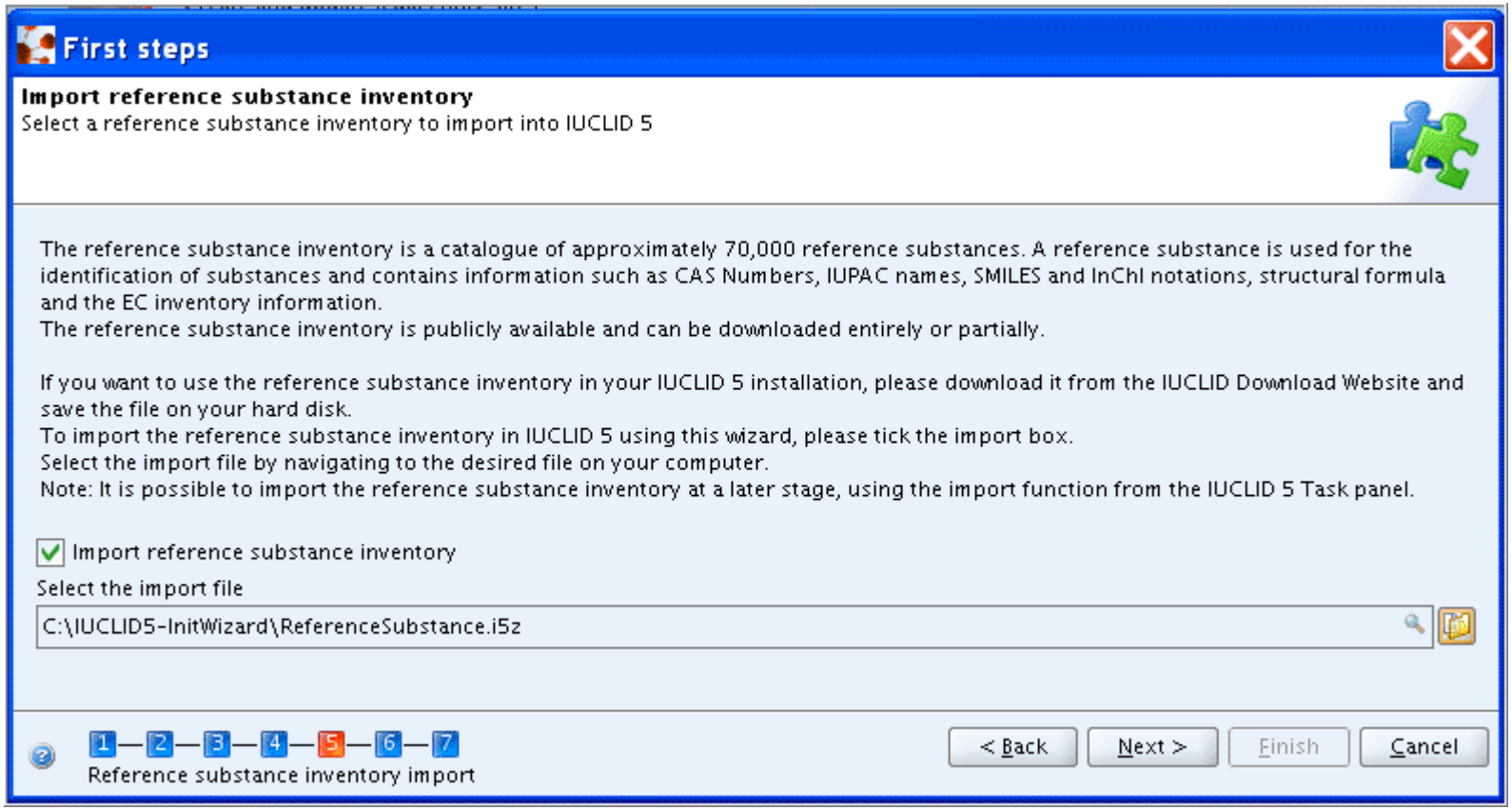
6. Step 4: Select the file for the EC inventory (see introductory remarks above). The EC Inventory will not be imported immediately. The import will start at the end of the First steps wizard. Depending on your machine speed and the size of the inventory, this import may take some time, i.e. up to half an hour.



7. Step 5: Select the file for the Reference substance inventory (see introductory remarks above). The Reference substance inventory will not be imported immediately. The import will start at the end of the first steps wizard together with the EC Inventory import. Depending on your machine speed and the size of the inventory, this bulk operation may take a very long time. The Reference substance inventory itself may take **up to several hours** for import!

Note

If you do not wish to import the complete Reference substances inventory into your IUCLID system, individual Reference substances files are available for download at the IUCLID web site.



8. Step 6: Create a new user account and assign a role to this user, which defines the user's access rights to the data. It is necessary to create a new user as working with the SuperUser is not supported.

    - Select the `Create user` checkbox.

      Fill in all fields. The user needs a `Login name` for identification during login. The `Full name` is used for proper user identification. The `Assigned role` is needed to administrate the access permissions (in a newly installed IUCLID 5 the roles "Administrator", "Full access" and "Read-only" are provided by default).

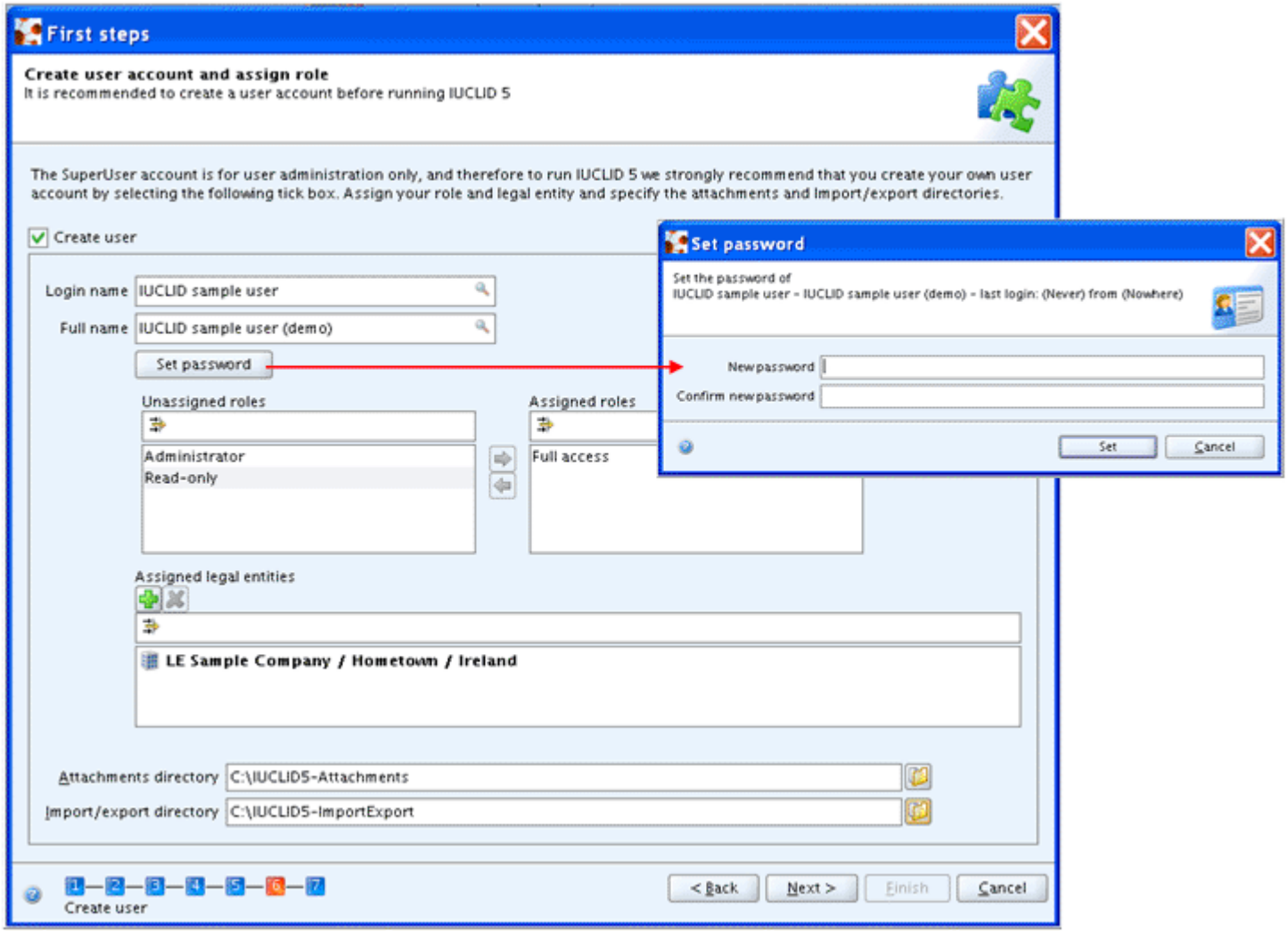
    - Enter a `Login name`, as it should be used for identification during login, and the `Full name` used for proper user identification.

- Optionally, click Set password and define a password.
- Click and highlight a role in the list of unassigned roles and assign it to the user by clicking the Right arrow. Assigning a Role is needed to administrate the access permissions (in a newly installed IUCLID, the roles "Administrator", "Full access" and "Read-only" are available by default).

Tip

It is recommended to create a User with the "Administrator" Role regardless of whether a stand alone or a distributed version of IUCLID is set up. Once a User has been created, the IUCLID Administrator (in case of a distributed version) can define different other User(s) and assign different Role(s) to them (see the IUCLID 5 End User Manual chapter D.16.1 Principles of administration tools for user settings).

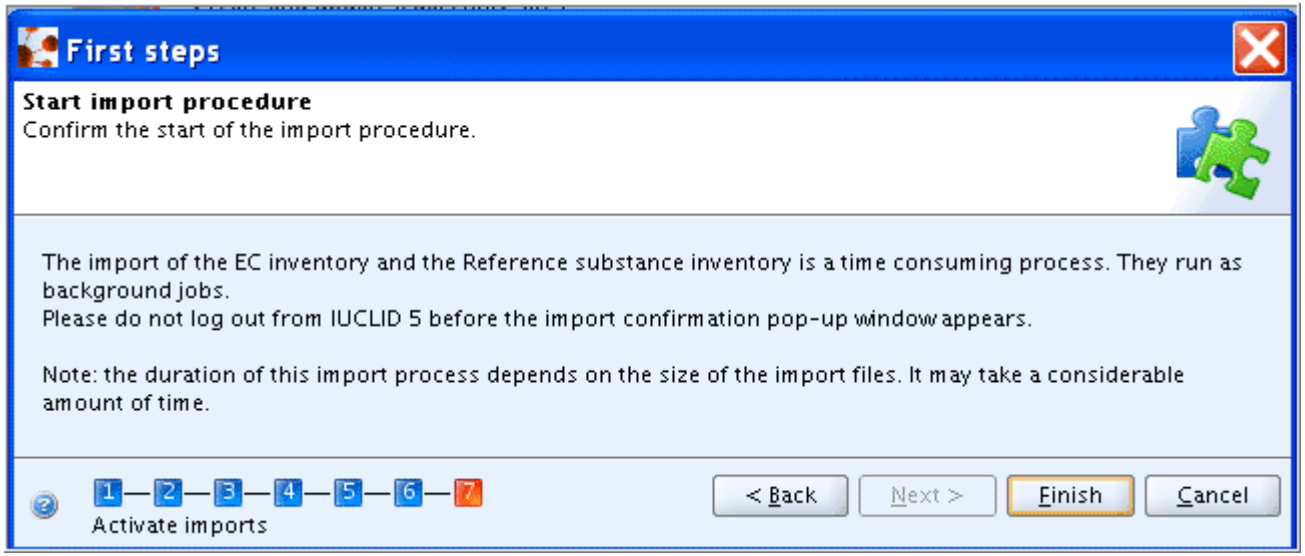
- Assign a Legal entity (normally the Legal entity imported in the third step of this wizard) by clicking the green plus button and performing a search for the desired Legal entity. In the Query field `Legal entity name`, enter the name of the desired Legal entity or an asterisk (*) as wildcard and click the **Search** button. In the Query results list, click the desired entry and then click the **Assign** button.
- Optionally, select default attachment and import/export directories. These settings can be made at a later stage as described in the IUCLID 5 End User Manual chapter D.16.5 Feature "User Preferences": How to set User Preferences .
- Click the **Next** button



9. Step 7: If you have selected an EC Inventory and/or Reference substances inventory file(s) during the wizard steps, you can now run the imports. Click the **Execute imports** button. Note again that these imports may take up to several hours, depending on your machine speed and the amount of data you are importing.

   Then click the **Finish** button. If you have launched any imports, you will now have to wait until the imports are completed. Afterwards, you should

log out and then log in again as a user for the newly defined account (remember: working as SuperUser is not supported).



3. Creating a dataset for a Substance and assigning a Reference substance

The tutorial in this chapter shows how to create a Substance dataset and assign a Reference substance to it.

Introduction

In IUCLID, there are three important parts related to the identification of a Substance:

- EC Inventory: This is the chemicals identifiers catalogue which is centrally managed and provided by the European Commission / European Chemicals Agency. The IUCLID feature EC Inventory allows browsing this catalogue, provided it was downloaded from the IUCLID web site. See the IUCLID 5 End User Manual chapter D.12 Inventories (View Inventory related information) .

- Reference substance inventory: This is a local inventory managed and upgraded by the users on their IUCLID installations as appropriate. See the IUCLID 5 End User Manual chapter D.11.1 Reference substance inventory .

Note

An inventory of ca. 70,000 Reference substances listed in the EC inventory can be downloaded from the IUCLID web site and imported into your IUCLID system.

- Substance dataset: This is the central core of information in IUCLID. It contains all data related to a chemical substance like the chemical identity including the substance composition, information on manufacture, use and exposure, information on the classification and labelling, and all required and available endpoint study summaries. A Substance dataset is the repository of data, which is used to create a Dossier for the submission substance. See the IUCLID 5 End User Manual chapter D.4 Substance (Create and update substance related information) .

When a Substance dataset is created for a given chemical substance, it is assigned to a Reference substance, which in turn is based on the EC Inventory or, if not listed, newly defined. The difference between the (submission) substance after which a Substance dataset is named and the assigned Reference substance is briefly explained based on the following examples of (i) a mono-constituent substance and (ii) a multi-constituent substance:

- Diethyl peroxydicarbonate:
  - Reference substance = Diethyl peroxydicarbonate as listed in EC inventory, with the following identifiers: EC 238-707-3, CAS 14666-78-5, C6H10O6
  - Submission substance = e.g. Diethyl peroxydicarbonate, i.e. named after the Reference substance as main constituent, but includes isododecane as stabilizing agent and, hence, an additive together with impurities which need to be specified in section *1.2 Composition*. The typical concentration of diethyl peroxydicarbonate in this substance is 22% with an upper limit of 27%.
- Mixture of 1,4-dimethylbenzene, 1,2-dimethylbenzene and 1,3-dimethylbenzene:
  - Reference substance = Mixture of 1,4-dimethylbenzene, 1,2-dimethylbenzene and 1,3-dimethylbenzene, with the following identifiers: EC 215-535-7, CAS 1330-20-7, C8H10
  - Submission substance = e.g. Mixture of 1,4-dimethylbenzene, 1,2-dimethylbenzene and 1,3-dimethylbenzene, i.e. named after Reference substance as main constituents, but with identification of all these constituents, i.e. 1,4-dimethylbenzene (30-40%), 1,2-dimethylbenzene (25-35%), 1,3-dimethylbenzene (20-30%), and impurities (water, 5-12%).

Workflow

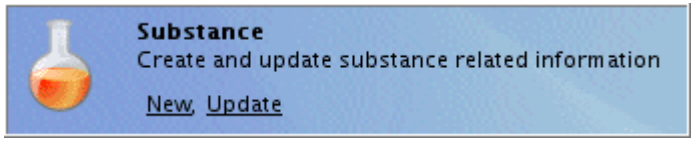
The creation of a Substance dataset and completion of sections 1 to 3 includes the following workflow:

- Launch the New Substance feature and define the Substance name and the Legal entity owner.
- Assign a Reference substance to the Substance dataset.
- In case of a newly created Reference substance, switch to the corresponding record and assign the respective identity from the EC inventory to that Reference substance; complete other identifier fields.
- Switch back to the Substance.
- Complete sections 1, 2 and 3 as appropriate.

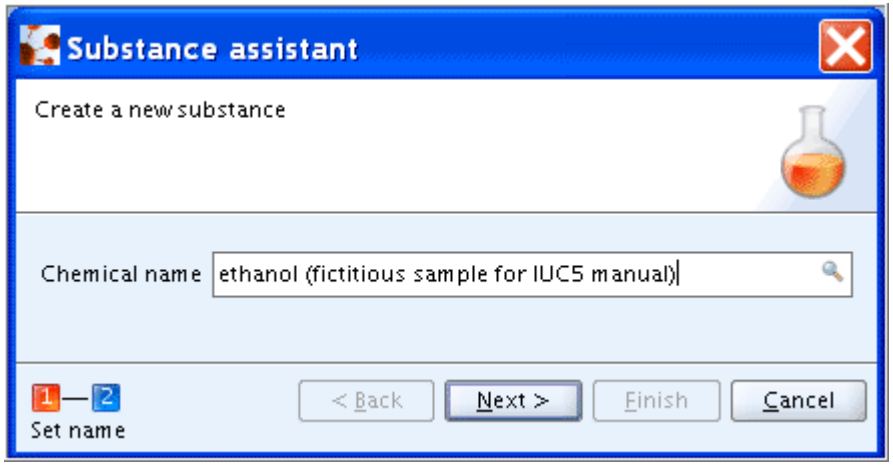
Step-by-step guide

The following step-by-step guide is illustrated by screenshots based on fictitious sample data.

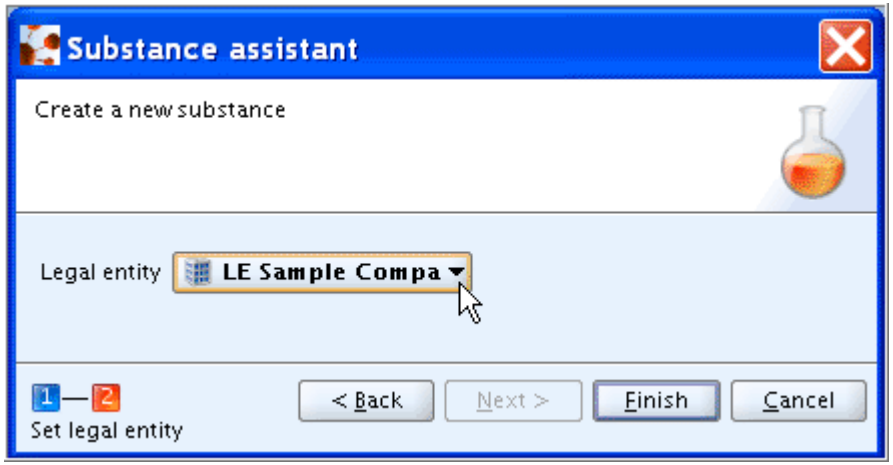
1. Select the command **New Substance** either from the IUCLID Task panel or the File menu on the Menu bar.



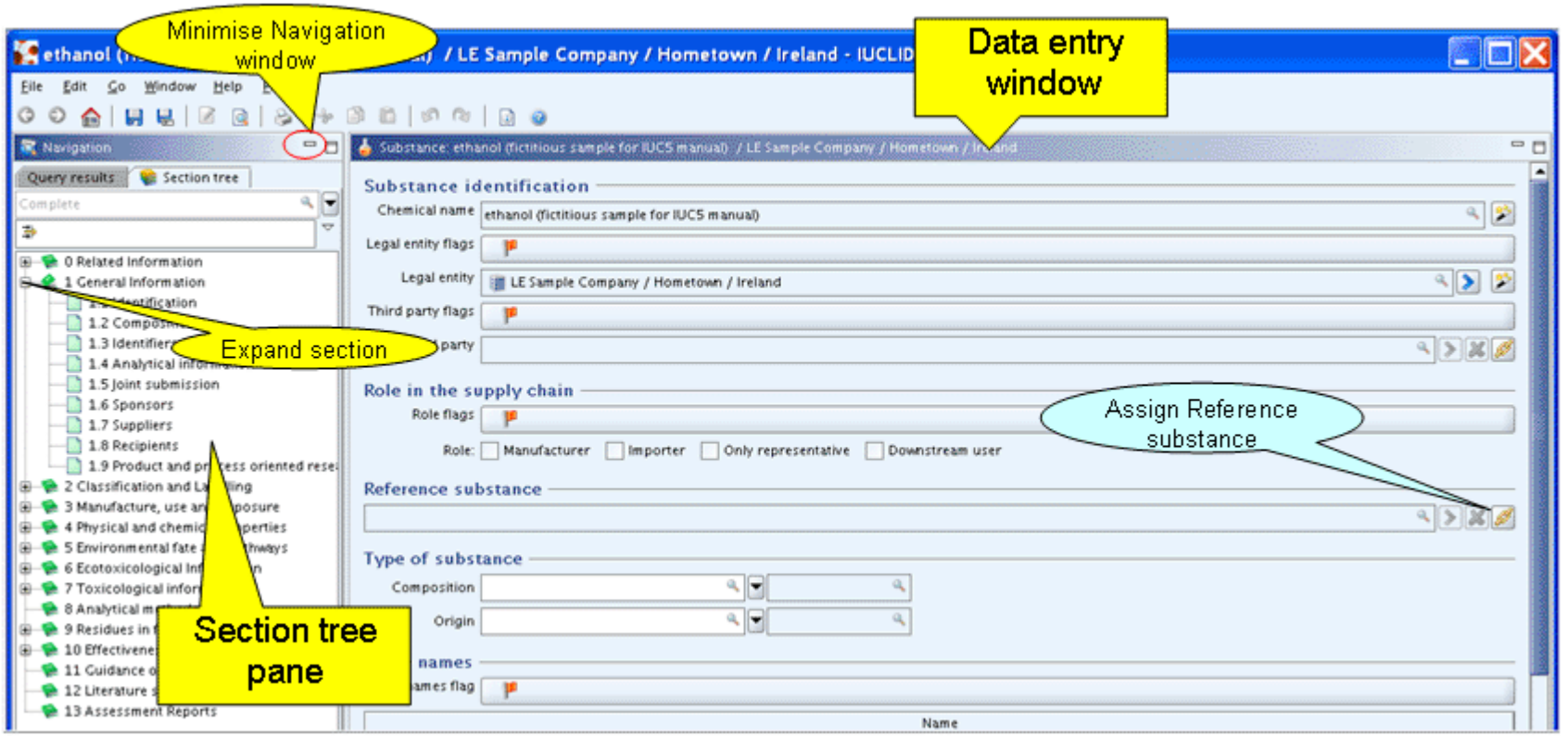
2. The Substance wizard comes up and guides you through following steps:
    - Enter the user-defined name of the Substance and click the **Next** button.



3. Select the Legal entity from the drop-down list and click the **Finish** button. (Note: Use the Legal entity defined for your company or, if not available yet, any other available Legal entity created at the IUCLID web site (i.e. "official" Legal entity, LEO). If necessary, a new Legal entity can be created later on and assigned to this dataset. See the IUCLID 5 End User Manual chapter D.9.2 Feature "Legal entity": How to create a Legal entity).



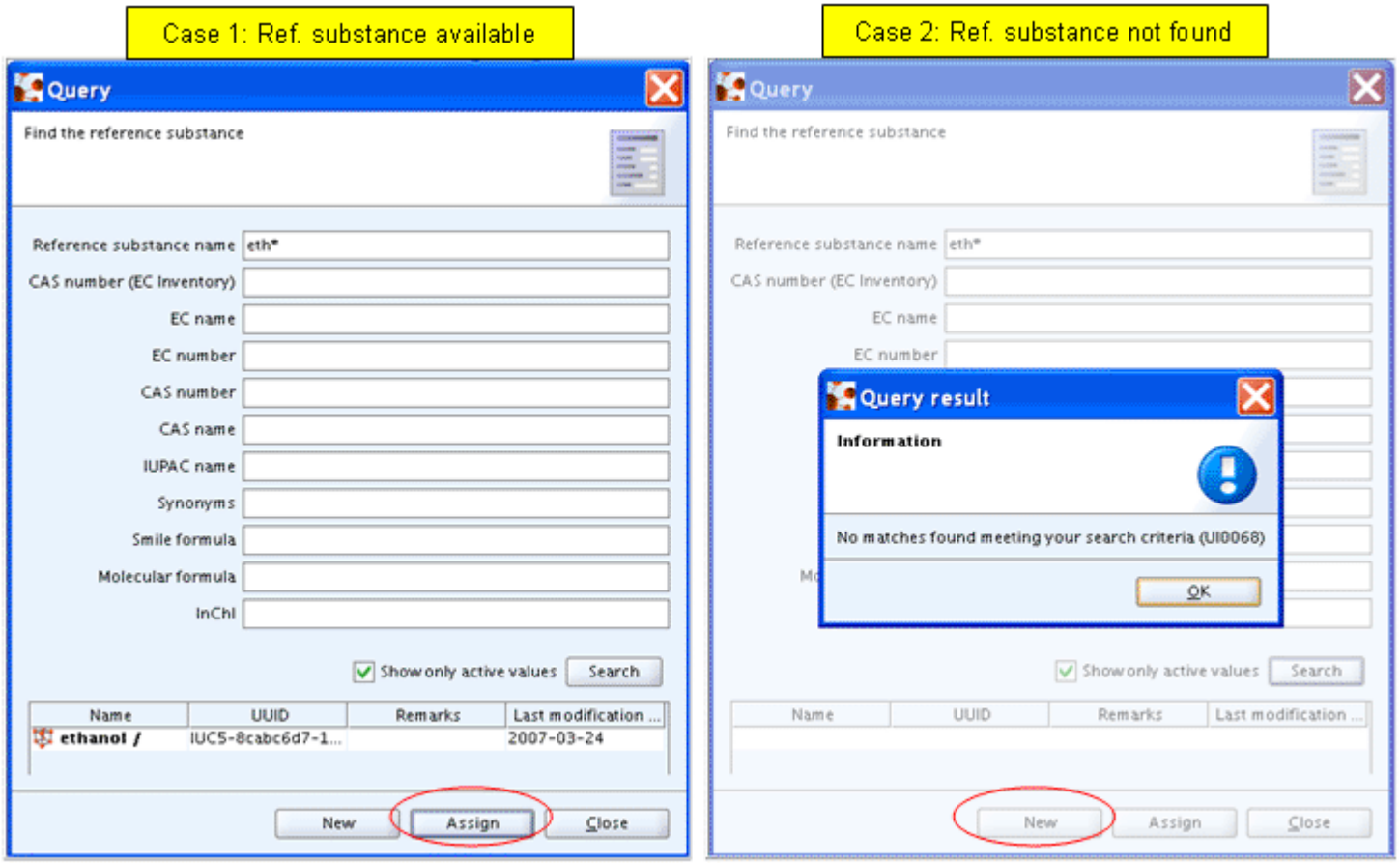
4. The newly created Substance dataset is displayed in the Data entry window and tabs **Query results** and **Section tree** appear in the Navigation window. In case of a smaller monitor, you may click the **Minimize** button on the Navigation bar (circled in the screenshot below) to enlarge the Data entry window.



5. To assign a Reference substance, click the button **Add reference** button in field `Reference substance` (see the screenshot above). In the appearing Query dialogue box, proceed as follows:

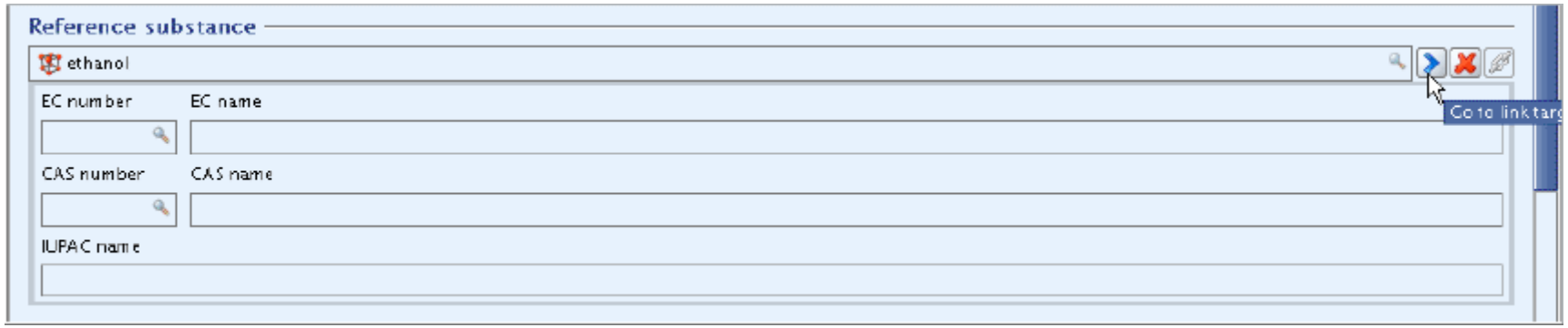
   - Case 1: Search for the desired Reference substance. For example enter "ethanol" or "eth*" in the search field `EC name` and click the **Search** button or press the Enter key.

   - Case 2: If the substance is not found, click the New button and enter an appropriate name, e.g. "ethanol". Then click the **Finish** button. (Note: The Reference substance can also be defined later using the corresponding feature (see the IUCLID 5 End User Manual chapter D.11.3 Feature "Reference substance - New": How to create a Reference substance) and assigned to this dataset.)

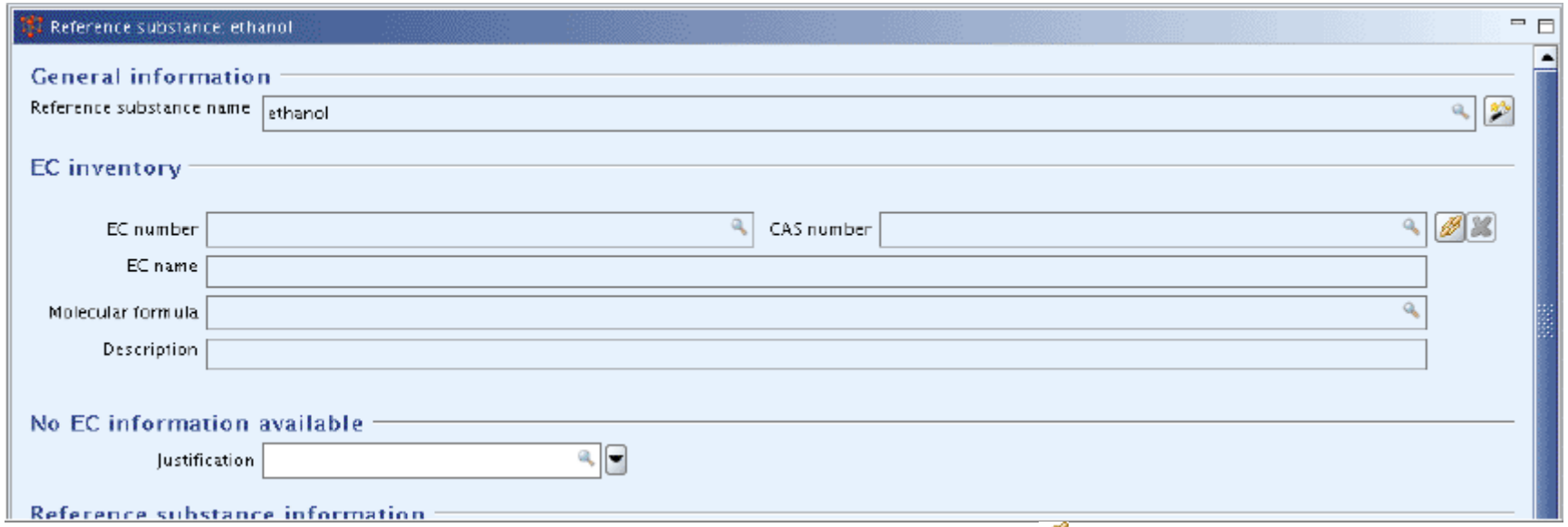


6. If a new Reference substance has been created, an EC inventory and/or other identifiers should be defined as follows:

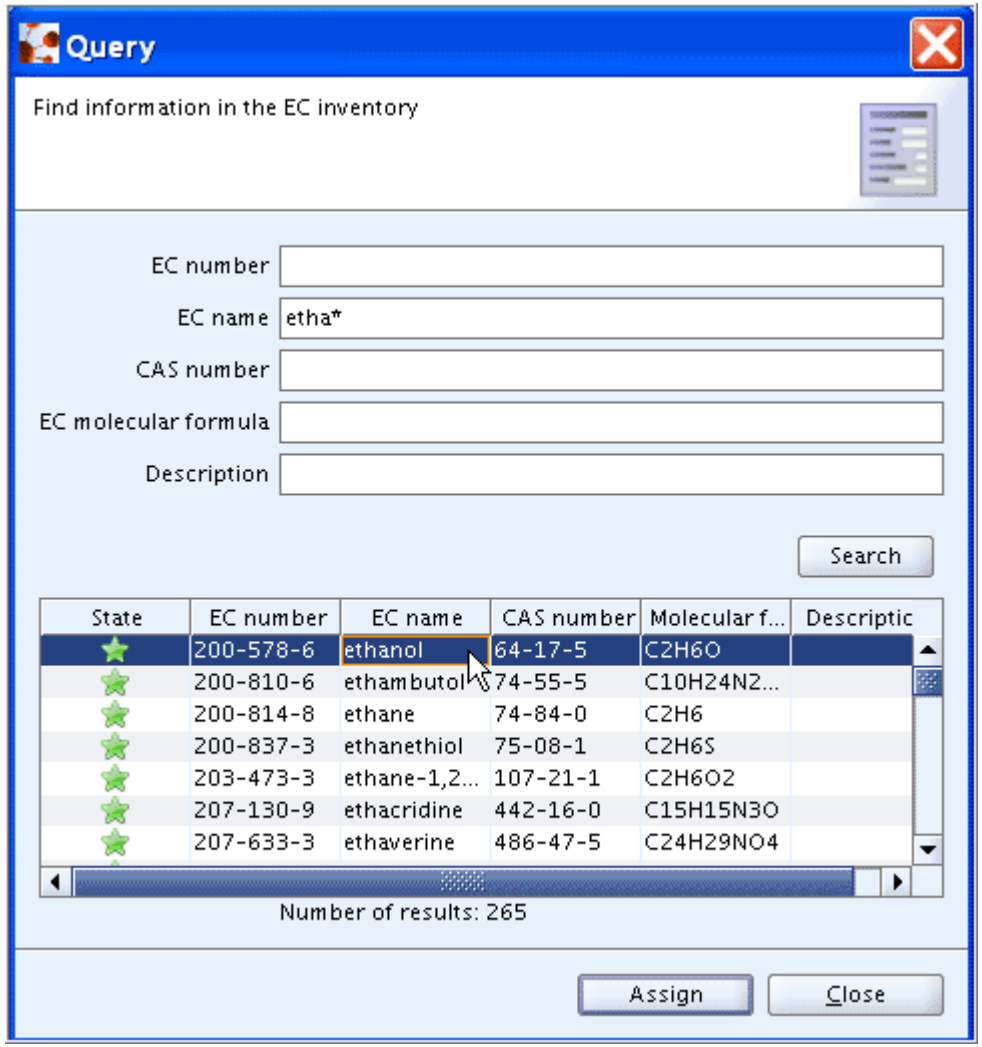
   - Switch to the Reference substance feature by clicking the **Goto** button ❯ to the very right.



7. An empty Reference substance record appears.

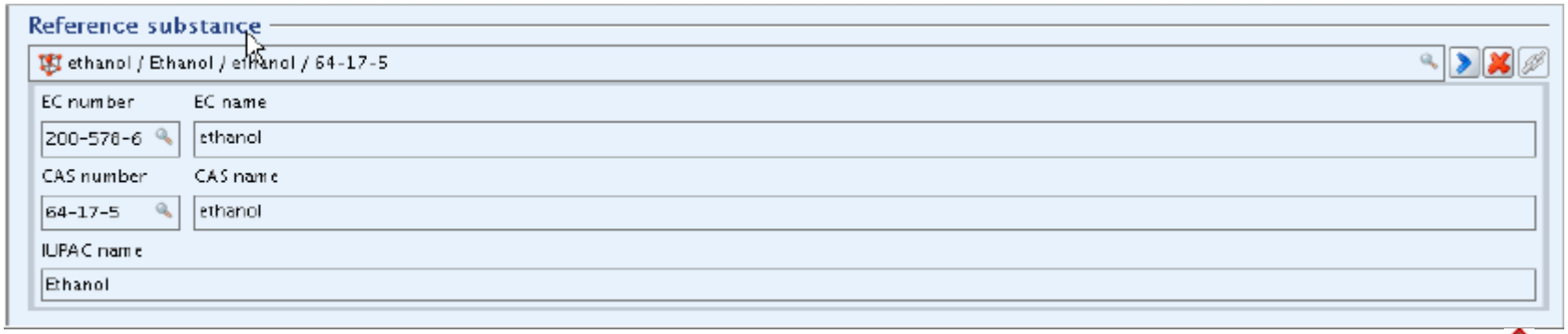


8. To assign the corresponding EC inventory identity, if available, press the **Add reference** button to the very right and in the Query dialogue appearing, search for the substance and click the **Assign** button. (Note: If data entry is locked, click the **Edit** button on the toolbar.)



9. EC number, EC name, CAS number, Molecular formula and Description (if any) are automatically entered in the Reference substance record. You may complete any other fields (e.g. CAS name, IUPAC name, Synonyms, SMILES notation) now or later.

- By clicking the **Back** button on the toolbar, you can then navigate back to the Substance dataset. The identifier fields of the assigned Reference substance are displayed.



10. The newly created Substance dataset is now related to a Reference substance and you can close the dataset by clicking the **Go Home** button or continue completing the dataset as instructed in chapter 4 Completing a Substance dataset.

Tip

Although the Reference substance can be assigned to a Substance any time, it is highly recommended to do this right when creating the Substance dataset because of the following reason: As shown in chapter 4.2 Entering/editing data in sections 4 to 13, each time you create a new Endpoint study record, the field `Test material identity` is automatically filled with the identifiers of the Reference substance. If the Reference substance is assigned later, this field will not be automatically updated. Instead, the substance identifiers would have to be entered manually in each record.

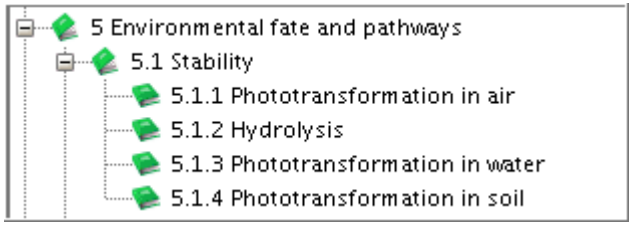
4. Completing a Substance dataset

The tutorial in this chapter shows how to complete sections of a Substance dataset. Sample data and instructions are given for

- Entering/editing data in sections 1 to 3 (chapter 4.1)
- Entering/editing data in sections 4 to 13 (chapter 4.2)

Introduction

A IUCLID dataset is structured into 13 main sections. Many of these sections are further broken down to subsections as exemplified in the following screenshot:



There is a striking difference as regards data entry between sections 1 - 3 and sections 4 -13 as follows:

- Sections 1 - 3: Data are entered directly into the subsections and all sections 1 to 3 are physically managed as one record. No further records can be created.
- Sections 4 -13: Data can only be entered into Endpoint study records or Endpoint summary records, which have to be created by the user.

This is illustrated on the user interface by different symbols: any title of subsections within sections 1 to 3 are preceded by a green or red leaf symbol, while any record in sections 4 to 13 is indicated by a green bullet. For more information see the IUCLID 5 End User Manual chapter D.4.6.1 Differences between sections 0 - 3 and sections 4 - 13 .

Note

Section *0 Related Information* contains special information on Templates, Categories and Mixtures and is not considered in this sample session for beginners, which explains the features and functions that are most commonly used for editing a Substance dataset based on hands-on examples.

Workflow

To edit and complete a Substance dataset the following workflow applies:

- Open the Substance dataset.
- Expand the section tree to display the subsections.
- Customise the view mode, i.e. display the sections required for a given regulatory programme.
- Complete sections 1, 2 and 3 as appropriate.
- Complete the Endpoint sections 4 to 13 as far as required.

4.1. Entering/editing data in sections 1 to 3

Introduction

IUCLID sections 1 to 3 comprise general and non-endpoint information. The following type of information is addressed:

- Section *1 General information*: General information on the substance includes its chemical identity as represented by the associated Reference substance, its composition, its various business relationships (identity of sponsors, suppliers or recipients and members of a joint submission/consortium), identifiers assigned by regulatory programmes (e.g. REACH registration number) and other IT systems (e.g. IUCLID 4 reference), analytical information and spectral data, and information on product and process oriented research and development (if applicable). For more information, see the IUCLID 5 End User Manual chapter E.1 Section 1: General Information.
- Section *2 Classification and labelling*: The classification and labelling information can be added to this section according to the Globally Harmonised System for Classification and Labelling (GHS) and /or according to the European Directives (67/548/EEC for substances and 1999/45/EC for preparations) and amendments and adoptions thereof. For more information, see the IUCLID 5 End User Manual chapter E.2 Section 2: Classification and Labelling.

- Section *3 Manufacture, use and exposure*: Information stored in this section includes the following: information on the manufacturing methods, estimated quantities of production, import and use, production/use sites, availability in the supply chain, uses and exposure scenarios, waste production, and chemical compounds resulting from the production or use of the substance. For more information, see the IUCLID 5 End User Manual chapter E.3 Section 3: Manufacture, Use and Exposure .

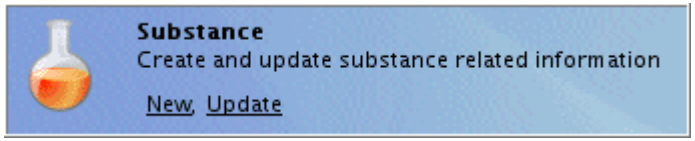
Note

Section 0 Related information is actually not a data entry section, but provides means to relate other IUCLID elements to a dataset or indicates any related information, i.e. Templates, Mixtures, Categories (see the IUCLID 5 End User Manual chapter B.4.2.1 General and non-endpoint information).

Step-by-step guide

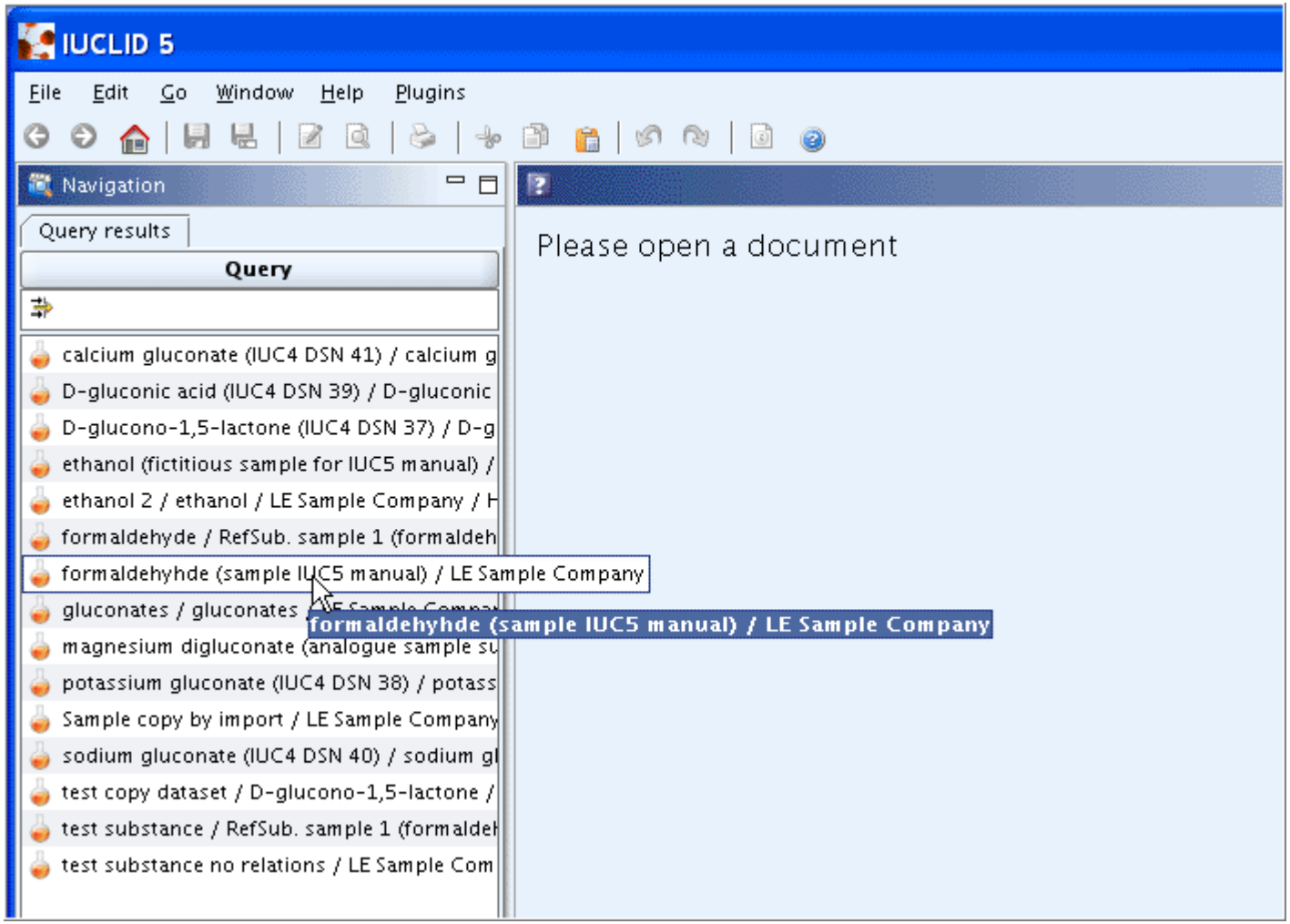
The following step-by-step guide is illustrated by screenshots based on fictitious sample data.

1. Select the command **Update Substance** from the IUCLID Task panel.



2. A screen comes up with an empty Data entry window on the right side and a **Query results** pane on the left (below the title bar **Navigation**) showing all substances available in your local IUCLID installation or the network you are connected to.

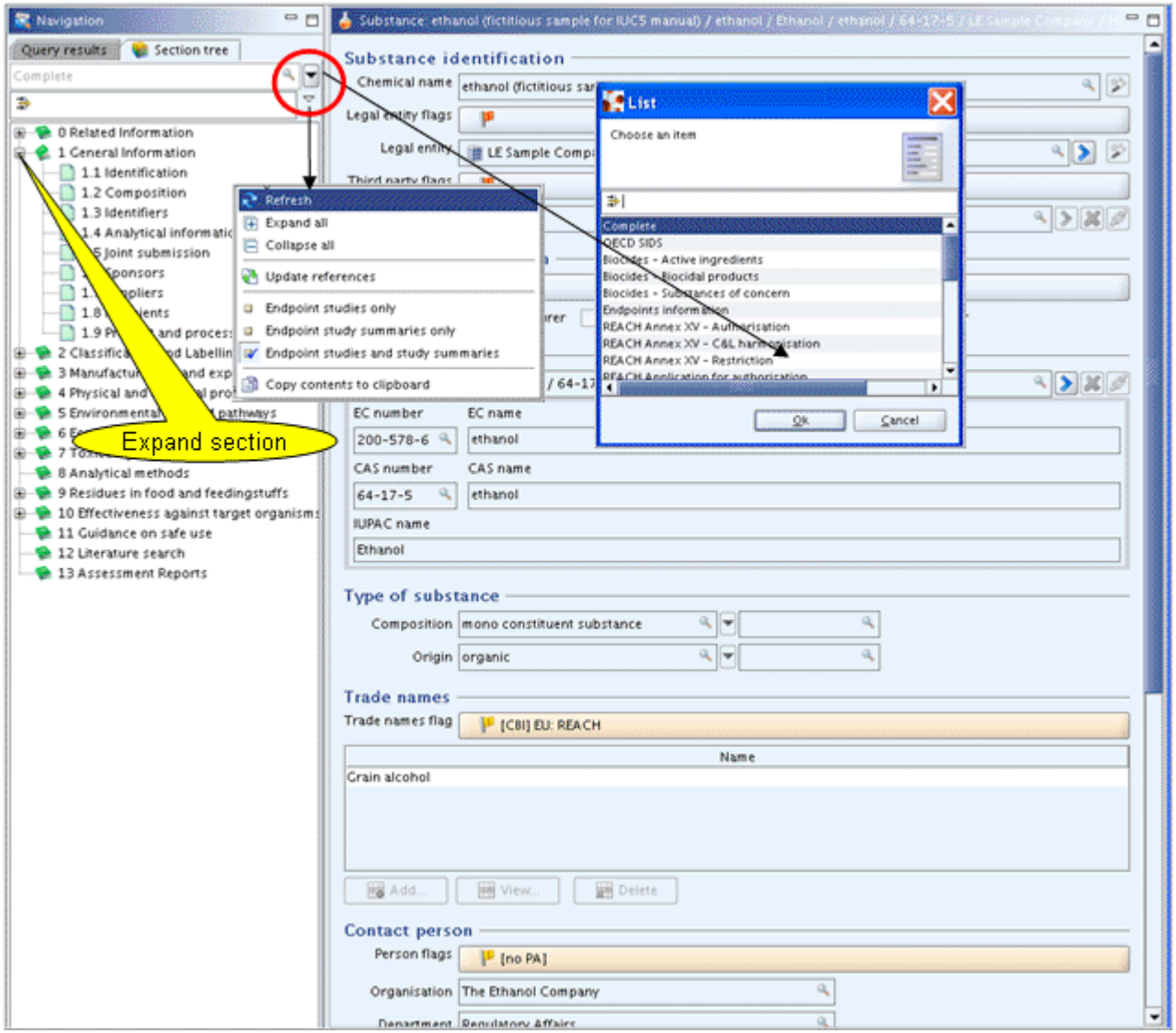
   Double-click the desired Substance (left mouse button) to open the corresponding dataset. If there is a large number of Substances listed, run a query as described in the following the IUCLID 5 End User Manual chapter D.4.3.2 Querying for a Substance in the Query results pane . (Note: You can also open the dataset from the context menu that comes up on right-clicking the Substance.)



3. When the Substance dataset is opened, the Navigation window provides, next to the **Query results** tab, a second tab, i.e. the **Section tree**. Click it to switch to the **Section tree pane**. Get acquainted with following features:

   - **Expand section tree**: Click the **Plus** symbol in front of any section (e.g. *1 General Information*) or the arrow next to the Find pane (red circle in the screenshot below) and from the drop-down list box select **Expand all**.

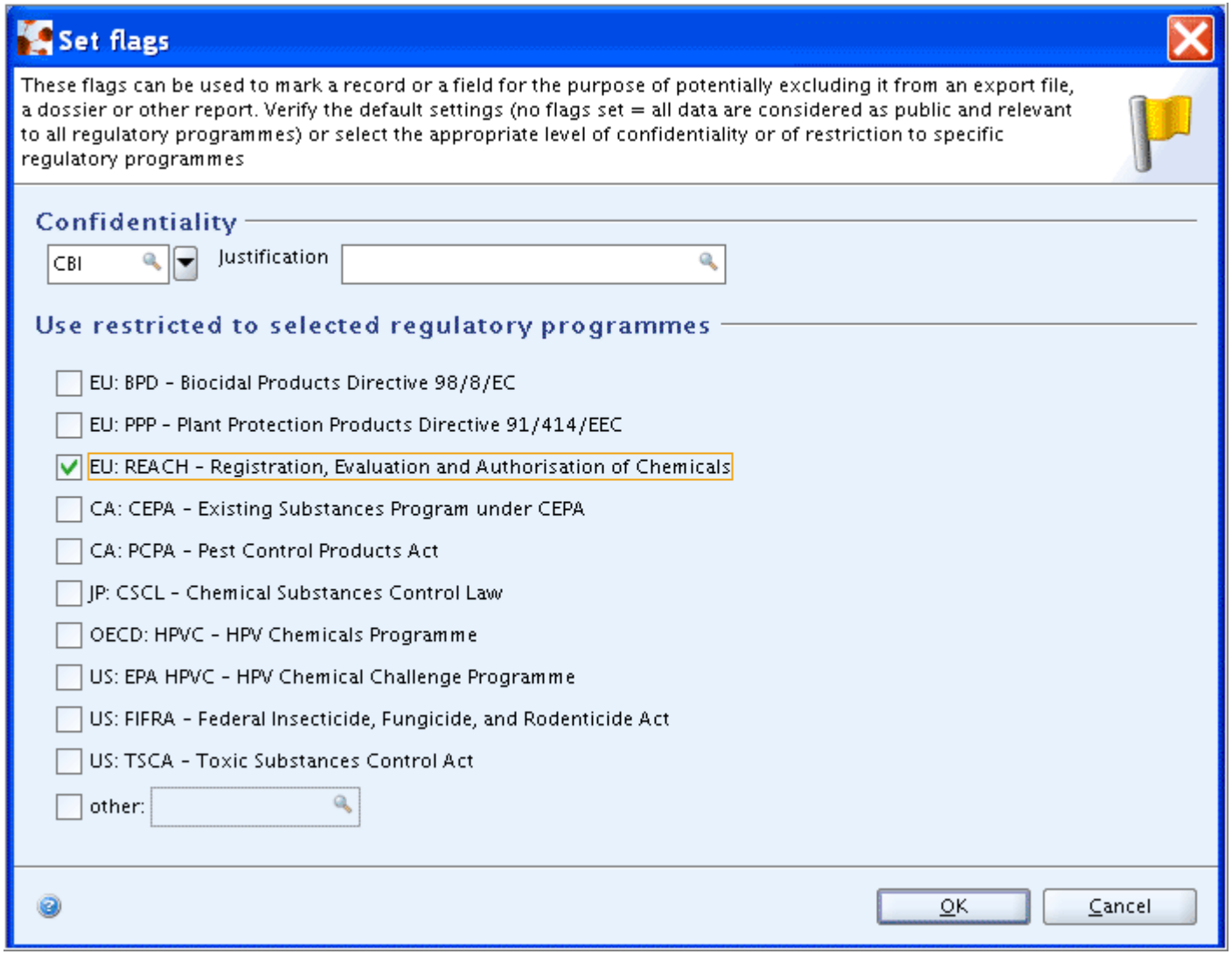
- **View mode selector**: Click the black arrow next to the view mode indicator (just below the Query/Section tree tabs) to open a drop-down list box for selecting the view mode. By default, the view mode "Complete" is set. Select another mode as appropriate, e.g. "REACH Registration 1 - 10 tonnes, standard requirements". The section tree then changes in such a way that the book symbols in front of the sections required for such a registration or submission are coloured red, while the symbol for all optional sections remains green. Some sections, which do not apply (i.e. biocides-related sections) are excluded.



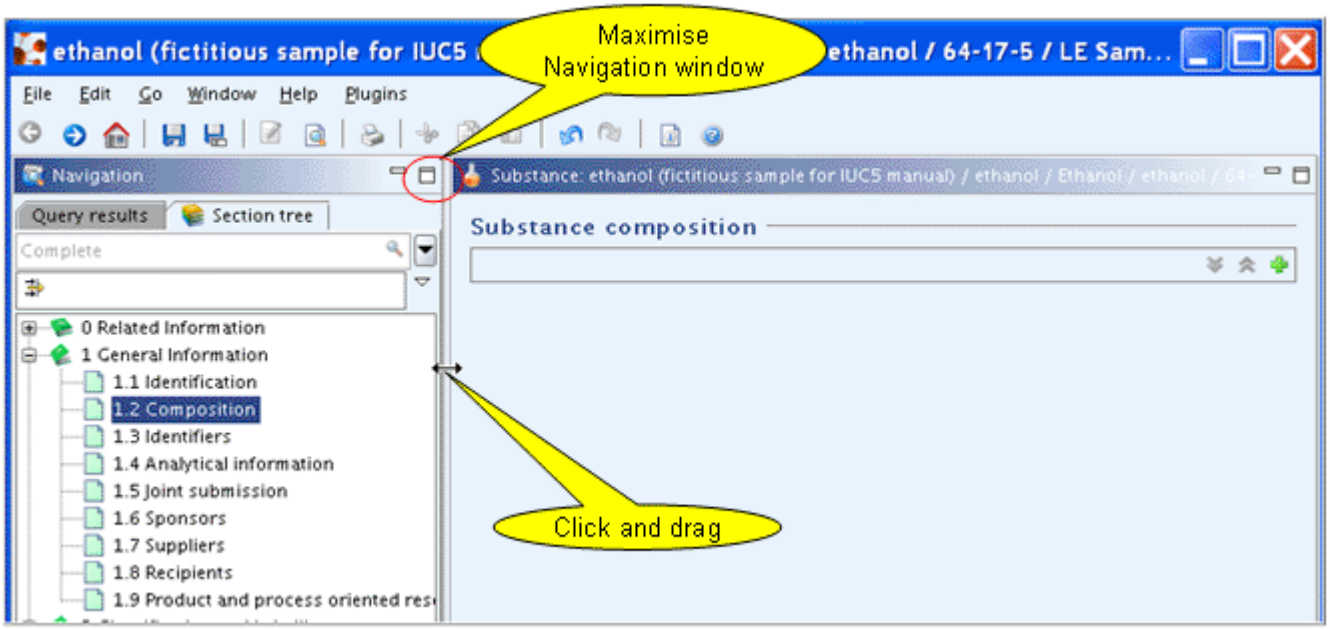
4. In IUCLID section *1.1 Identification*, complete the fields under headings `Role in the supply chain`, `Type of substance`, `Trade name` and `Contact person`, as illustrated in the screenshot above.

Tip

Throughout the IUCLID sections, flags dialogue boxes are provided either related to specific parts (e.g. `Trade names flag` and `Person flag` in the screenshot above) or to an entire record. These dialogue boxes have always the same design and include both the `Confidentiality flag` and `Regulatory purpose flags`, which can be used to filter out the flagged data in subsequent operations such as exporting, printing or Dossier creation. For example, set flags "CBI" (confidential business information) and "EU: REACH" for `Trade names flag`.

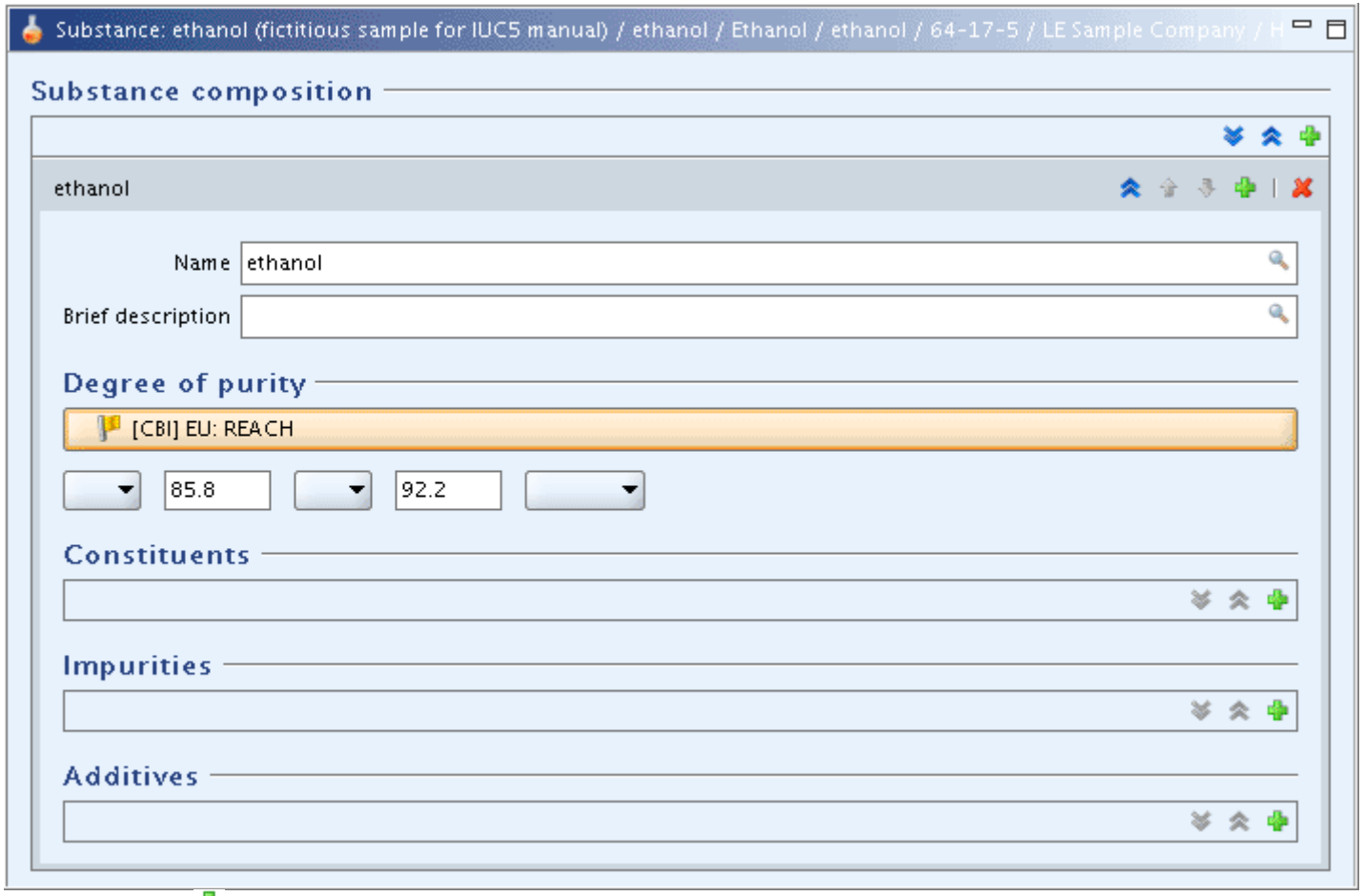


5. Navigate to section `1.2 Composition` by double-clicking the respective section title in the Section tree pane (if necessary, click the **Maximise** button on the Navigation bar or hover the mouse directly on the divider between the Navigation and the Data entry window until the pointer changes to a double-headed arrow. Then click and drag the line to the left or right).



6. In section `1.2 Composition`, complete the fields in the repeatable block, which allows to specify multiple compositions for the substance (needed for substances with e.g. different impurity profiles):

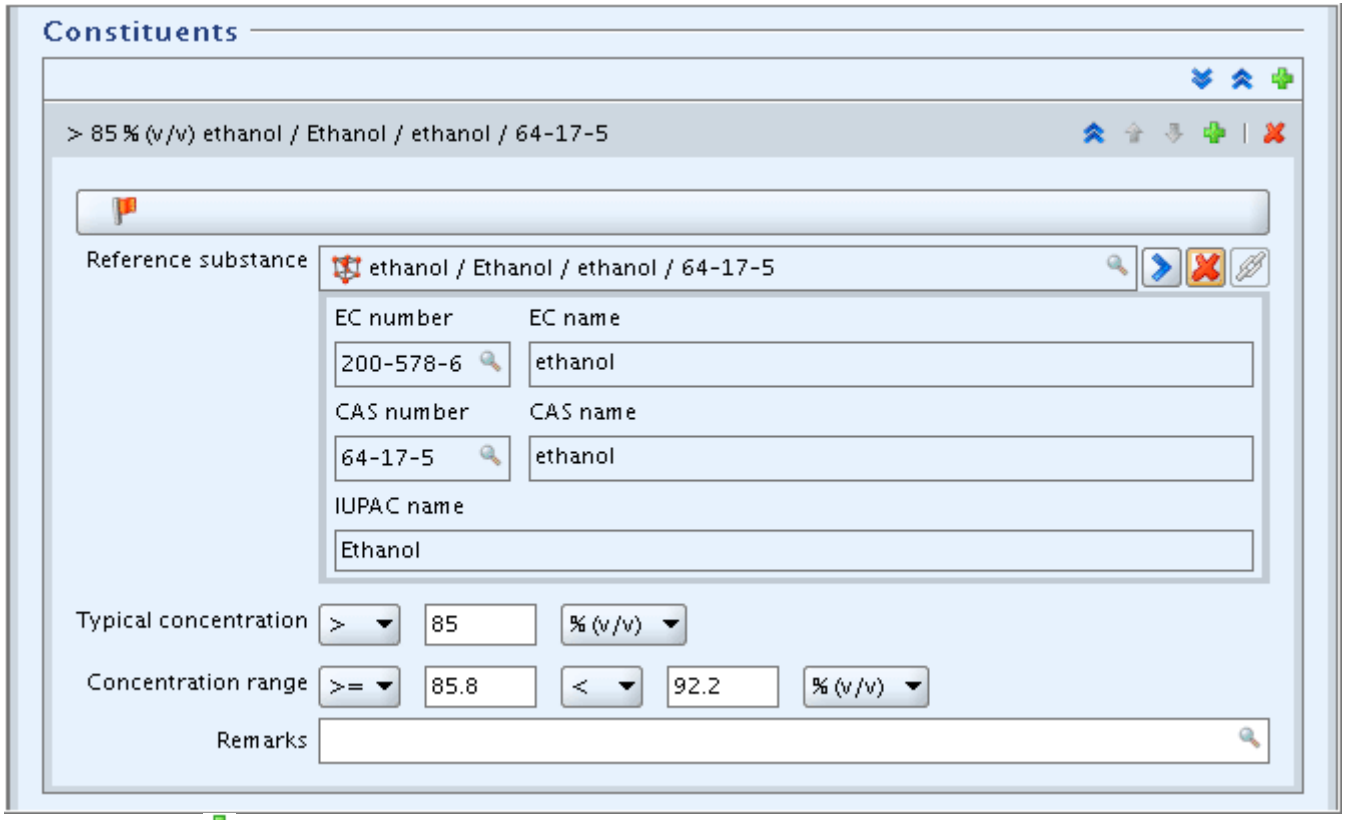
   - Click the Add symbol ✚ to expand the block `Substance composition`.
   - Enter the name you wish to assign to this composition (or composition profile) and specify the typical degree of purity of the substance.
   - Set the Confidentiality and/or Regulatory purpose flags related to the degree of purity if so required (see the following screenshot).



7. Click the **Add** symbol to open the block `Constituents`.

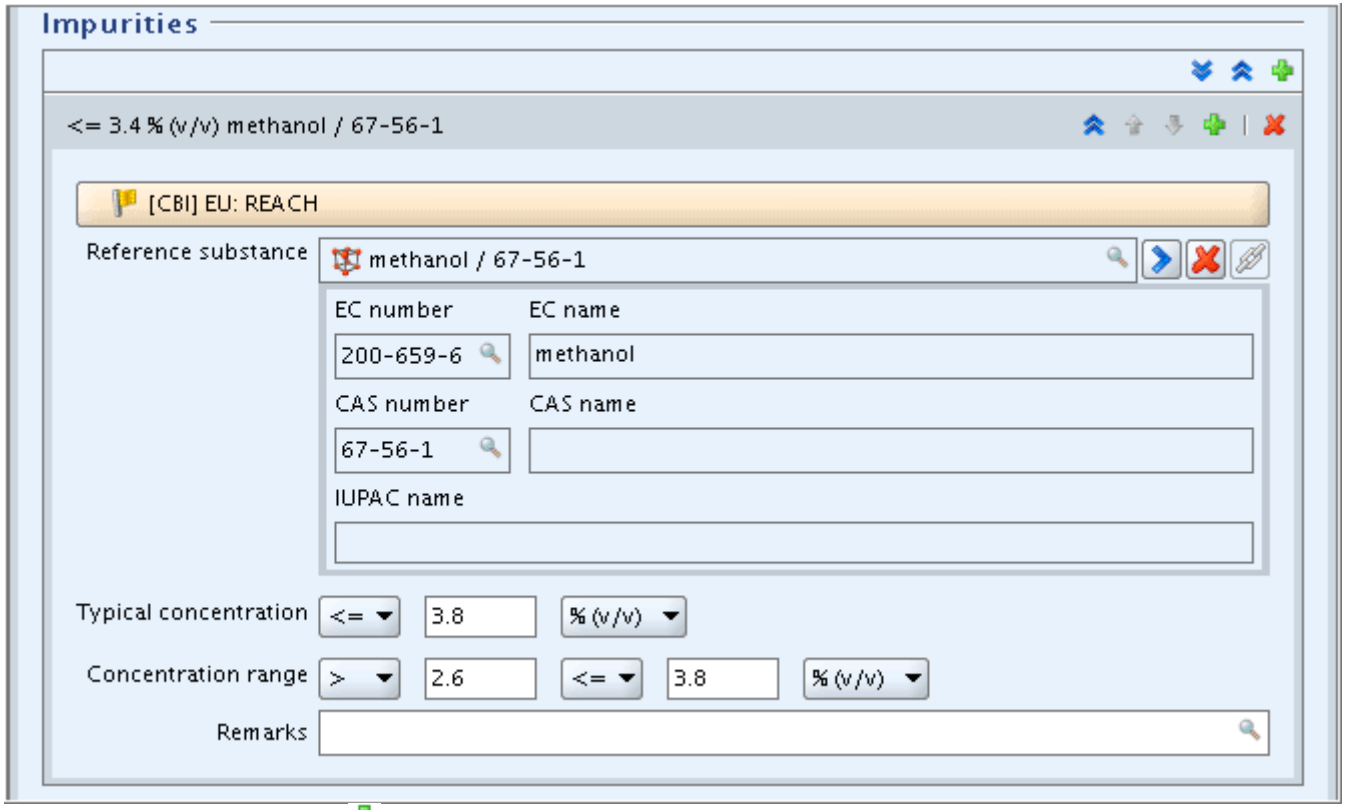
- Specify the constituent by assigning the respective Reference substance, which is identical with that for the Substance in case of a mono-constituent (i.e. ethanol). See step 4 (Case 1) on assigning a Reference substance to the Substance in chapter 3 Creating a dataset for a Substance and assigning a Reference substance.

- Complete the fields `Typical concentration` and `Concentration range` in the `Constituents` block. The field `Remarks` can be used for any relevant information (e.g. for giving a brief justification in case of deviation of the 80% rule for multi-constituent substances).



8. Click the **Add** symbol to open the block `Impurities`.

- Specify the first impurity by assigning the respective Reference substance (e.g. methanol). See steps 4 and 5 on assigning a Reference substance to the Substance. Be aware to click the **Edit** button on the toolbar if the Reference substance record is locked.
- From the Reference substance record go back to the `Impurities` block, again click the **Edit** button and complete the fields.



9. Repeatedly click the **Add** symbol for the blocks `Constituents`, `Impurities` and/or `Additives` to record all substances as appropriate.

10. Complete any other subsections of sections 1, 2 and 3. See guidance in the IUCLID 5 End User Manual chapter E.1 Section 1: General Information , E.2 Section 2: Classification and Labelling and E.3 Section 3: Manufacture, Use and Exposure, respectively.

4.2. Entering/editing data in sections 4 to 13

Introduction

IUCLID sections 4 to 11 are also called "Endpoint sections". In this context, an endpoint is meant as an information requirement or data point with regard to

the physico-chemical properties of the substance, environmental fate and behaviour, ecotoxicological information, toxicological information and specific information (e.g. residues in food and feedingstuffs) according to a given regulatory programme, e.g. the standard information requirements set out in the EU REACH Annexes VI to XI.

A IUCLID Endpoint section provides the container for storing "endpoint study" data, e.g. a study on vapour pressure to be entered in section *4.6 Vapour pressure* or a study on repeated dose toxicity (oral) to be entered in section *7.5.1 Repeated dose toxicity: oral*. The term "study" has a rather generic meaning in that it refers to any experimental study, but also to an estimation or prediction method including (Q)SAR, read-across, weight of evidence evaluation, data waiving or any other type of information being relevant for a given information requirement. For more information see the IUCLID 5 End User Manual chapter B.4.2.2 Summaries of study reports and other information .

The collection of endpoint-related information in IUCLID is based on summarising descriptions of full study reports. These study summaries can be very condensed or very detailed. However, a study summary should provide sufficient information to make an assessment of the relevance of the study. Very detailed study summaries are also termed "robust study summaries", if they address all relevant study items (see the IUCLID 5 End User Manual chapter B.4.2.2.3.1 Definition of key studies, supporting studies, robust study summaries).

In IUCLID, study summaries are managed using Endpoint study records, which are templates with predefined fields and freetext prompts intended to help the user summarise a study (see the IUCLID 5 End User Manual chapter D.4.7.1 What is an Endpoint study record?). Each Endpoint study record of sections 4 to 10 is structured into the following main parts:

- Administrative data
- Data source
- Material and methods
- Results and discussion
- Overall remarks, attachments
- Applicant's summary and conclusions

Under these headings certain data entry fields are subsumed which are common to all Endpoint study records, in addition to endpoint-specific data entry fields. Because many fields are only relevant for robust study summaries, a system of detail levels has been implemented in IUCLID. This allows displaying

either only the basic fields or all fields (see the IUCLID 5 End User Manual chapter D.4.7.6 Switching between display type "basic fields" (detail level 1) and "all fields" (detail level 2)).

Almost all IUCLID Endpoint study records are modelled on the so-called OECD harmonised templates, which are standard formats for reporting endpoint study summaries related to any type of a chemical (e.g. pesticides, biocides, industrial chemicals) (see the IUCLID 5 End User Manual chapter D.4.7.1 What is an Endpoint study record?).

IUCLID does not prescribe how detailed the study summaries should be recorded. The fields provided should be considered as a maximum degree of detail. Older study reports or literature sources often do not provide the details for which many fields prompt for on a robust study summary level. On the other hand, more recently conducted studies and any new studies can be summarised in a very detailed manner. Refer to the relevant guidance for the respective chemical programme on how detailed studies need to be summarised. In the case of existing IUCLID 4 datasets prepared in the context of the OECD High Production Volume Chemicals Programme, EU Risk Assessment or for other purposes, which will be used for EU REACH, a pragmatic approach may have to be considered to avoid unnecessary additional work for adjusting these datasets to the new format in IUCLID 5.

Note

Sections *11 Guidance on safe use*, *12 Literature search* and *13 Assessment Reports* are not used for recording endpoint study summaries, but are also related to endpoint information.

Step-by-step guide

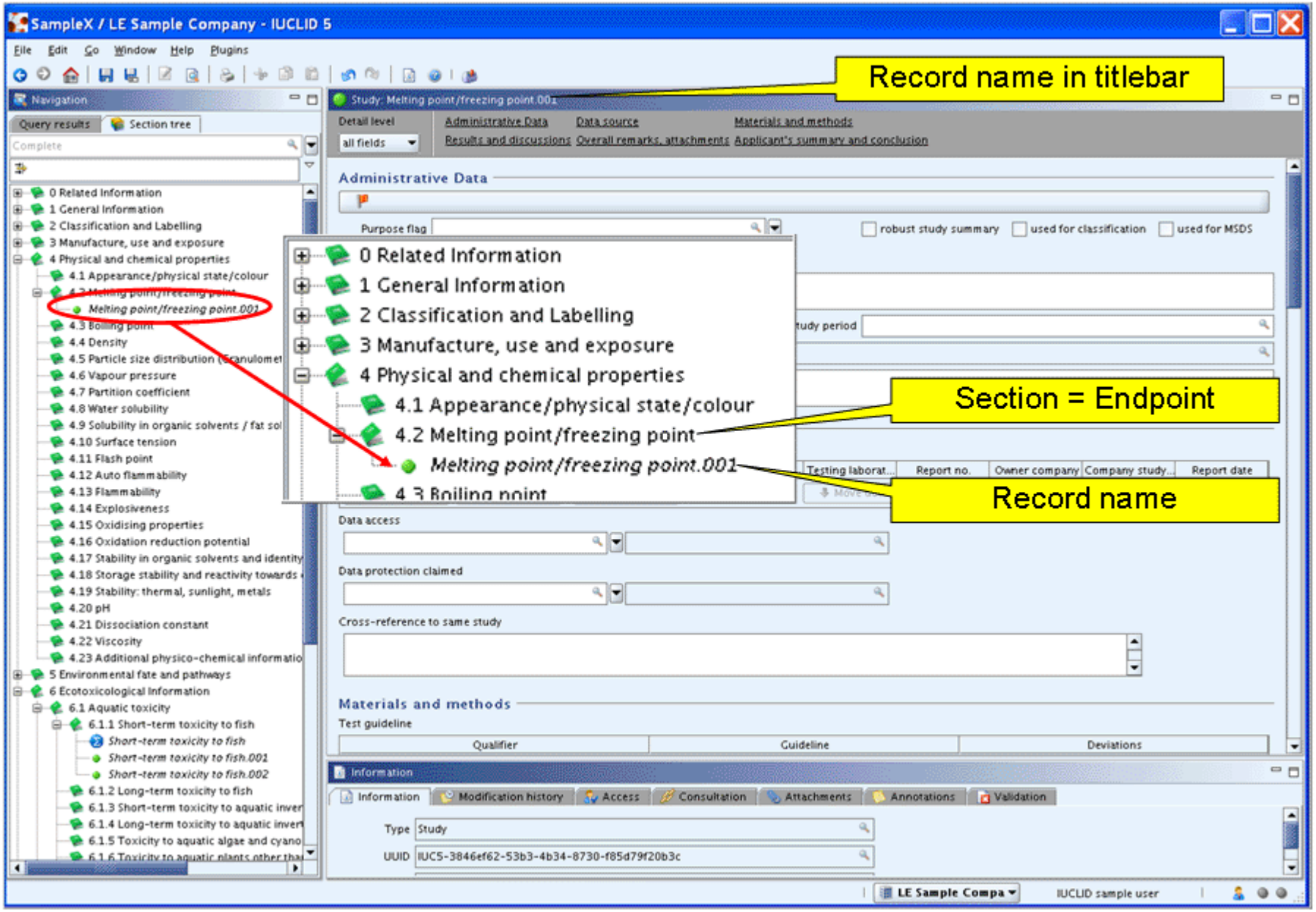
The following step-by-step guides are illustrated by screenshots based on fictitious sample data.

Creating an Endpoint study record

1. Open the Substance dataset as instructed in 4.1 Entering/editing data in sections 1 to 3.
2. Verify if the view mode "REACH Registration 1 - 10 tonnes, standard requirements" is selected (see chapter 4.1 Entering/editing data in sections 1 to 3).
3. Click the Plus symbol in front of section *4 Physical and chemical properties* to display all subsumed subsections.

4. Right-click section *4.2 Melting point/freezing point* and from the menu displayed, click the **New Endpoint study record** command.

5. A new record appears indicated by a green bullet  . A default record name is generated and displayed both in the section tree pane and the record titlebar. This record name consists of the section title followed by a dot and a consecutive number, e.g. "Melting point/freezing point.001", as shown in the following screenshot.


SampleX / LE Sample Company - IUCLID 5
File Edit Go Window Help Plugins
Record name in titlebar
Navigation
Query results
Section tree
Study: Melting point/freezing point.001
Detail level
all fields
Administrative Data
Data source
Materials and methods
Results and discussions
Overall remarks, attachments
Applicant's summary and conclusion
Administrative Data
Purpose flag
robust study summary
used for classification
used for MSDS
0 Related Information
1 General Information
2 Classification and Labelling
3 Manufacture, use and exposure
4 Physical and chemical properties
4.1 Appearance/physical state/colour
4.2 Melting point/freezing point
Melting point/freezing point.001
4.3 Boiling point
Section = Endpoint
Record name
Testing laborat...
Report no.
Owner company
Company study...
Report date
Data access
Data protection claimed
Cross-reference to same study
Materials and methods
Test guideline
Qualifier
Guideline
Deviations
Information
Modification history
Access
Consultation
Attachments
Annotations
Validation
Type
Study
UUID
IUC5-3846ef62-53b3-4b34-8730-f85d79f20b3c
LE Sample Compa
IUCLID sample user

Renaming an Endpoint study record

1. Select the record in the section tree pane and either press the F2 key or right-click the record and from the menu displayed, click the **Rename** command.

2. Edit the record name as appropriate and then click OK.

Tip

It can be useful to add additional information or even replace the default record name by information that gives an overview of the value of that record on the fly. Example: "Hommel (1987)/key.001" (indicates the Author and Year and that the record contains a key study). For more information see the IUCLID 5 End User Manual chapter D.4.7.3 Renaming an Endpoint Study Record .

Entering handbook data for section 4.2 Melting point/freezing point

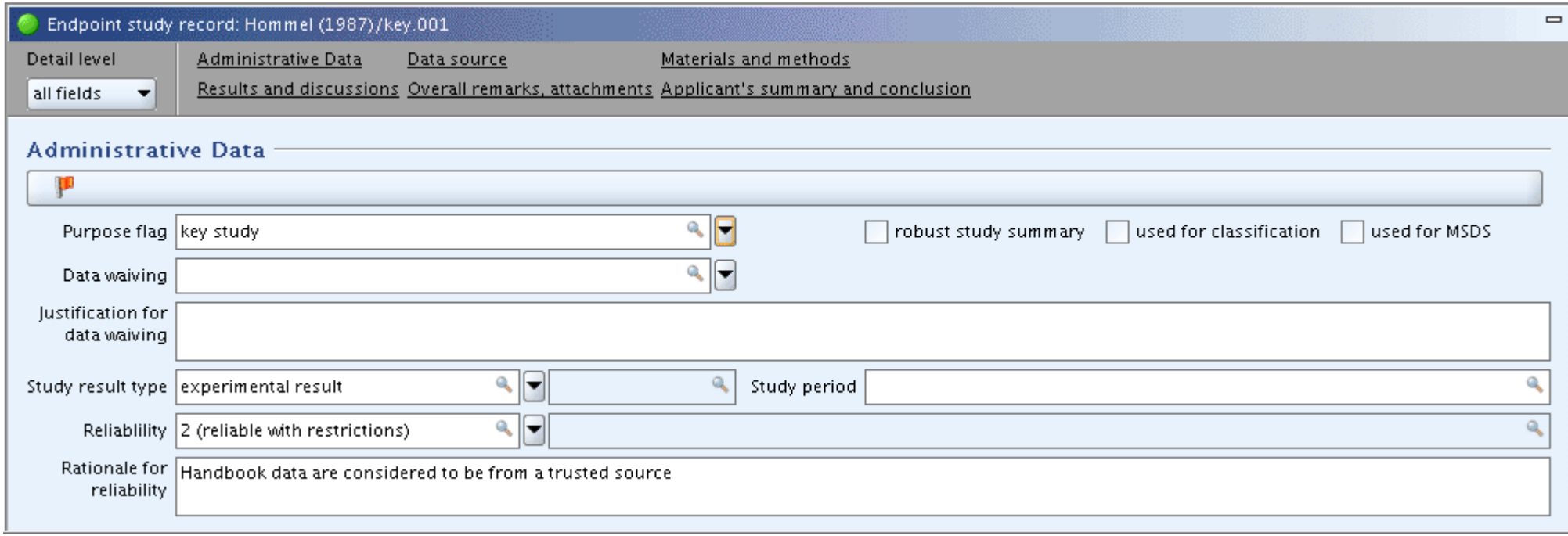
This use case includes the entry of (limited) handbook data. It is assumed that the data are from a trusted source and can therefore be used as key study. (Note: Refer to the relevant guidance document for the regulatory programme as to whether handbook data are accepted to cover endpoints for physico-chemical properties.)

1. The newly created record in section *4.2 Melting point/freezing point* should be open and displayed in the Data entry window. If not, double-click the record in the Section tree.

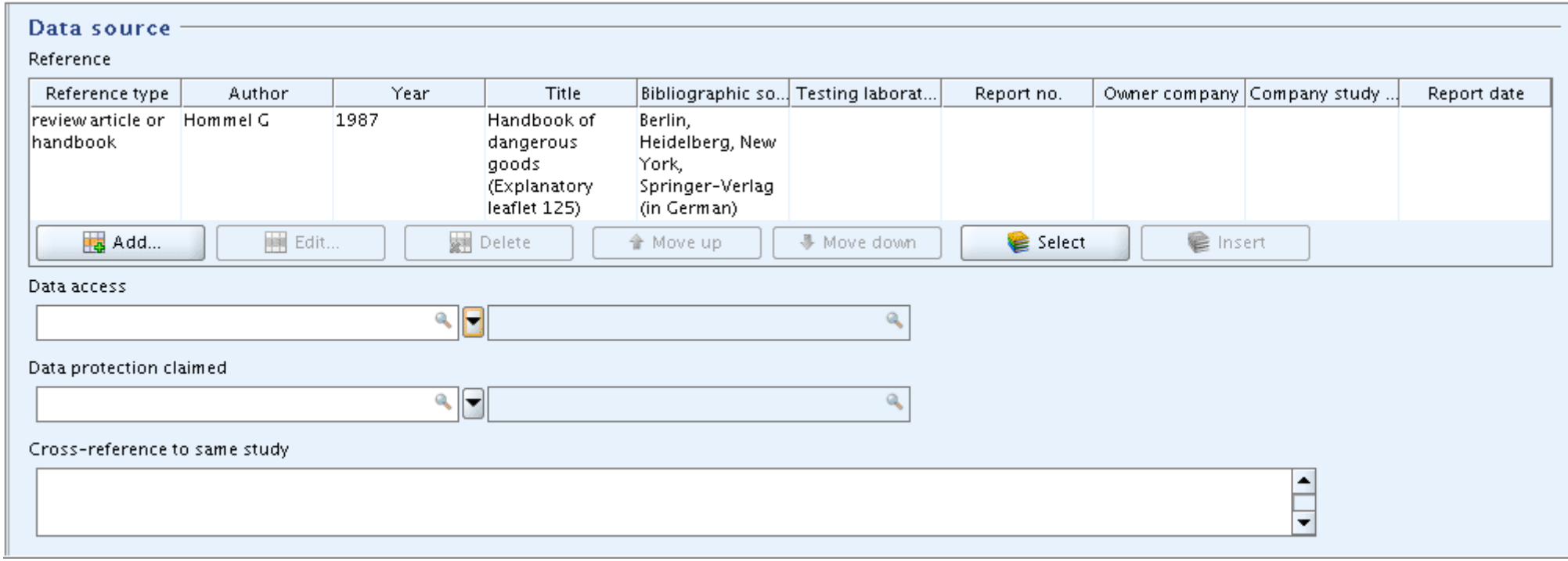
Tip

Any newly created record will automatically be in the Edit mode. When you re-open a record, you need to click the **Edit** button  on the toolbar.

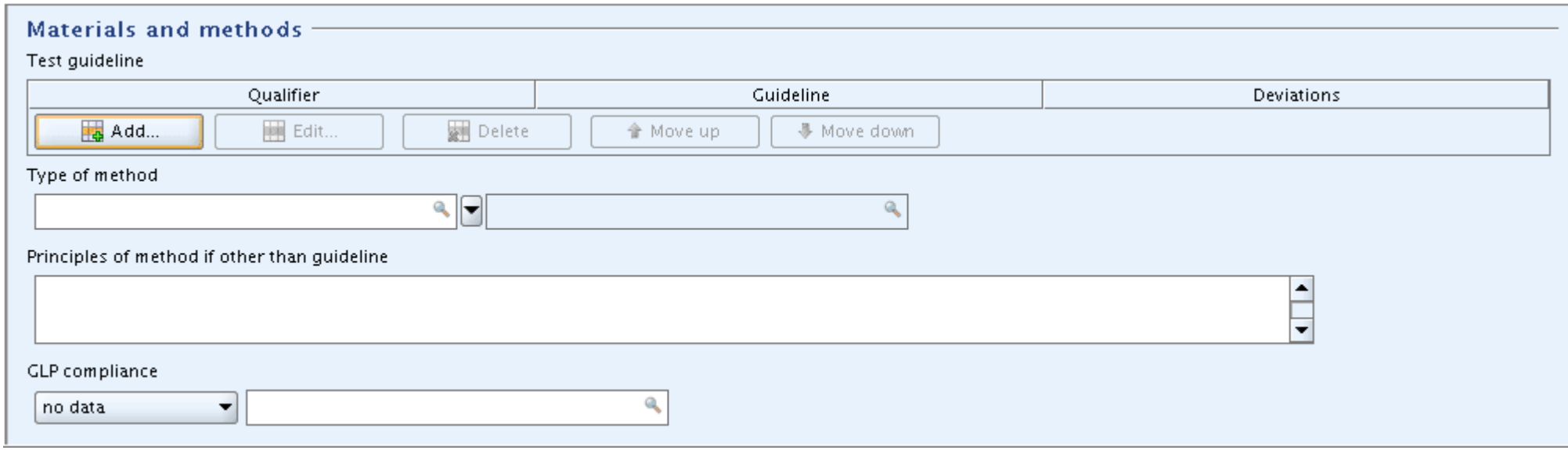
2. Part "Administrative Data": complete the appropriate fields as shown in the following screenshot:



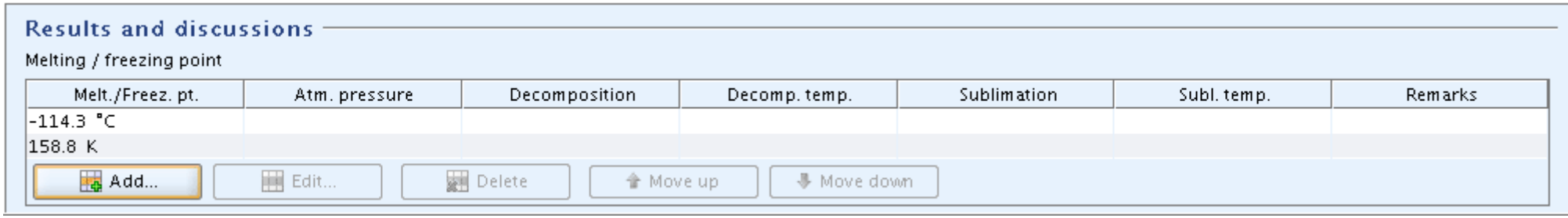
3. Part "Data Source": In field block `Reference`, click the **Add** button and in the dialogue opened, select the Reference type and enter the bibliographic reference information as shown in the following screenshot. Other fields in this part are not applicable.



4. Part "Materials and methods": The only field that can be completed in this example is the field `GLP compliance`.



5. Part "Results and discussions": In field block `Melting / freezing point`, click the **Add** button and in the dialogue opened, enter the freezing point in degree Centigrade. If required, repeat this procedure and enter the corresponding value in kelvin.



6. If you continue creating another Endpoint study record, a dialogue will ask you to save the modified data. Confirm by clicking the **Save** button.

Important

If you discontinue working with IUCLID for a longer time (i.e. more than two hours), it is recommended to click the **Save** button on the toolbar to make sure that the data entered are saved. Otherwise a session timeout might occur causing IUCLID to stall. The data could then not be saved anymore.

Entering the basic data of a study in section 6.1.1 Short-term toxicity to fish

This use case includes the entry of the basic data of a study in an Endpoint study record. It is assumed that only limited information is available from a publication and and executive summary of a study report. But the study report itself is not available yet. This use case is intended to demonstrate the Detail level switch, how to use basic fields only, launching the online help, handle a comprehensive drop-down list, use a Freetext template and the Undo function.

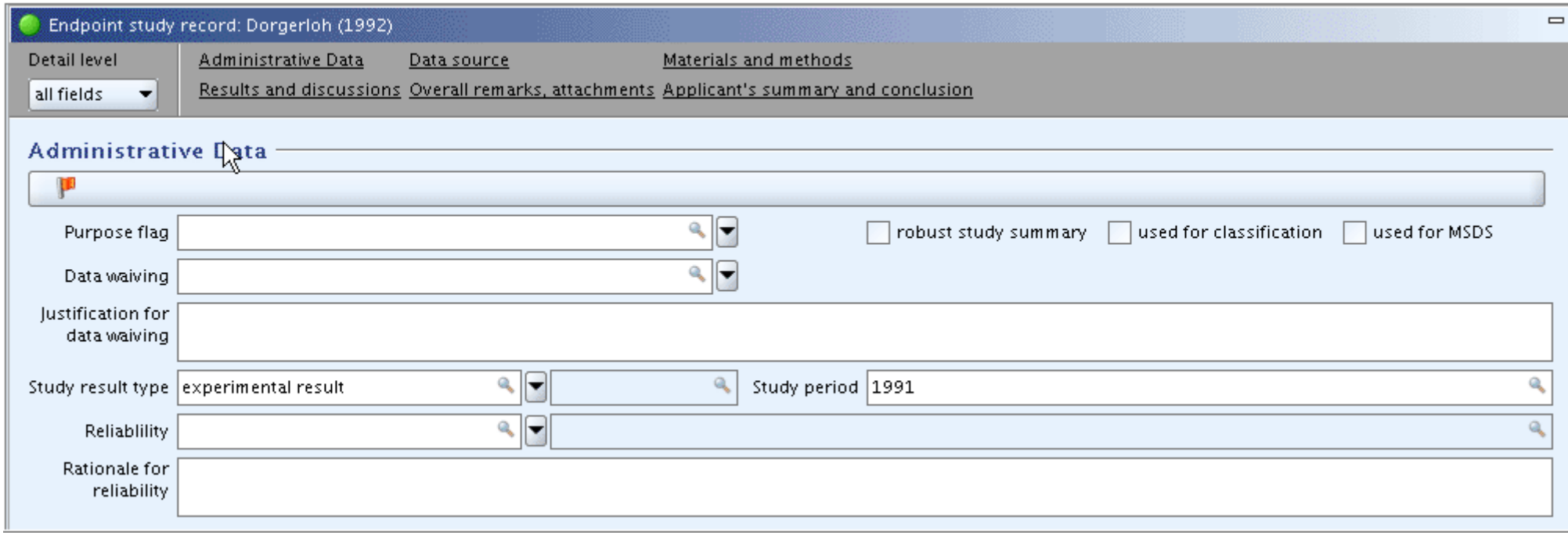
1. Create a new Endpoint study record in section *6.1.1 Short-term toxicity to fish*.
2. Rename the record to "Dorgerloh (1992)"
3. Click the Detail level button below the record title bar and from the menu displayed, select "basic fields".

Note

As described in the IUCLID 5 End User Manual chapter D.4.7.1 What is an Endpoint study record? , IUCLID allows displaying either

the basic fields only or all fields, i.e. including additional fields, which are normally only relevant for robust study summaries. The field labels of any additional fields are set in blue colour, while the label of all basic fields is black.

4. Part "Administrative Data": In field `Study result type`, select "experimental study". In field `Study period`, enter "1991" as assumingly indicated in the publication. Other fields are left empty for the time being.



5. Part "Data Source":

   - In field block `Reference`, enter the two references shown in the screenshot:

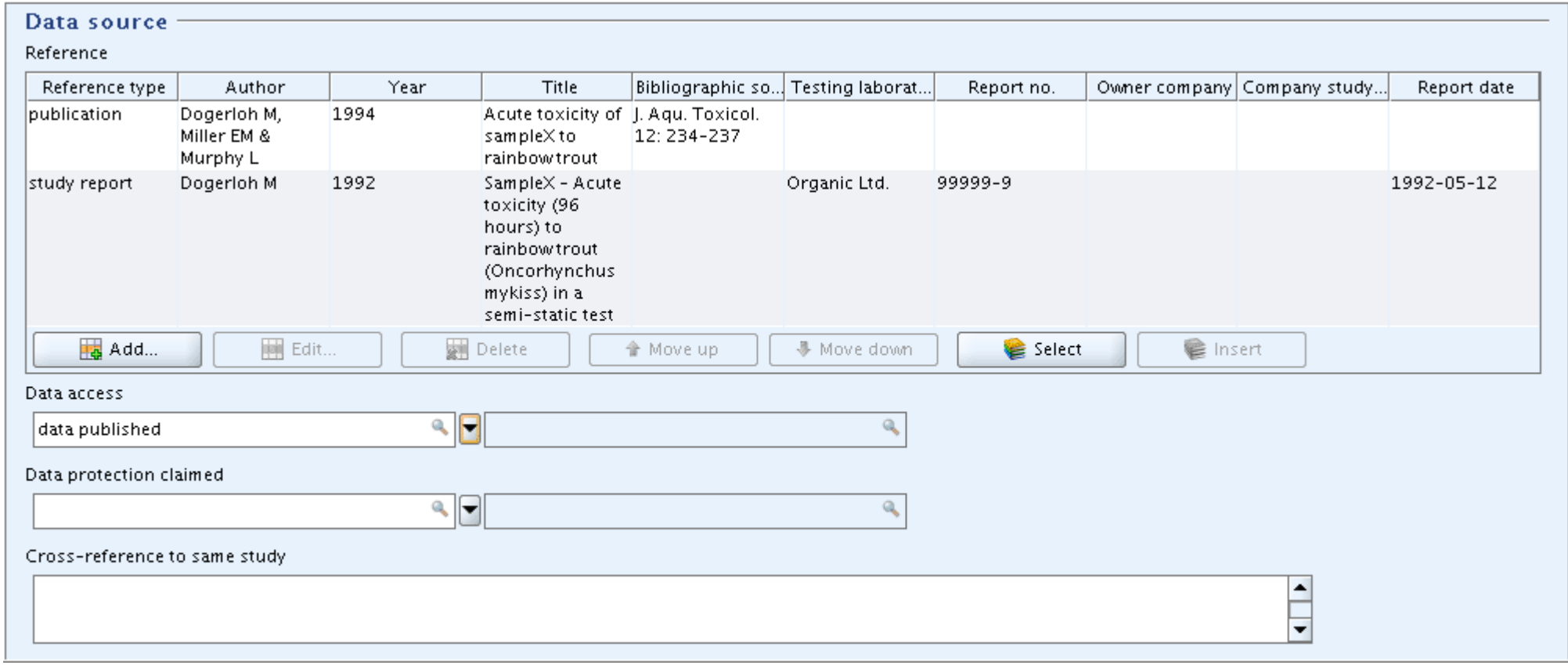
     - Launch the context-sensitive online help from within any field via the F1 key or by clicking the **Help** button on the toolbar.

     - Customise the size of the Help window as appropriate (If you need to look up online help for fields frequently, it can be useful to position both the Help window and the IUCLID screen in such a way that both windows are visible without having to switch back and forth. However, the context-sensitive help for each field has to be explicitly evoked by pressing the F1 key or clicking the **Help** button

.)

- Enter the bibliographic data as appropriate.

- In field `Data access`, select the item "data published".

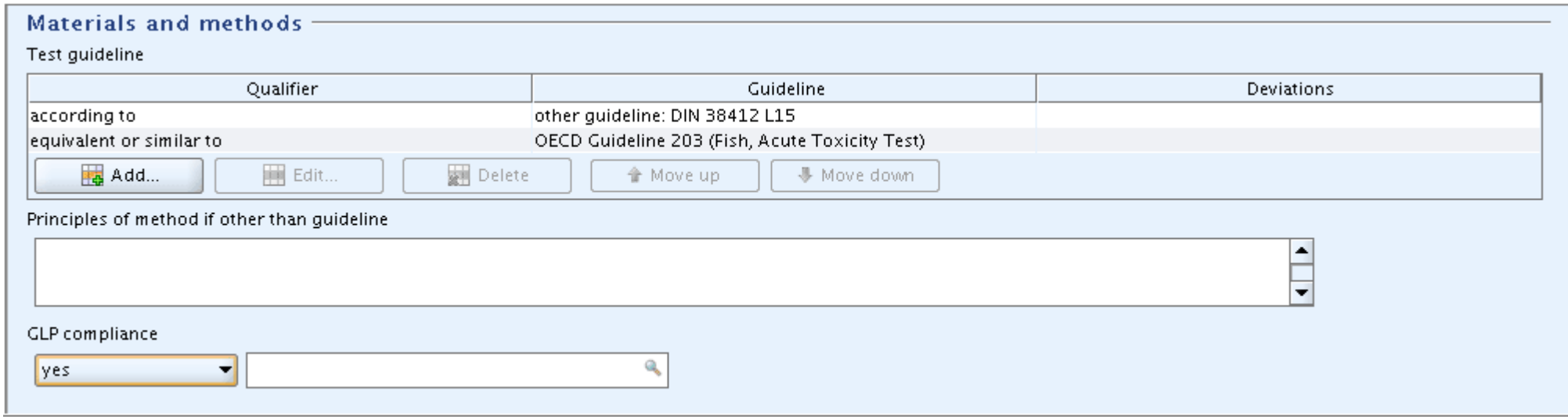


6. Part "Materials and methods":

- Enter the guideline given in the data source: Select "according to" in the field `Qualifier`. Select "other guideline" in the field `Guideline`, because the guideline used is not listed in the picklist, and enter "DIN 38412 L15" in the associated text field.

- Indicate that this guideline is equivalent to OECD Guideline 203: Repeat this procedure, but select the appropriate items from the picklists as shown in the screenshot below.

- Select "yes" in the field `GLP compliance`.



7. Part "Test materials":

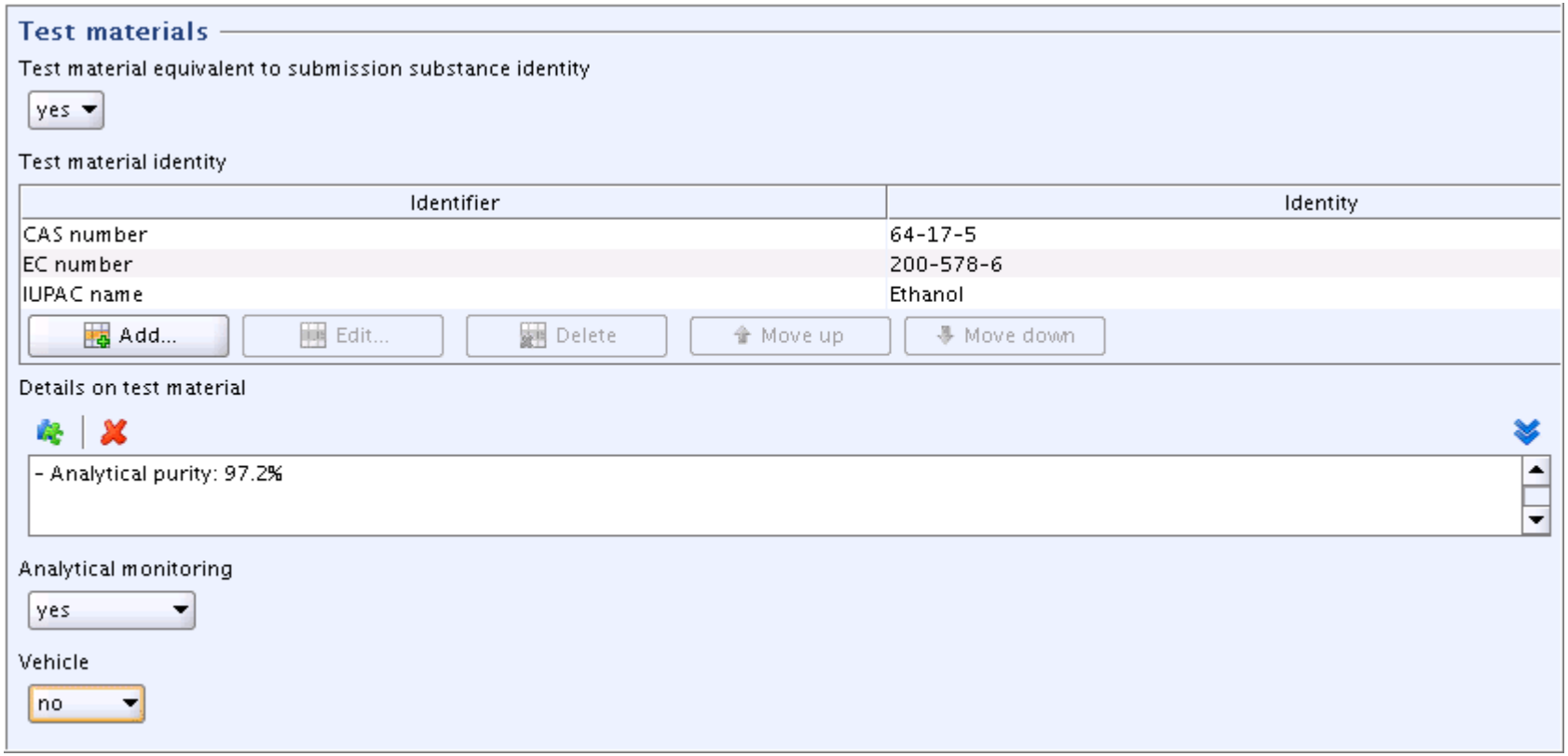
- Fields related to the identity of the test material are filled automatically based on the Reference substance assigned to the Substance dataset (see chapter 3 Creating a dataset for a Substance and assigning a Reference substance). You can add any additional identifiers.

Note

If the study was conducted with another than the submission substance (i.e. as identified by the Reference substance) and used as read-across, you would have to update these fields accordingly.

- Field `Details on test material`: Click the puzzle-like icon below the field label. In the Freetext templates dialogue box that opens, edit the Freetext template provided in such a way that only the item "- Analytical purity:" is kept, while all other items are deleted. Specify as shown in the screenshot below.

- Complete the fields `Analytical monitoring` ("yes") and `Vehicle` ("no").



8. Parts "Test organisms", "Study design" and "Test conditions": Enter the basic data as shown in the screenshot below.

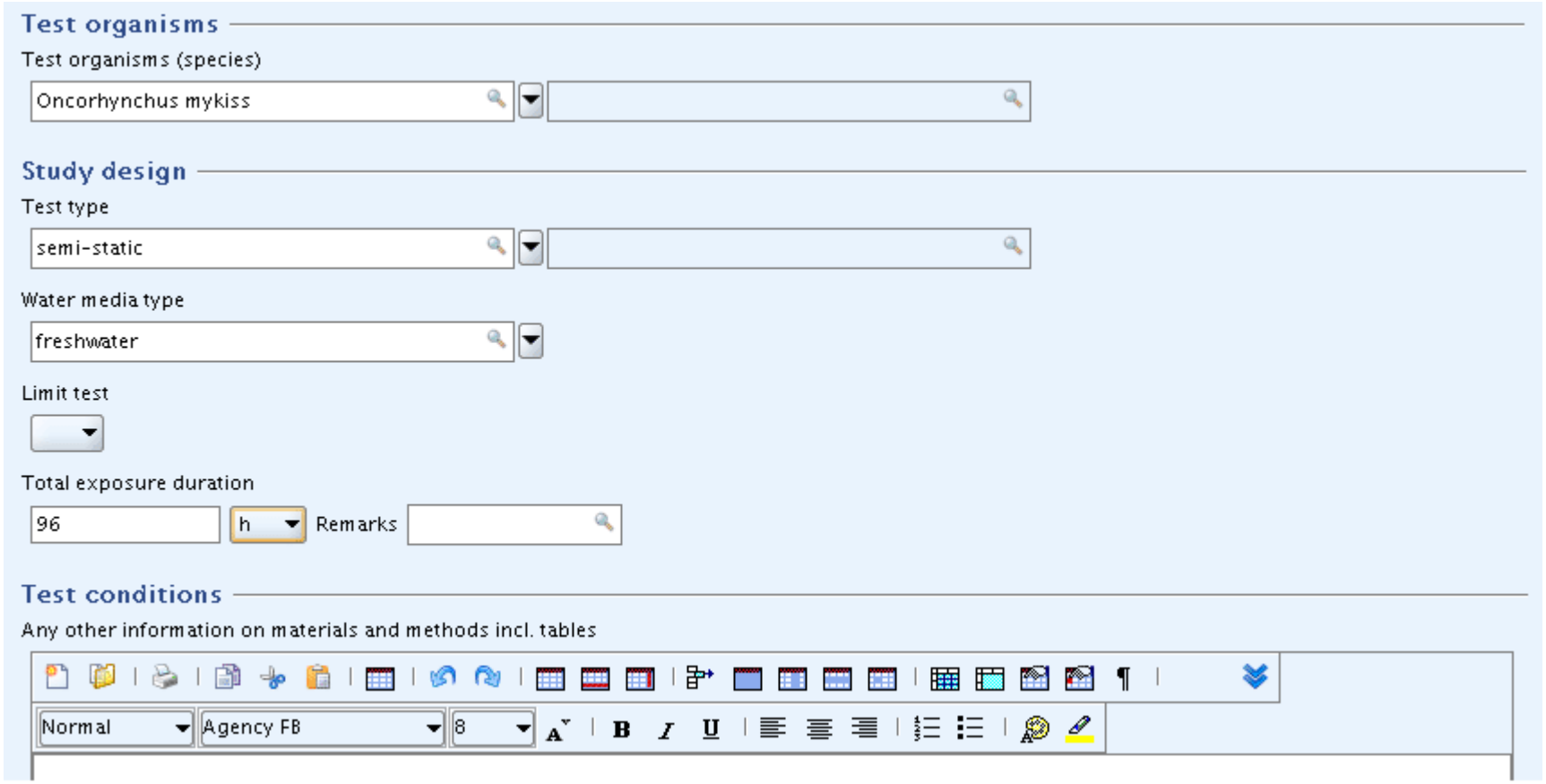
Tip

In case of very comprehensive picklists provided in a drop-down combo box, you can find the desired item quickly by using either of the following methods:

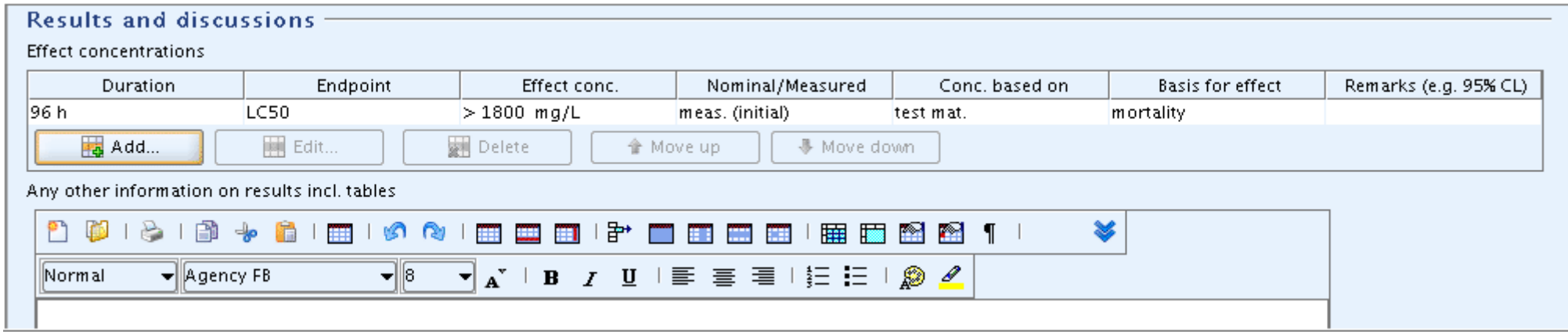
- Click the drop-down arrow and in the picklist that opens, click into the Find pane and enter an adequate part of the item. For example, "my" will immediately find any item that contains this string, e.g. "Oncorhynchus mykiss". You need not use

wildcards (*) and such on the-fly queries are not case-sensitive.

- Just start typing the item of your choice in the list field. The autofill function of IUCLID will display the first entry in the list starting with the letter(s) you enter. For example, typing "O" or "o" will extend to "Oncorhynchus gorbuscha". When you then click the drop-down arrow, the first entry in the list starting with that/these letter(s) will be displayed directly and you can find the desired item (e.g. "Oncorhynchus mykiss") right away.



9. Part "Results and discussions": In the field block `Effect concentrations`, click the **Add** button and in the dialogue opened, enter the LC50 value and the parameters shown in the following screenshot:

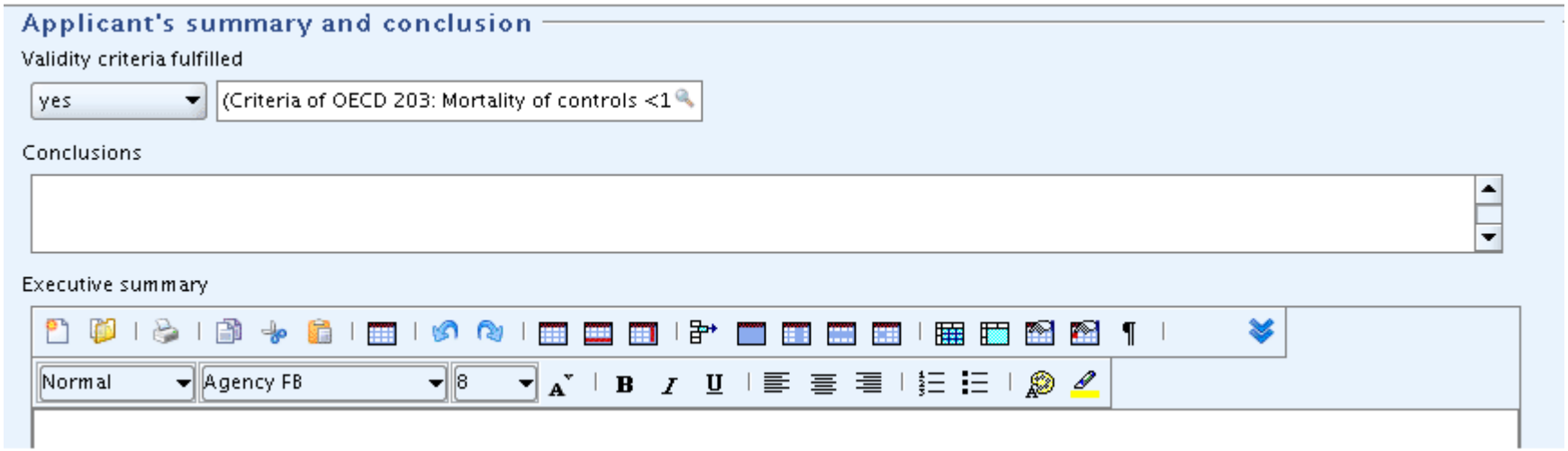


10. Part "Overall remarks, attachments": Nothing to add for this sample study.

11. Part "Applicant's summary and conclusion": In field `Validity criteria fulfilled`, select "yes" and add a brief explanation in the related text field.

Tip

In print-outs, the supplementary text field related to the list field is not separated by any delimiter. This might cause confusing text combinations. It is therefore recommended to include any supplementary text in parentheses to get it set aside from the list item. This is not required if the picklist item end with a colon as for "other:".



12. Test the Undo function: Delete the entry in field `Validity criteria fulfilled` by selecting the blank item. Then click the **Undo** button on the toolbar. The previous picklist item will be re-entered, but not the related text field.

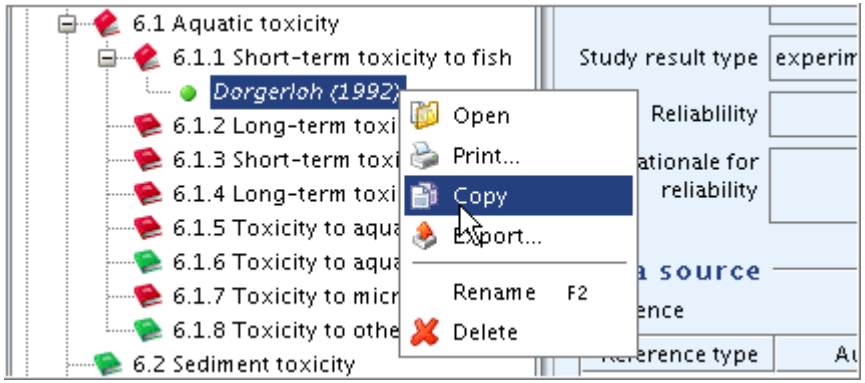
Note

Using the Undo command, the most recent edit operations can be undone in most cases. There are a few exceptions to this rule as demonstrated with the example above.

Copying an Endpoint study record

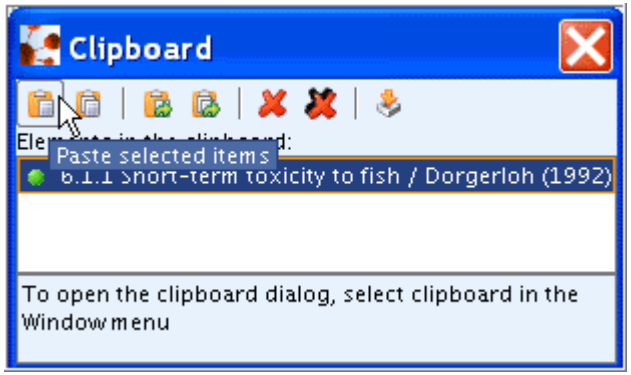
Use case: To demonstrate the Copy function it is assumed that the Endpoint study record prepared in the sample above shall be expanded to a robust study summary, while the first draft record shall be stored. Proceed as follows:

1. Right-click the record "Dorgerloh (1992)" in the section tree pane and from the menu displayed, click the **Copy** command.

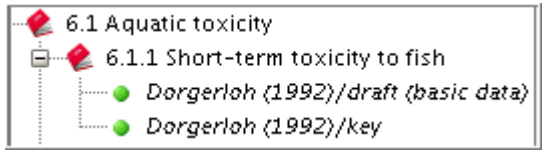


2. The clipboard manager is opened and the copied record is displayed.

3. Select and highlight the copied record in the clipboard and click the **Paste selected items** button. The record will then appear in the section tree under the same name as the orginal one.



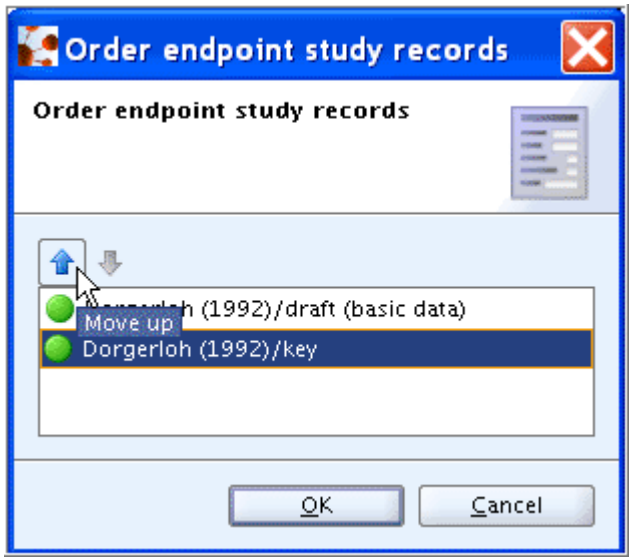
4. Rename one record to "Dorgerloh (1992)/draft (basic data)" and the other one to "Dorgerloh (1992)/key".



Ordering Endpoint study records

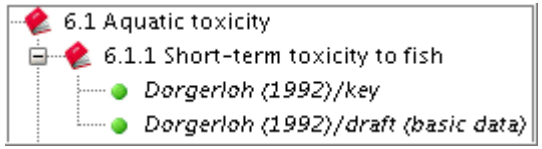
Use case: Reorder records in the section tree to position the record designated as "key study" first (useful in case of many records per Endpoint section). Proceed as follows:

1. Right-click the section title *6.1.1 Short-term toxicity to fish* and from the menu displayed, click the **Order records** command.



2. In the dialogue box, highlight the record designated as "key study", click the **Move up arrow** to position it first and then click **OK**.

3. The key study then appears as first record.



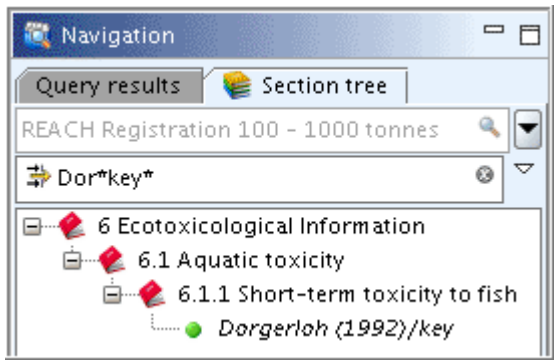
Quickly finding specific Endpoint study records in the section tree

Use case: Especially if a section contains a large number of Endpoint study records, the query / filter method should be used to quickly filter for specific records.

To query and find a record

1. Click into the Find or Filter pane below the title bar of the section tree pane.

2. Enter an adequate part of the record name and all records containing this search string in their names will be filtered out and displayed immediately. For example, "Dor" (without quotation marks) will select records starting with this string. "Dor*key" will find the record "Dorgerloh (1992)/key".



Tip

Use wildcards (*) for any characters preceding or following a search string.

Entering additional data for a robust study summary in section 6.1.1 Short-term toxicity to fish

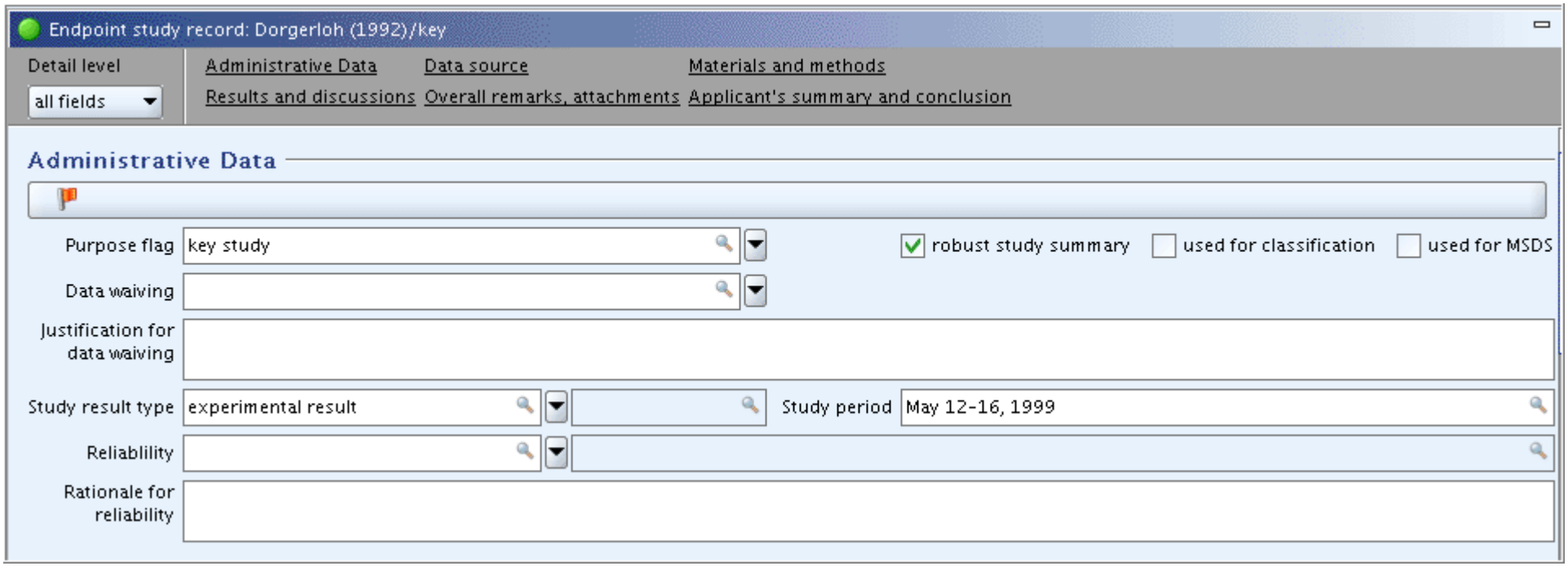
Use case: It is assumed that the full study report is now available and can be used to prepare a robust study summary. This use case is intended to demonstrate the Detail level "all fields", the Navigation links to the main parts of an Endpoint study record, the use of comprehensive Freetext templates, sorting of items in repeatable blocks of fields, using a rich text field and uploading a predefined table, and other edit functions.

1. Find the record "Dorgerloh (1992)/key" in the section tree and double-click it to open it.

2. Click the **Edit** button on the toolbar to allow editing of the record.

3. Click the **Detail level** button below the record title bar and from the menu displayed, select "all fields".

4. Part "Administrative Data": Complete the field `Purpose flag`, select the checkbox for "robust study summary" and specify the study period in the corresponding field as shown in the following screenshot. (Note: Fields `Reliability` and `Rationale for reliability` will be completed later, when the study has been evaluated and the robust study summary is completed.)

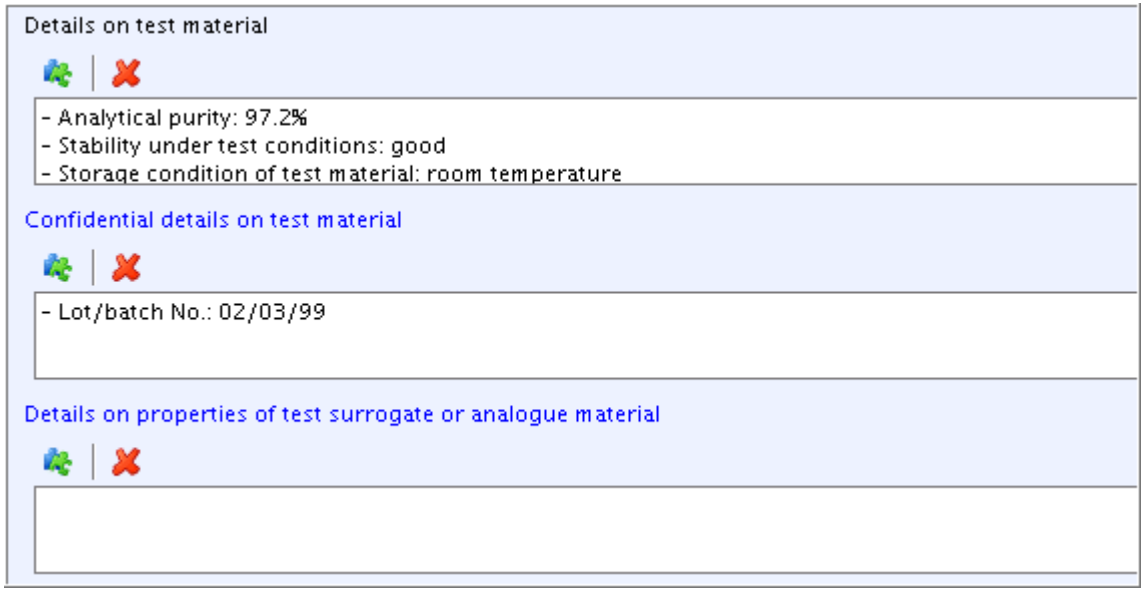


5. Part "Test materials":

   - Add additional information in field `Details on test material`. Click the Freetext template icon below the field label. In the Freetext templates dialogue box that opens, edit the Freetext template provided in such a way that only the needed items are kept, while all other items are deleted. Specify as shown in the screenshot below.

- Field `Confidential details on test material`: Select the item "- Lot/batch No.:" from the Freetext template and add data as shown in the screenshot below. (Note: Any information that can be claimed confidential (e.g. composition, impurities, lot/batch no.) should be included in this field, because this will allow to filter out such data from any print-out or export file.)

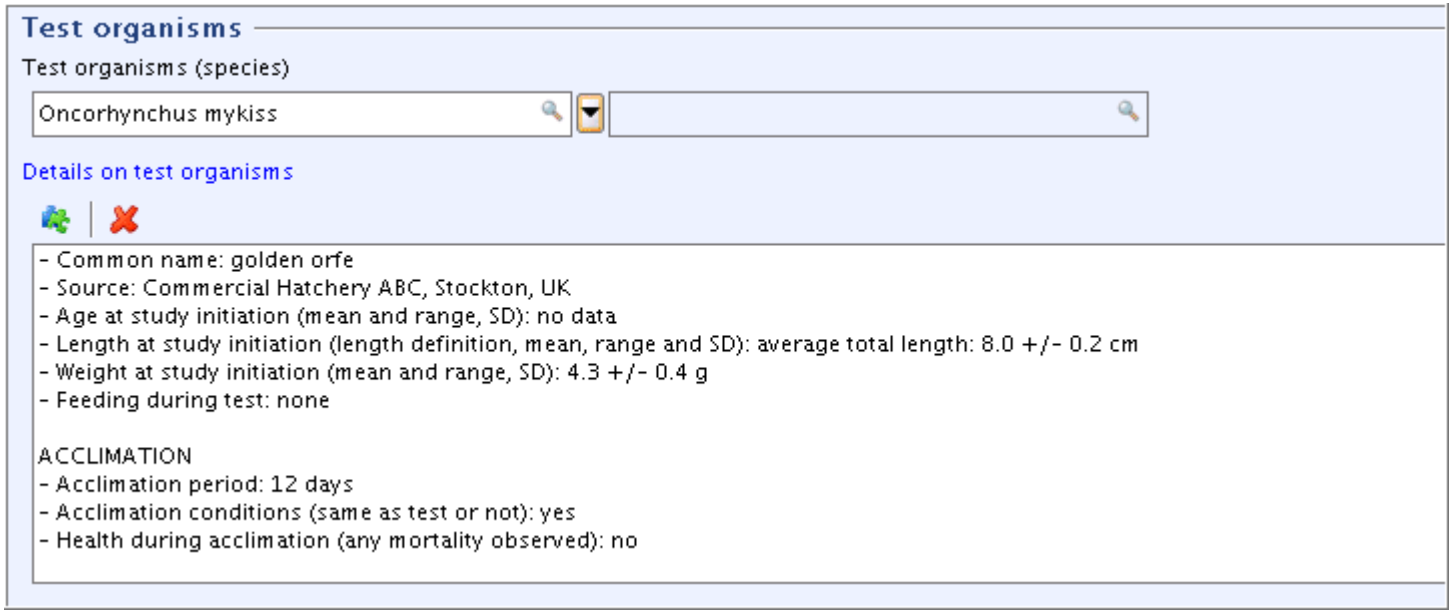
- Field `Details on properties of test surrogate or analogue material`: Leave this field empty, because it is only relevant in case of read-across from another substance, e.g. an analogue or surrogate.



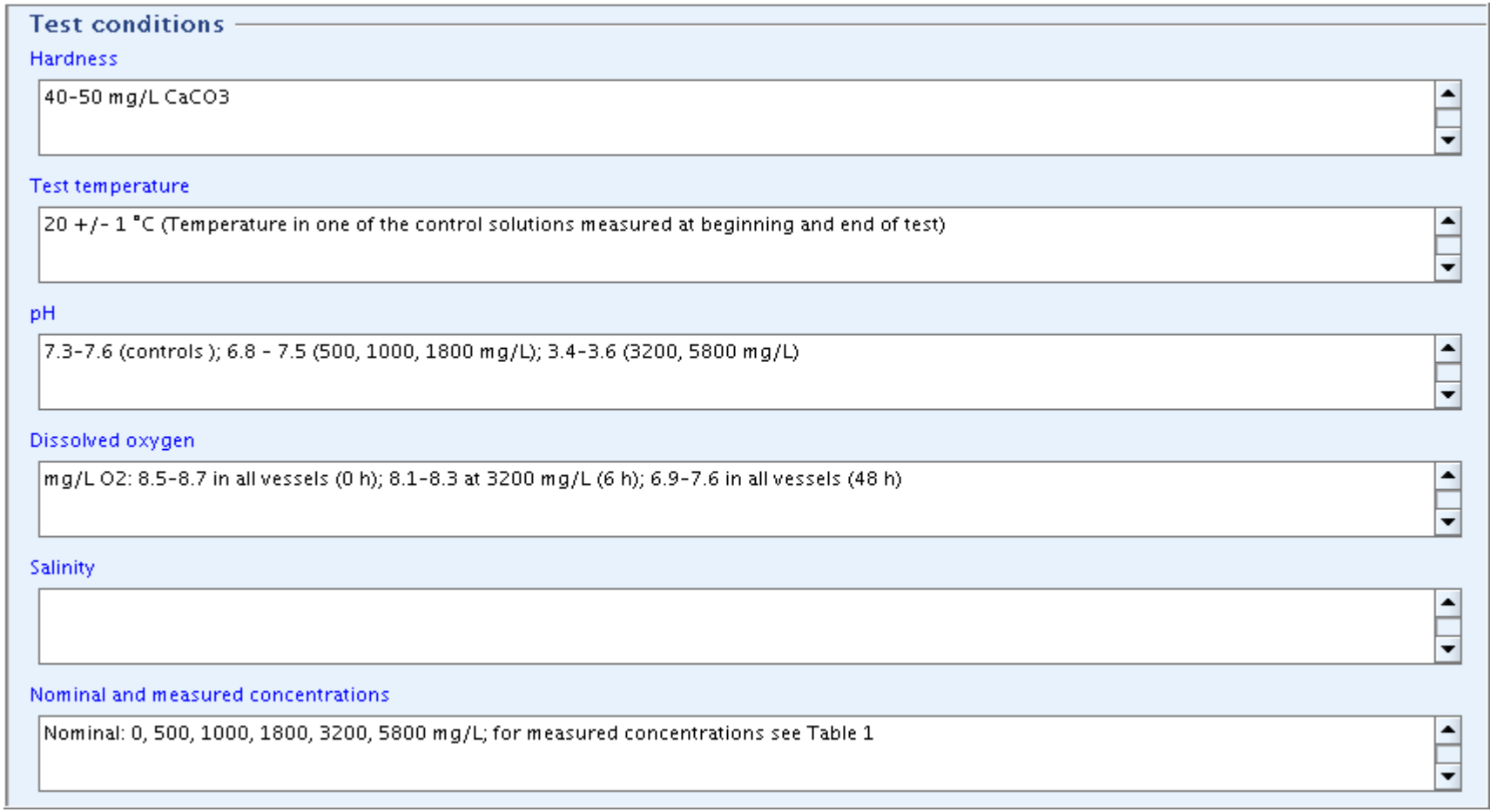
6. Part "Test organisms", field `Details on test organisms`: Select and edit the Freetext template as shown in the following screenshot.

Tip

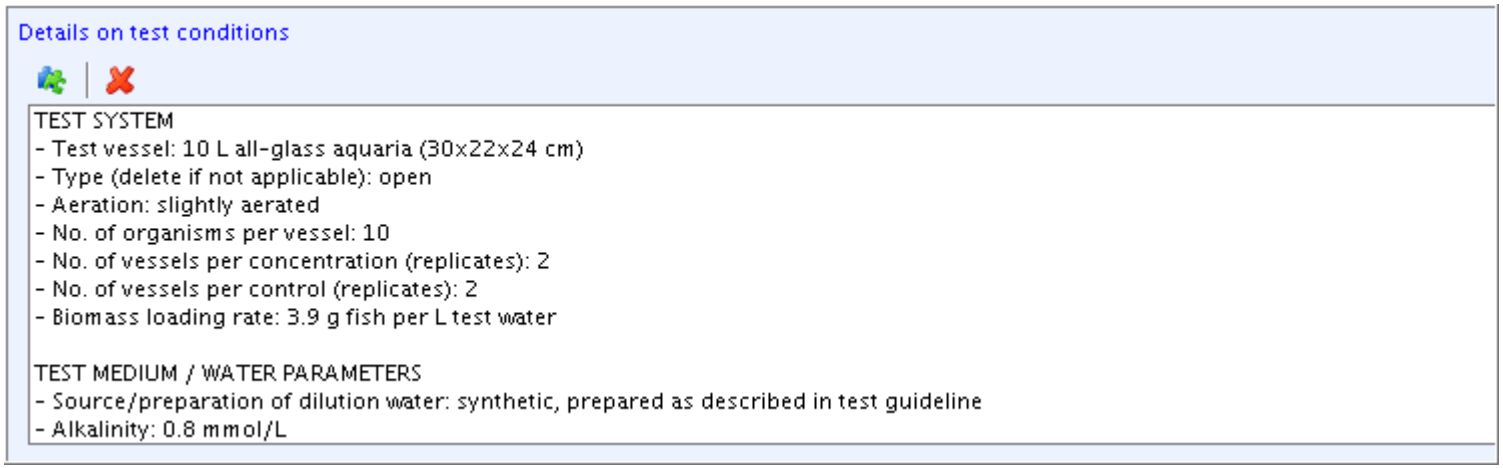
Click the **Unfold button** on the upper right of the field to expand the field or the **Fold button** to minimise the display area.



7. Part "Test conditions": Complete the fields `Hardness`, `Test temperature`, `pH`, `Dissolved oxygen`, and `Nominal and measured concentrations` as shown in the following screenshot.



8. Part "Test conditions" (cont'd), field `Details on test conditions`: Select and edit the Freetext template as shown in the following screenshot.



9. Field `Any other information on materials and methods incl. tables`: Upload a predefined or other available table into this rich text field as follows:

   - Click the **Open file** button on the toolbar of the rich text editor.
   - From the **Open** dialogue box displayed, select the file you wish to upload into the field, and then click the **Open** button.
   - Edit the table as appropriate.

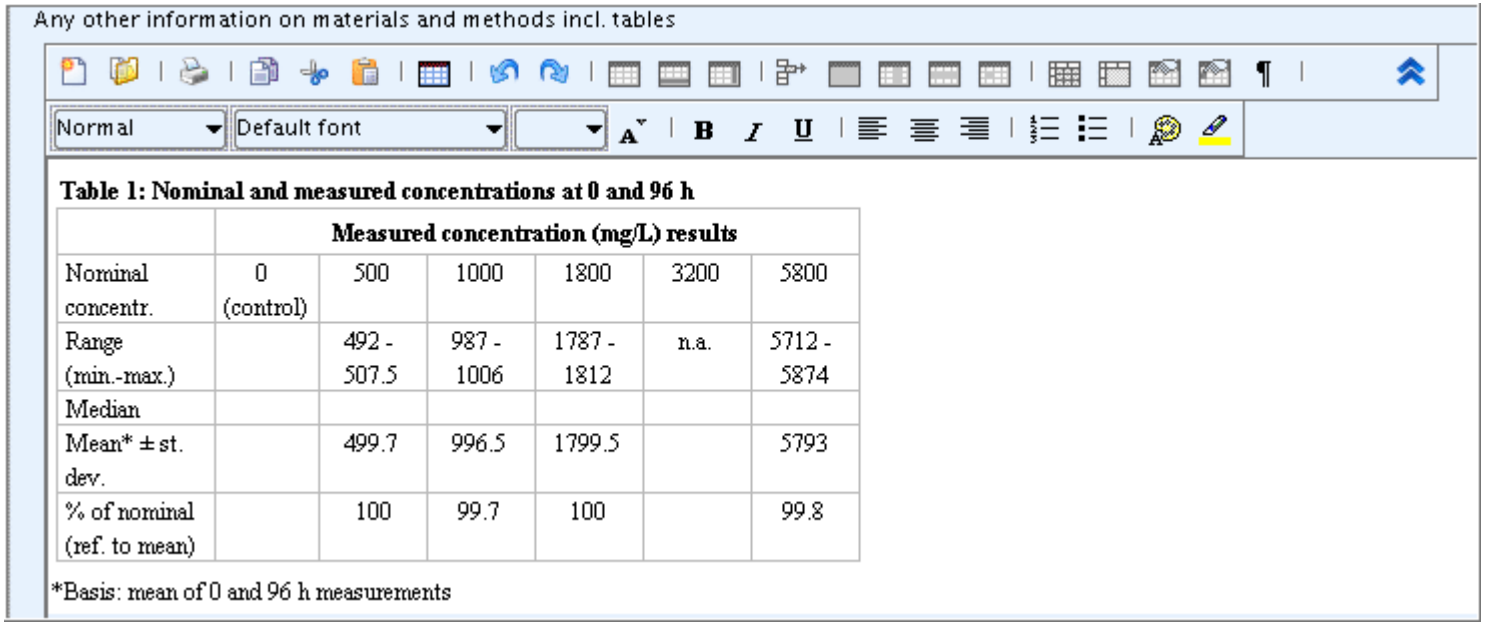
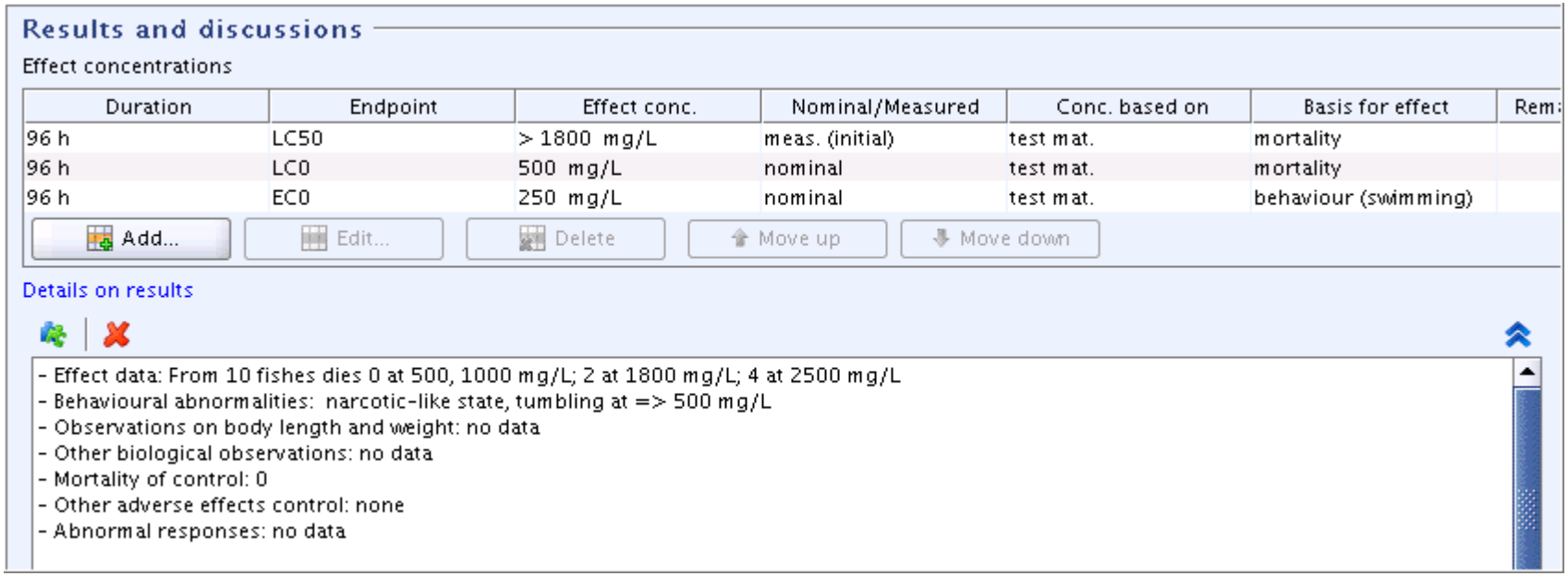


Table 1: Nominal and measured concentrations at 0 and 96 h

	Measured concentration (mg/L) results					
Nominal concentr.	0 (control)	500	1000	1800	3200	5800
Range (min.-max.)		492 - 507.5	987 - 1006	1787 - 1812	n.a.	5712 - 5874
Median						
Mean* ± st. dev.		499.7	996.5	1799.5		5793
% of nominal (ref. to mean)		100	99.7	100		99.8

*Basis: mean of 0 and 96 h measurements

10. Part "Results and discussions": Add additional effect concentration data in the field block `Effect concentrations` and details in the field `Details on results` as shown in the following screenshot:



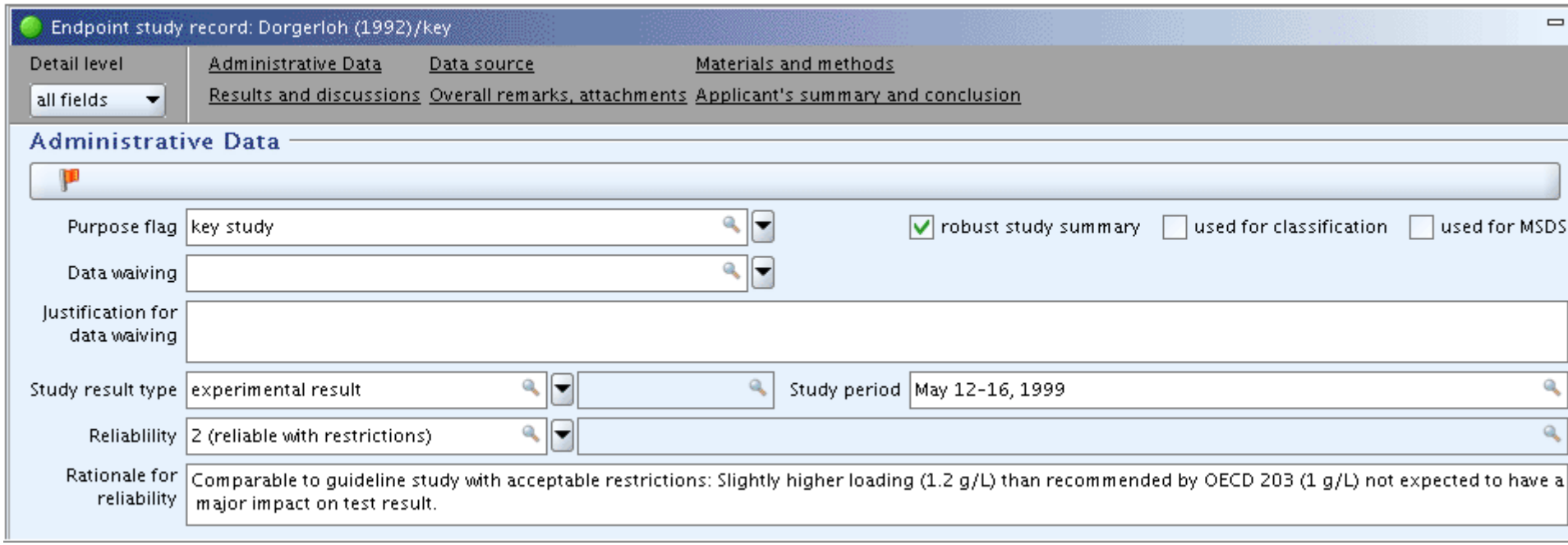
11. Part "Administrative Data": The fields `Reliability` and `Rationale for reliability` still need to be completed based on the inherent quality of the test report or publication and hence, the adequacy of data. Proceed as follows:

    - Click the link "Administrative data" in the navigation bar just below the title bar to jump directly to that part.

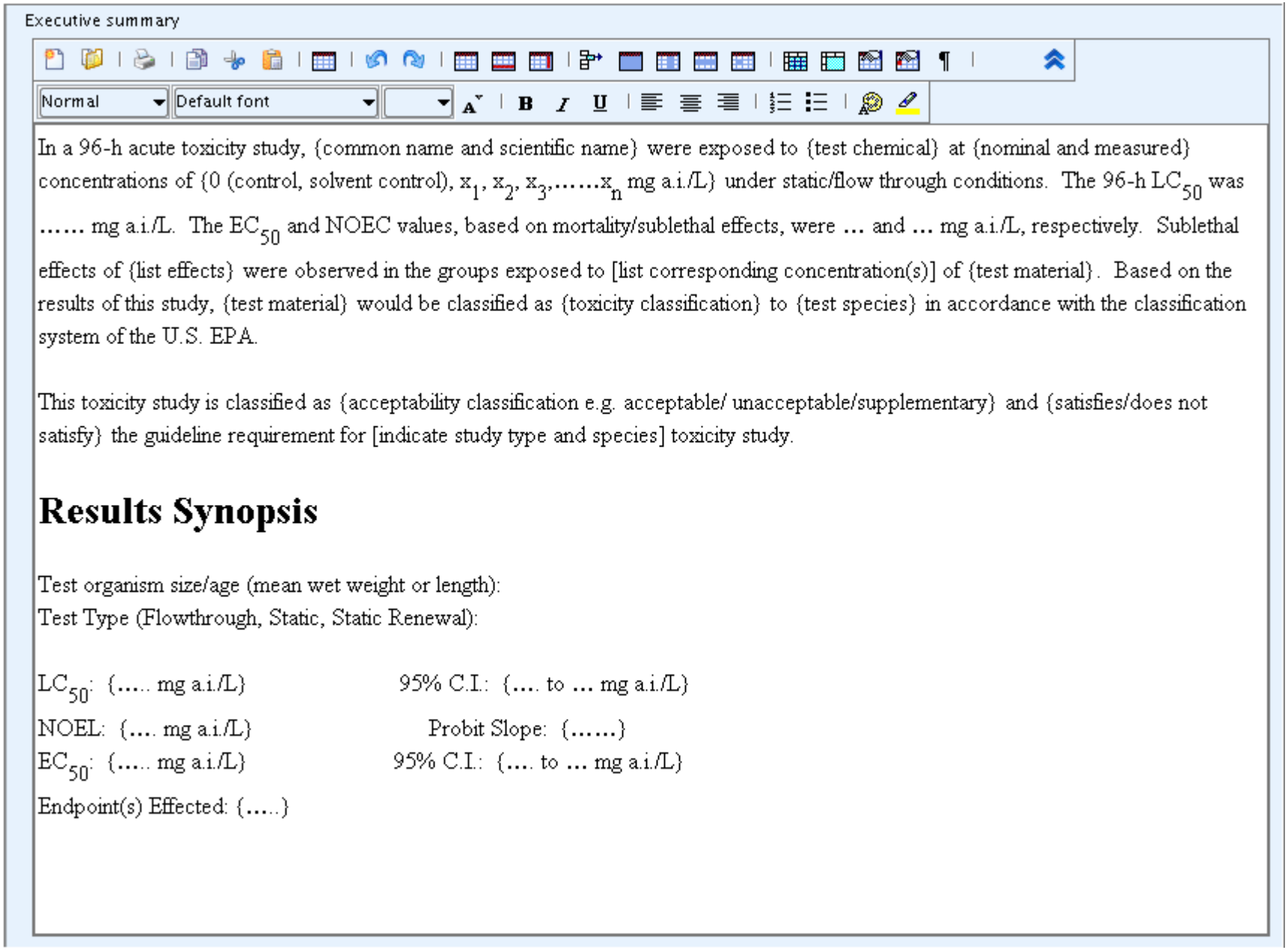
    ### Tip

    Using the links on the navigation bar is particularly helpful in case of very comprehensive Endpoint study records or if you prefer to start editing or viewing with a particular part, e.g. "Results and discussion".

    - Complete the fields `Reliability` and `Rationale for reliability` as shown in the following screenshot.
    - Click the link "Applicant's summary and conclusions" to jump to that part and proceed.



12. Part "Applicant's summary and conclusion":



In a 96-h acute toxicity study, {common name and scientific name} were exposed to {test chemical} at {nominal and measured} concentrations of {0 (control, solvent control), x_1, x_2, x_3,.....x_n mg a.i./L} under static/flow through conditions. The 96-h LC_{50} was ..... mg a.i./L. The EC_{50} and NOEC values, based on mortality/sublethal effects, were ... and ... mg a.i./L, respectively. Sublethal effects of {list effects} were observed in the groups exposed to [list corresponding concentration(s)] of {test material}. Based on the results of this study, {test material} would be classified as {toxicity classification} to {test species} in accordance with the classification system of the U.S. EPA.

This toxicity study is classified as {acceptability classification e.g. acceptable/ unacceptable/supplementary} and {satisfies/does not satisfy} the guideline requirement for [indicate study type and species] toxicity study.

Results Synopsis

Test organism size/age (mean wet weight or length):
Test Type (Flowthrough, Static, Static Renewal):

LC_{50}: {..... mg a.i./L} 95% C.I.: {.... to ... mg a.i./L}
NOEL: {.... mg a.i./L} Probit Slope: {.....}
EC_{50}: {..... mg a.i./L} 95% C.I.: {.... to ... mg a.i./L}
Endpoint(s) Effected: {.....}

5. Printing the Substance dataset

The tutorial in this chapter shows how to print

- an Endpoint study record with basic fields only
- an Endpoint study record with all fields
- the complete Substance dataset

Step-by-step guide

To print the sample Endpoint study record "Dorgerloh (1992)/key" with basic fields only

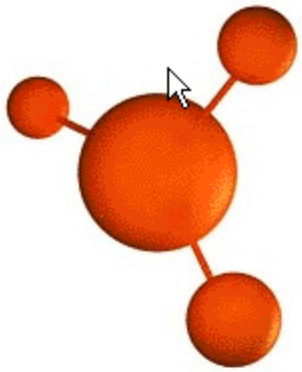
1. Right-click this record in the section tree or select the **Print** command from the **File** menu.
2. The Print assistant comes up and guides you through several steps of a self-explanatory Print dialogue: Verify or change the default properties, for which the record shall be printed. In Step 5, select the detail level "Basic level". Specify output path, file name and other print options, and click the **Finish** button.
3. Open the html file from for viewing it.

To print this record with all fields, follow the same procedure, except for selecting detail level "All fields - including confidential test material information".

To print the complete dataset

1. Double-click any record in sections 0 to 3. Make sure one of the subsections is displayed in the data entry window, e.g. section *1.1 Identification*.
2. Select the **Print** command from the **File** menu.
3. The Print assistant comes up and guides you through several steps of a self-explanatory Print dialogue: Verify or change the default properties, for which the records shall be printed, specify output path, file name and other print options, and click the **Finish** button.

The following screenshot show part of the print-out of the sample Endpoint study record:



IUCLID 5

INTERNATIONAL UNIFORM CHEMICAL INFORMATION DATABASE

Printing Date 2007-03-31 19:21:16 CEST

Restriction of specific regulatory purposes

EU: BPD, EU: PPP, EU: REACH, CA: CEPA, CA: PCPA, JP: CSCL, OECD: HPVC, US: EPA HPVC, US: FIFRA, US: TSCA, other:

Confidentiality

CBI, IP, no PA

Owner	ethanol (fictitious sample for IUC5 manual) / ethanol / Ethanol / ethanol / 64-17-5 / LE Sample Company / Hometown / Ireland
Owner legal entity	LE Sample Company / Hometown / Ireland

Endpoint study record: Dorgerloh (1992)/key

UUID	IUC5-1539298a-0a9c-4e6b-8b7b-77377715156a
Dossier UUID	[]
Author	IUCLID sample user / LE Sample Company / Hometown / Ireland
Date	2007-03-31 19:08:03 CEST
Remarks	

Administrative Data

[]

Purpose flag	key study (X) robust study summary ( ) used for classification ( ) used for MSDS		
Study result type	experimental result	experimental result	May 12-16, 1999
Reliability	2 (reliable with restrictions)		

The complete print-out is shown in the IUCLID 5 End User Manual chapter D.4.7.13 Printing Endpoint study records.

6. Creating a Dossier

The tutorial in this chapter shows how to create a Dossier, which is very similar to the creation of a print-out.

Introduction

A Dossier is a write-protected copy of the raw data stored in a Substance dataset. An Ownership protection option can be set, which prevents Endpoint study / summary records provided with a Dossier from being copied. This can be relevant if a Dossier is made available to another party, but the submitter does not want to allow copying Endpoint records. For further details, see the IUCLID 5 End User Manual chapter D.8 Dossier (create Dossier and browse Dossier data) .

Step-by-step guide

To create a Dossier for a Substance datset, follow these steps:

1. Go Home  to the Task panel if you are not already there.
2. Under **Substance**  , click **Update**.
3. In the **Query results** pane, right-click the desired Substance (i.e. the sample dataset) and from the menu displayed, click the **Create dossier** command.
4. The Create dossier assistant comes up and guides you through a several steps dialogue: Verify or change the default properties (i.e. for which the records shall be included in the dossier), specify specific dossier information, and click the **Finish** button.
5. The Dossier created appears in a new tab of the Navigation window, called Components. Each component of a Dossier is listed, i.e.:
    - The Dossier itself:

    - The Dossier title includes the Dossier template type, the name of the Substance / Reference substance, the CAS No., Legal entity, date and the user-defined name.

    - The Dossier information entered during the process of Dossier creation is displayed (read-only) in the Data entry window. You can directly navigate to the Dossier subject. See the screenshot below.

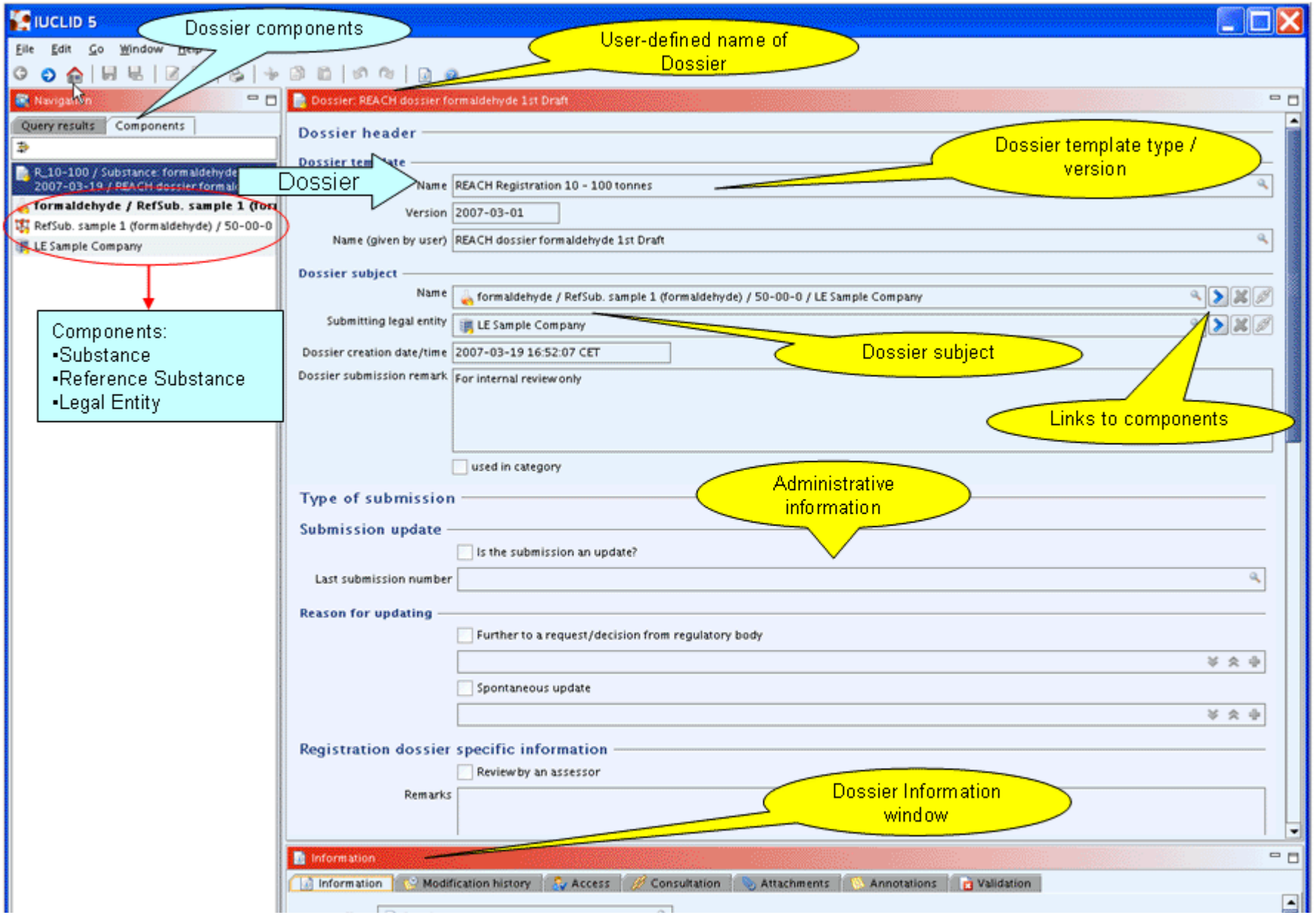
    - The Dossier-related Information window.

- The source Substance dataset.

- The Reference substance referred to in the Substance.

- The Legal entity the Substance is assigned to.

The following screenshot shows an example of Dossier components and Dossier information:


IUCLID 5
File Edit Go Window Help
Dossier components
User-defined name of Dossier
Navigation
Query results
Components
R_10-100 / Substance: formaldehyde
2007-03-19 / REACH dossier formal
formaldehyde / RefSub. sample 1 (for
RefSub. sample 1 (formaldehyde) / 50-00-0
LE Sample Company
Dossier
Components:
•Substance
•Reference Substance
•Legal Entity
Dossier: REACH dossier formaldehyde 1st Draft
Dossier header
Dossier template type / version
Name REACH Registration 10 - 100 tonnes
Version 2007-03-01
Name (given by user) REACH dossier formaldehyde 1st Draft
Dossier subject
Name formaldehyde / RefSub. sample 1 (formaldehyde) / 50-00-0 / LE Sample Company
Submitting legal entity LE Sample Company
Dossier creation date/time 2007-03-19 16:52:07 CET
Dossier submission remark For internal review only
Dossier subject
Links to components
used in category
Type of submission
Administrative information
Submission update
Is the submission an update?
Last submission number
Reason for updating
Further to a request/decision from regulatory body
Spontaneous update
Registration dossier specific information
Review by an assessor
Remarks
Dossier Information window
Information
Information
Modification history
Access
Consultation
Attachments
Annotations
Validation

7. Exporting the Substance dataset

The tutorial in this chapter shows how to export a complete Substance dataset or individual records.

Step-by-step guide

To export the complete Substance dataset

1. Click the Query results pane if it is not already active or select the command **Update Substance** from the IUCLID Task panel.
2. Select the Substance dataset to be exported:
   - Either right-click it and from the menu displayed, click the **Export** command.
   - Or click it and then select the **Export** command from the **File** menu.
3. The Export assistant comes up and guides you through a several steps Export dialogue: Verify or change the default properties, for which the records shall be exported, specify output path, file name and other options, and click the **Finish** button.

To export individual record(s) of a Substance dataset

1. Right-click the record name in the section tree and from the menu displayed, click the **Export** command..
2. The Export assistant comes up and guides you through a several steps Export dialogue: Verify or change the default properties, for which the records shall be exported, specify output path, file name and other options, and click the **Finish** button.

For more information, see the IUCLID 5 End User Manual chapter D.4.7.14 Exporting Endpoint study records .

8. Importing the Substance dataset

The tutorial in this chapter shows how to import a complete Substance dataset or individual records.

Prerequisite is that you have a IUCLID export file stored on your computer, e.g. as created in the preceding exercise (see chapter C.7 Exporting the Substance dataset). If you import an already existing Substance dataset, any identical records will be automatically deselected by default. To test the import of a Substance dataset that is not yet available on your IUCLID installation, you may delete the Substance dataset after exporting it (right-click it in the Query results pane and select the **Delete** command).

Step-by-step guide

To import a IUCLID export file of a Substance dataset

1. Go Home to the Task panel if you are not already there.
2. Under **Import** , click **Import**.

3. The Import assistant comes up and guides you through a several steps Import dialogue: Select the input path and file name; verify or change the default properties, for which the records shall be imported, select/deselect all or individual records to be imported, and click the **Finish** button.

For more information, see the IUCLID 5 End User Manual chapter D.14 Import (import data from other IUCLID 5 systems) .

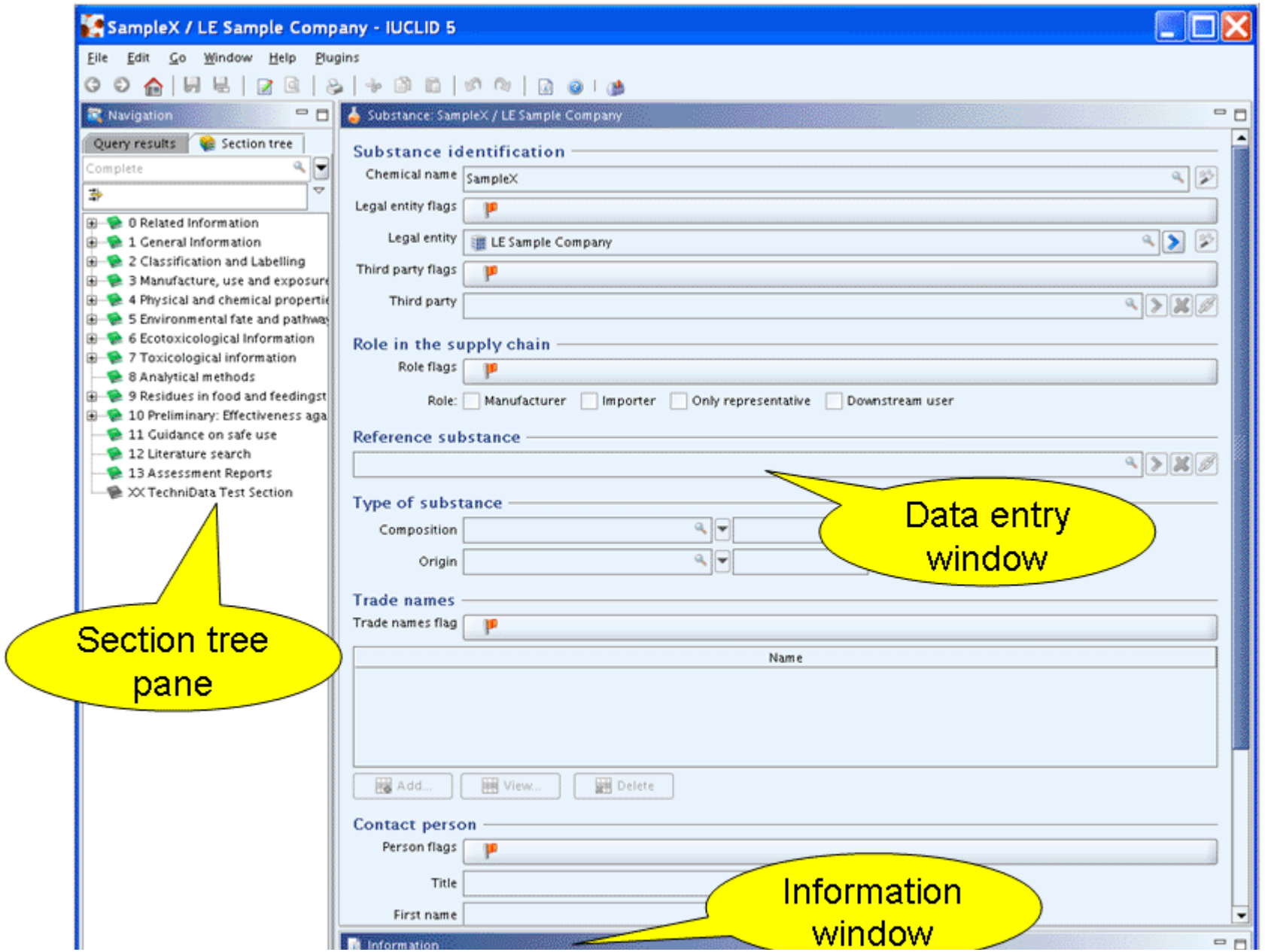
9. Making annotations

The tutorial in this chapter shows how to make annotations on records on the raw data level and on records provided with a Dossier.

Introduction

The Annotations feature is primarily designed for the use by regulatory authorities, e.g. the European Chemicals Agency or Competent Authorities of the Member States, when evaluating the data submitted by the applicant. However, it may also be used by the Legal entity compiling a Substance dataset, for example, in the context of the internal review process.

The Annotations feature can be found on the Annotations tab of the Information window, which is provided just below the Data entry window, as shown in the following screenshot:


SampleX / LE Sample Company - IUCLID 5
File Edit Go Window Help Plugins
Navigation
Query results
Section tree
Complete
0 Related Information
1 General Information
2 Classification and Labelling
3 Manufacture, use and exposure
4 Physical and chemical properti
5 Environmental fate and pathwa
6 Ecotoxicological Information
7 Toxicological information
8 Analytical methods
9 Residues in food and feedingst
10 Preliminary: Effectiveness aga
11 Guidance on safe use
12 Literature search
13 Assessment Reports
XX TechniData Test Section
Substance: SampleX / LE Sample Company
Substance identification
Chemical name
SampleX
Legal entity flags
Legal entity
LE Sample Company
Third party flags
Third party
Role in the supply chain
Role flags
Role:
Manufacturer
Importer
Only representative
Downstream user
Reference substance
Type of substance
Composition
Origin
Trade names
Trade names flag
Name
Add...
View...
Delete
Contact person
Person flags
Title
First name
Information
Section tree pane
Data entry window
Information window

Tip

You can minimise / maximise the Information window by clicking the respective **Minimise** or **Maximise** button in the upper right corner of the title bar of this window.

An annotation record consists of the following three tabs:

- Data: Constitutes the actual annotation entry screen.
- Information: Contains general technical information:
  - Record ID: Displays the UUID (**U**niversal **U**nique **ID**entifier) assigned to the annotation record.
  - Linked record ID: Displays the UUID assigned to the record the annotation record refer to.
  - Linked record type: Displays the type of the linked record.
  - Linked record date: Displays the date of the linked record.
- Modification: Shows the modification history of the current annotation document.

Annotations can be created for any IUCLID element. As a general rule, the Annotations tab provided in the Information window is related to the very record displayed in the above Data entry window. This can be the Dossier, an Endpoint study or summary record of any Substance contained in the Dossier, the Legal entity or the Legal entity site, etc.

For more information, see the IUCLID 5 End User Manual chapter D.4.9 How to use the Information window .

9.1. Annotating raw data

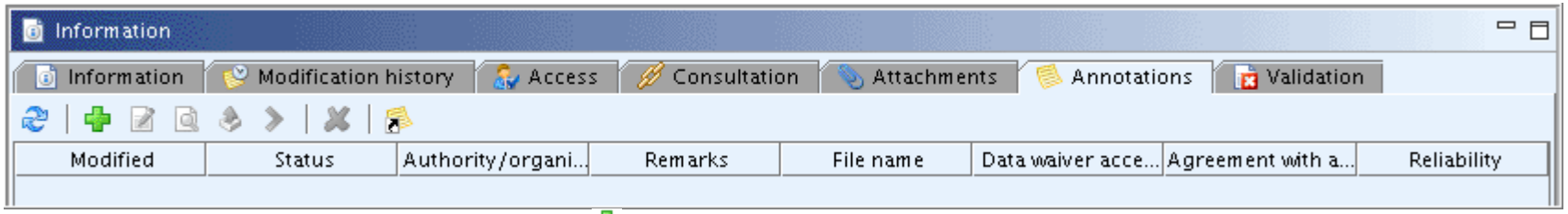
Although sections 0 to 3 of a Substance dataset are technically handled as one record in IUCLID (see the IUCLID 5 End User Manual chapter D.4.6.1 Differences between sections 0 - 3 and sections 4 - 13), individual annotations can be created for each subsection. The following hands-on example demonstrates how to manage an annotation record for an Endpoint study record. The same principles apply for annotating any other IUCLID element, except

that the Annotation template for Endpoint study records provides additional endpoint-related annotation fields.

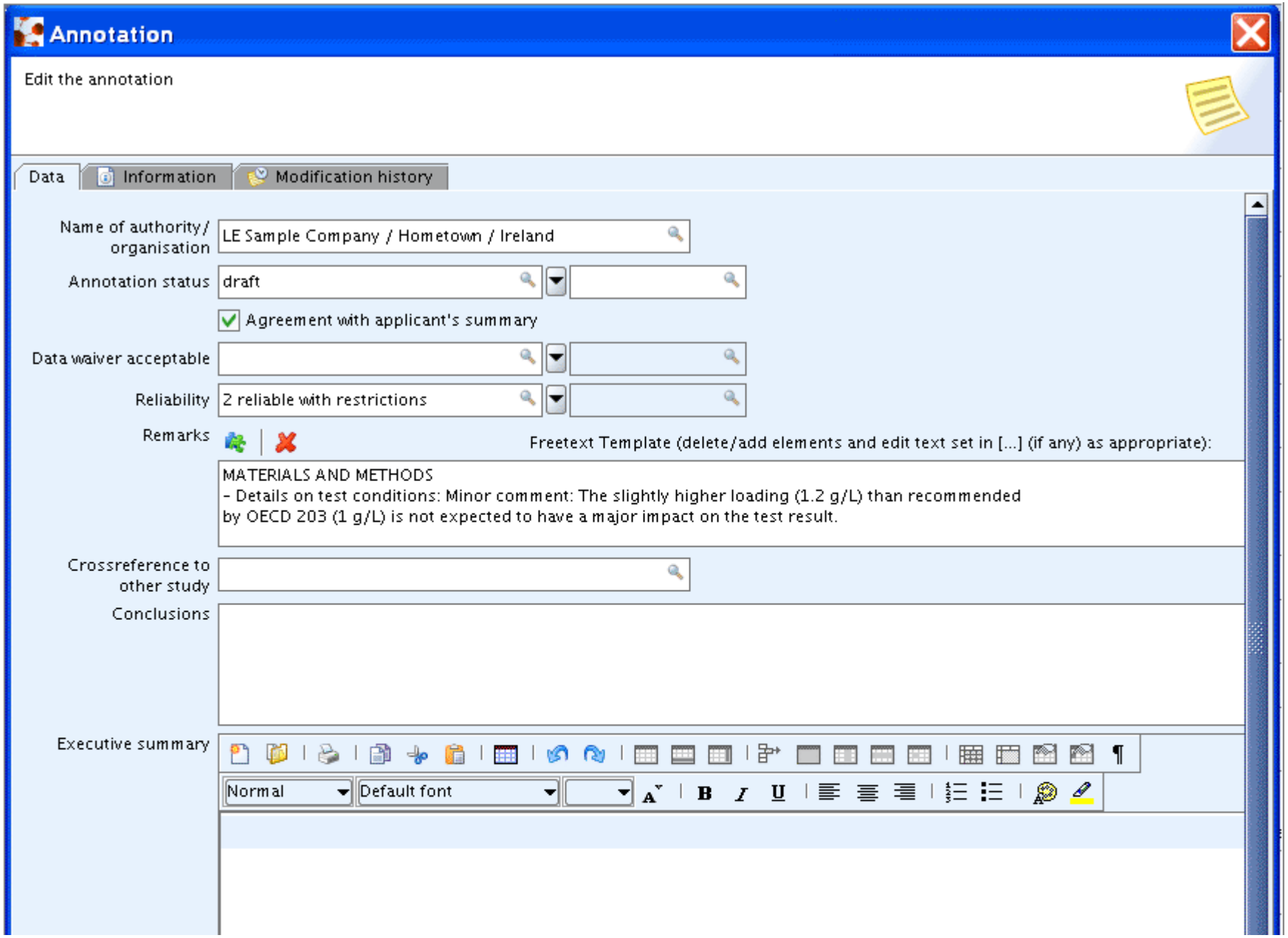
Step-by-step guide

To add an annotation related to the sample Endpoint study record

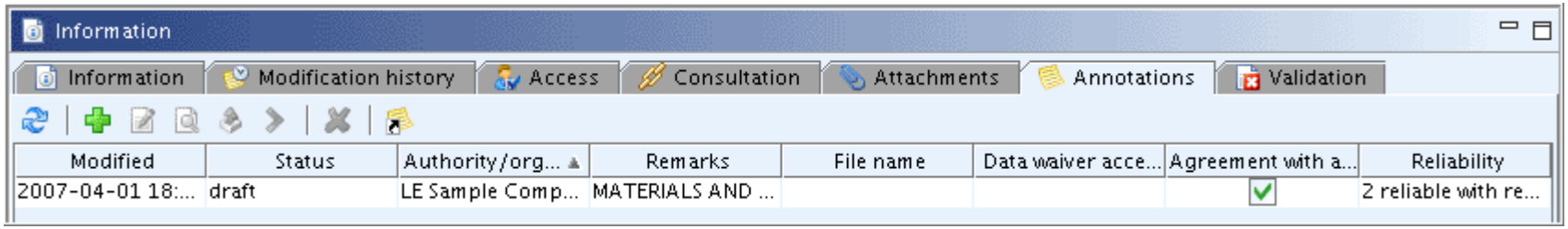
1. Find the record "Dorgerloh (1992)/key" in the section tree and double-click it to open it.
2. In the Information window, click the Annotations tab to access this feature.



3. On the Annotations toolbar, click the **Add** button .
4. In the Annotation template appearing, complete the appropriate fields, as shown in the screenshot below. In the fields `Conclusions` and `Executive summary`, the submitter's proposal may be adopted or revised as appropriate.
5. Click the **Save** or **Save with comment** button if you wish to add any comment, which will appear in the modification history only.


Annotation
Edit the annotation
Data
Information
Modification history
Name of authority/ organisation
LE Sample Company / Hometown / Ireland
Annotation status
draft
Agreement with applicant's summary
Data waiver acceptable
Reliability
2 reliable with restrictions
Remarks
Freetext Template (delete/add elements and edit text set in [...] (if any) as appropriate):
MATERIALS AND METHODS
- Details on test conditions: Minor comment: The slightly higher loading (1.2 g/L) than recommended
by OECD 203 (1 g/L) is not expected to have a major impact on the test result.
Crossreference to other study
Conclusions
Executive summary
Normal
Default font

After clicking the **Save** button, the annotation record is displayed in table-view as follows:



9.2. Annotating a Dossier

The Annotations feature can also be used to make annotations on any Dossier component and any record withing each component. As a general rule, the Annotations tab provided in the Information window is related to the very record displayed in the Data entry window. This can be the Dossier, an Endpoint study or summary record of any Substance contained in the Dossier, the Legal entity or the Legal entity site etc.

Important

Any annotations made on raw data are not included in Dossiers. Vice versa, any annotations made on Dossier data are confined to the Dossier and are not related to the corresponding raw data records.

Step-by-step guide

First the Dossier needs to be opened as follows:

1. Go Home to the Task panel if you are not already there.
2. Under **Dossier** , click **View**. A screen comes up with empty windows on the right side and a **Query results** pane on the left (below the title bar **Navigation**) showing all Dossiers available in your local IUCLID installation or the network you are connected to.
3. Double-click the desired Dossier to display it in the Components pane together with all its components, as shown in the screenshot below.

4. If there is a large number of Dossiers listed, run a query as described for Substances in the IUCLID 5 End User Manual chapter D.4.3.2 Querying for a Substance in the Query results pane .

5. When the desired Dossier has been selected, it is displayed in the Components pane together with all its components, i.e.:

    - The Dossier itself:

        - The Dossier title includes the Dossier template type, the name of the Substance / Reference substance, the CAS No., Legal entity, date and the user-defined name.

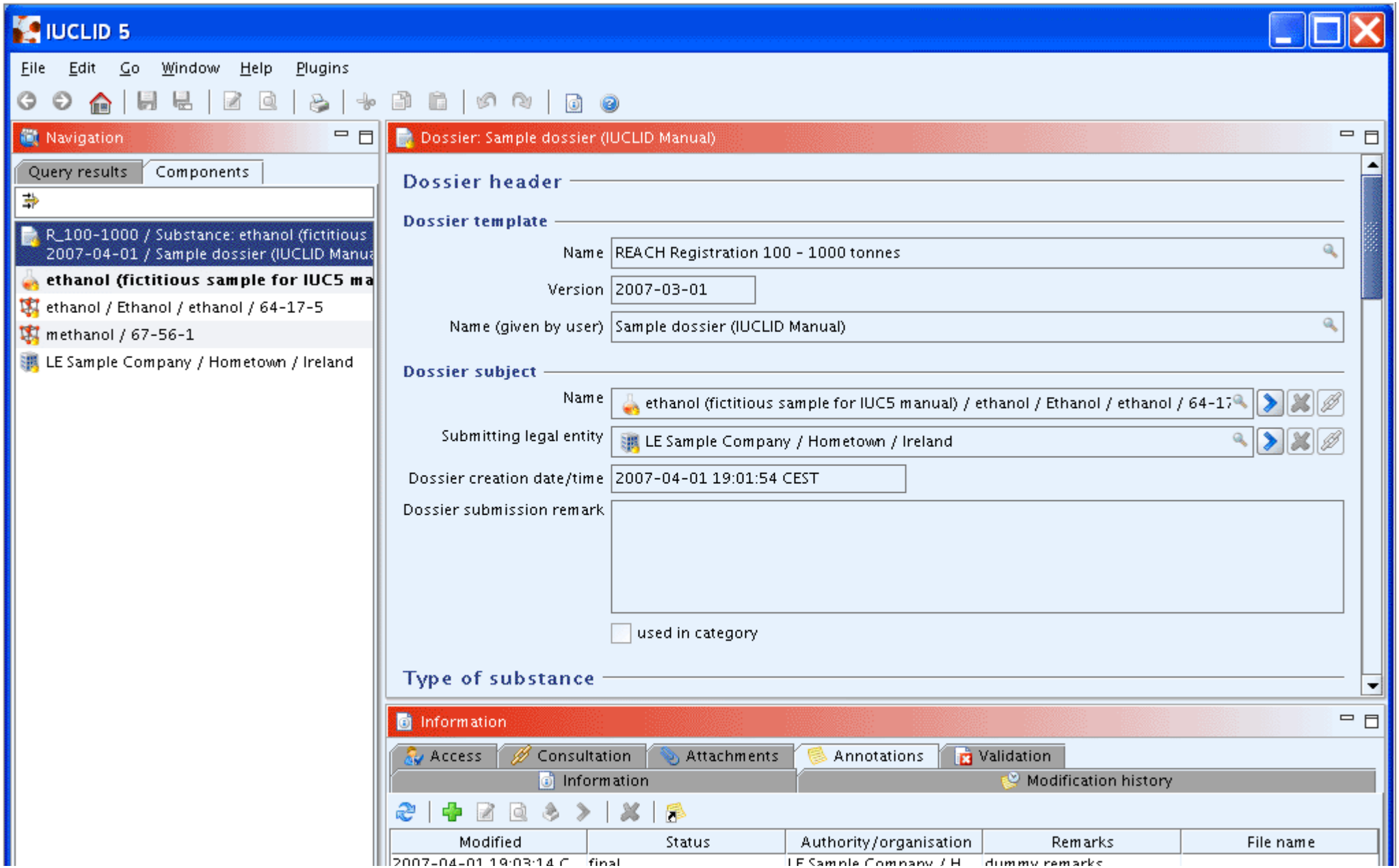
        - The Dossier information entered during the process of Dossier creation is displayed (read-only) in the Data entry window.

        - The Dossier-related Information window including the Annotations tab.

    - The source Substance dataset (in **bold**).

    - The Reference substance referred to in the Substance.

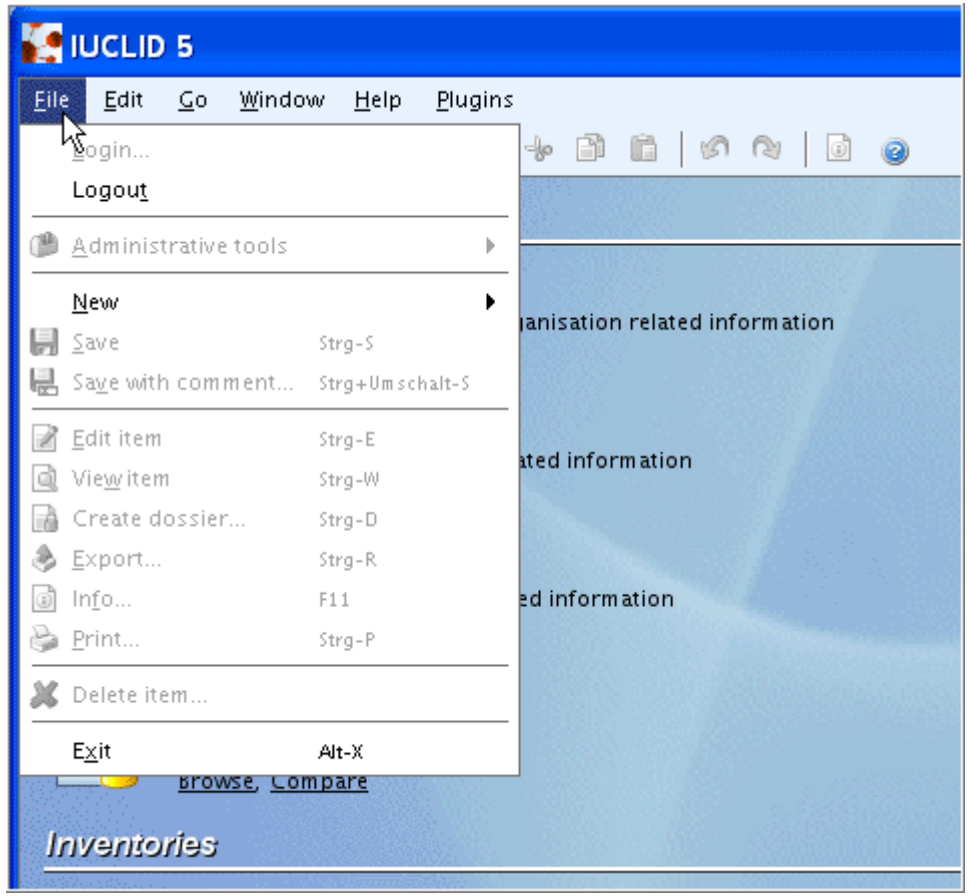
    - The Legal entity the Substance is assigned to.


IUCLID 5
File Edit Go Window Help Plugins
Navigation
Query results
Components
R_100-1000 / Substance: ethanol (fictitious
2007-04-01 / Sample dossier (IUCLID Manua
ethanol (fictitious sample for IUC5 ma
ethanol / Ethanol / ethanol / 64-17-5
methanol / 67-56-1
LE Sample Company / Hometown / Ireland
Dossier: Sample dossier (IUCLID Manual)
Dossier header
Dossier template
Name
REACH Registration 100 - 1000 tonnes
Version
2007-03-01
Name (given by user)
Sample dossier (IUCLID Manual)
Dossier subject
Name
ethanol (fictitious sample for IUC5 manual) / ethanol / Ethanol / ethanol / 64-17
Submitting legal entity
LE Sample Company / Hometown / Ireland
Dossier creation date/time
2007-04-01 19:01:54 CEST
Dossier submission remark
used in category
Type of substance
Information
Access
Consultation
Attachments
Annotations
Validation
Information
Modification history
Modified
Status
Authority/organisation
Remarks
File name
final
dummy remarks

To add annotations to the Dossier, open the desired Dossier component and navigate to the element where you wish to comment on. For example, add an annotation to the Dossier itself or open the Substance dataset, navigate to Endpoint record(s) and add annotations related to these records. As to how to create annotations see the preceding exercise.

10. Logging out

To log out from your user account or exit IUCLID, select the respective **Logout** or **Exit** command from the File menu.



European Commission

IUCLID 5 Guidance and support

Vol. 2: Getting Started
June 2007

http://iuclid.eu