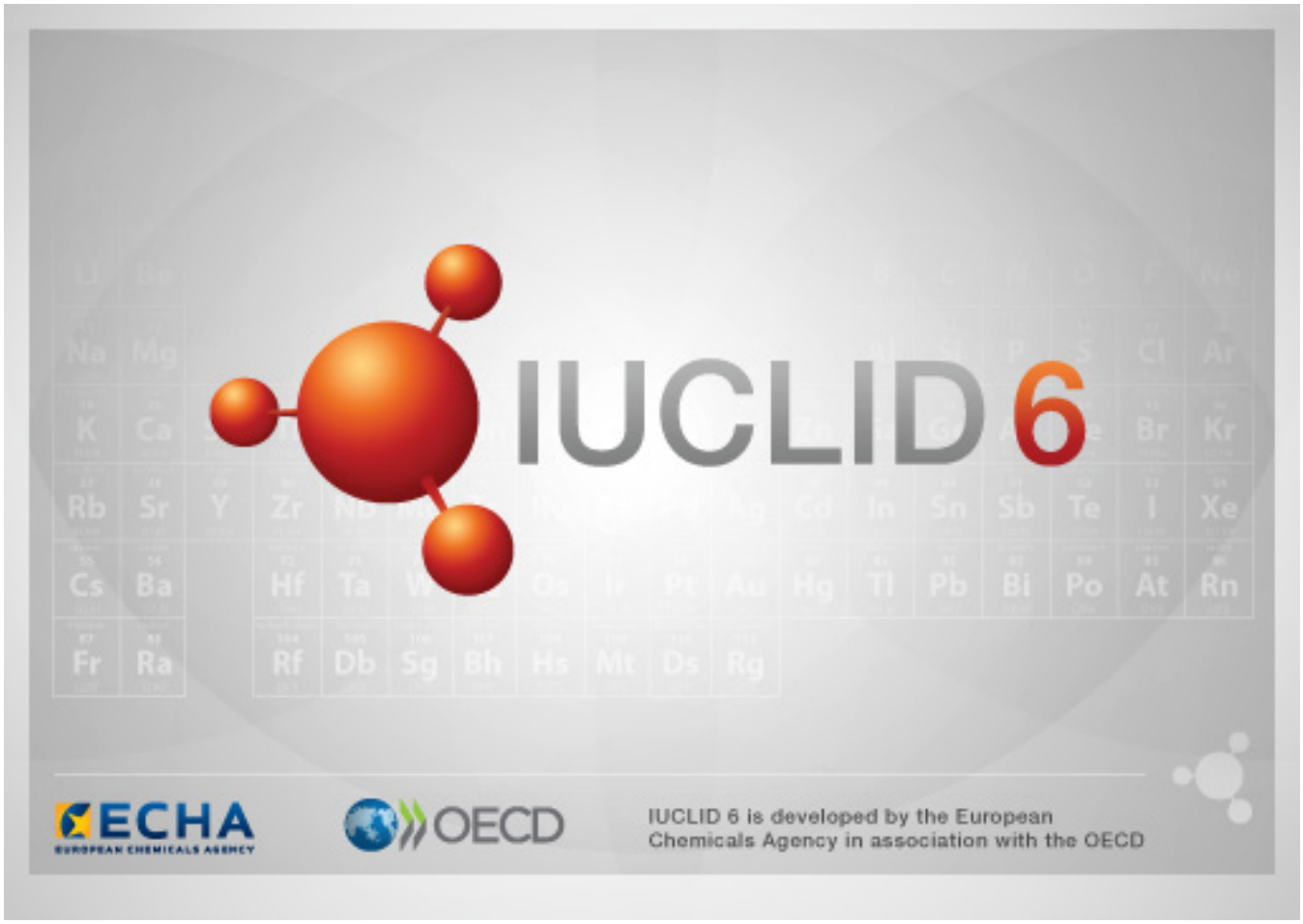
Functionalities of IUCLID 6



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Changes to this document

Date	Modification
29/04/2016	First version
21/06/2016	Added a description of how to prevent the locking of the *User*, SuperUser. Stated the default passwords given to *Users* when they are imported, or created by importation of a CSV file. Updated the description of the Validation assistant in sections *19.4.3.2. Validation assistant report toolbar* and *19.4.3.4. Validation assistant report table*. Added a description of how to backup and restore data using a separate software tool that is supplied with IUCLID 6 Desktop. Added information on how to update IUCLID 6 and its plugins.

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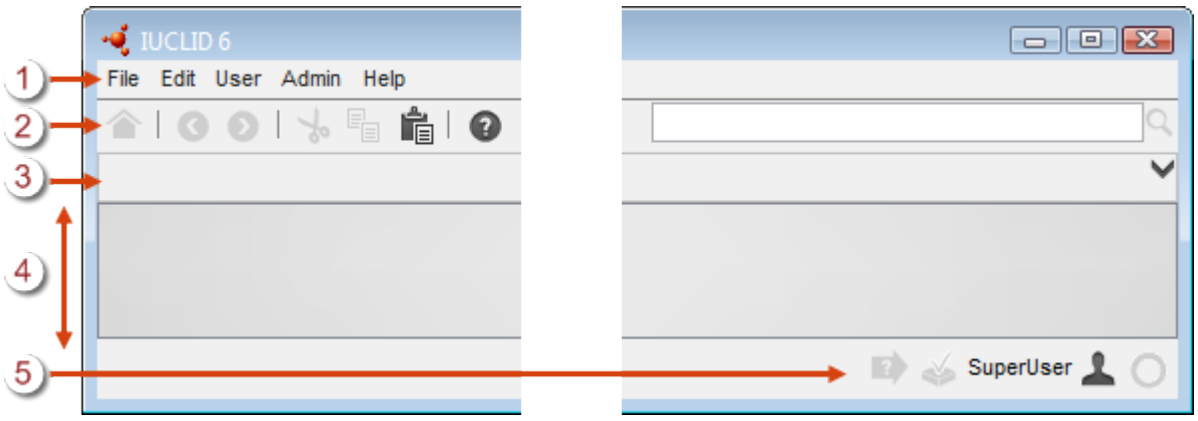
1. Overview of the interface

The graphical user interface of IUCLID 6 has a main window with fixed menus for functions displayed at the top and bottom of it. Between the upper and lower menu areas, there is an area that can show either a home page, or various fields for the management of data. The latter is divided into three panels: *Navigation*, *Data* and *Information*. The overall structure of the interface is shown below.

Figure 1: Structure of the interface of IUCLID 6



Key for Figure 1:

1. The main menus;
2. The upper menu toolbar;
3. The area for system messages. The black downward pointing arrow at the right expands the area to show all messages;
4. The main inner window which shows either the home page, or a page divided into three panels: *Navigation*, *Data*, and *Information*;
5. The lower menus toolbar, which shows the available plugins, the current *User*, and the background jobs.

Some of the functions of IUCLID 6 are displayed in their own pop-up windows. In some cases, the pop-up window contains a wizard that allows for the input of data in a structured and sequential manner. Examples include *Export*, and the creation of a *Dossier*. The parts of the main window are described below.

1.1. Technical terms

The following technical terms refer specifically to the use of IUCLID 6 and its interface.

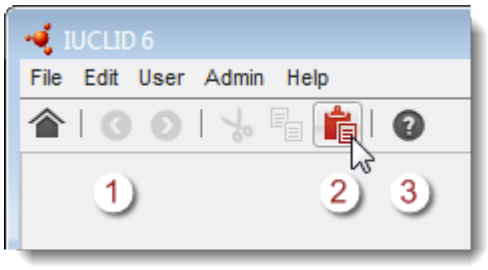
Table 1: Some technical terms

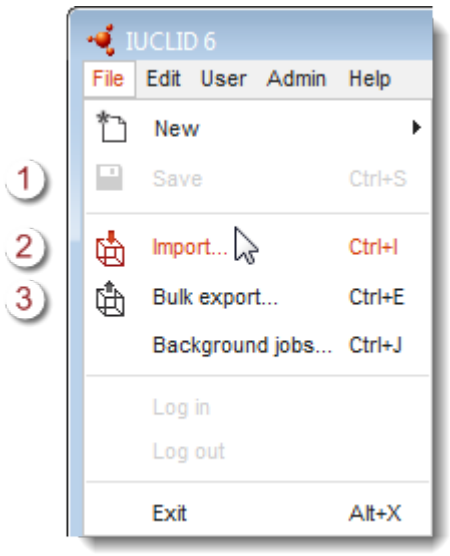
Term	Description
Data object	A *data object* in IUCLID 6 is any discrete piece of data, serving a unique and specialist purpose, that can be created, modified, and deleted independently via the interface.
Field	A *field* is a piece of data that exists as part of a data object. There can be many fields in one data object.
Block	A *block* is a set of fields grouped because of common business behaviour or database dependency. They are grouped and commonly identified to allow the functionality to be reused throughout the application.
Entity	An *entity* is a type of data object in IUCLID 6 that can be managed from the sections on the home page that are labelled *Main tasks* and *Inventories*. Examples include *Substance* and *Legal entity*. Typically, entities can be re-used across various different data objects.
Document	A *document* is a page that contains functionality for creating, viewing or modifying an entity, a record, or a summary. A *document* is also a standard set of data that exists in a *Substance* as a node in the table of contents.

1.2. States of icons, menu items and buttons in the interface

In the interface, icons, menu items, and buttons that contain links to functions can be shown in three different states. Dark grey means that the link is active. A very pale grey means that the link is not active either because the function is not relevant, or is blocked for security reasons. The colour orange indicates that the mouse pointer is currently hovering over at item so that a primary/left click follows the link. In some cases, right-click gives access to a menu. An example of the colours used it shown below.

Figure 2: Hues and shades used in the interface





Key for Figure 2:

1. The icon or menu item is disabled;
2. The cursor is hovering over a clickable area;
3. The icon or menu item is clickable.

1.3. Common functionalities in the interface

The following functionalities are used throughout the interface.

1.3.1. Free text template

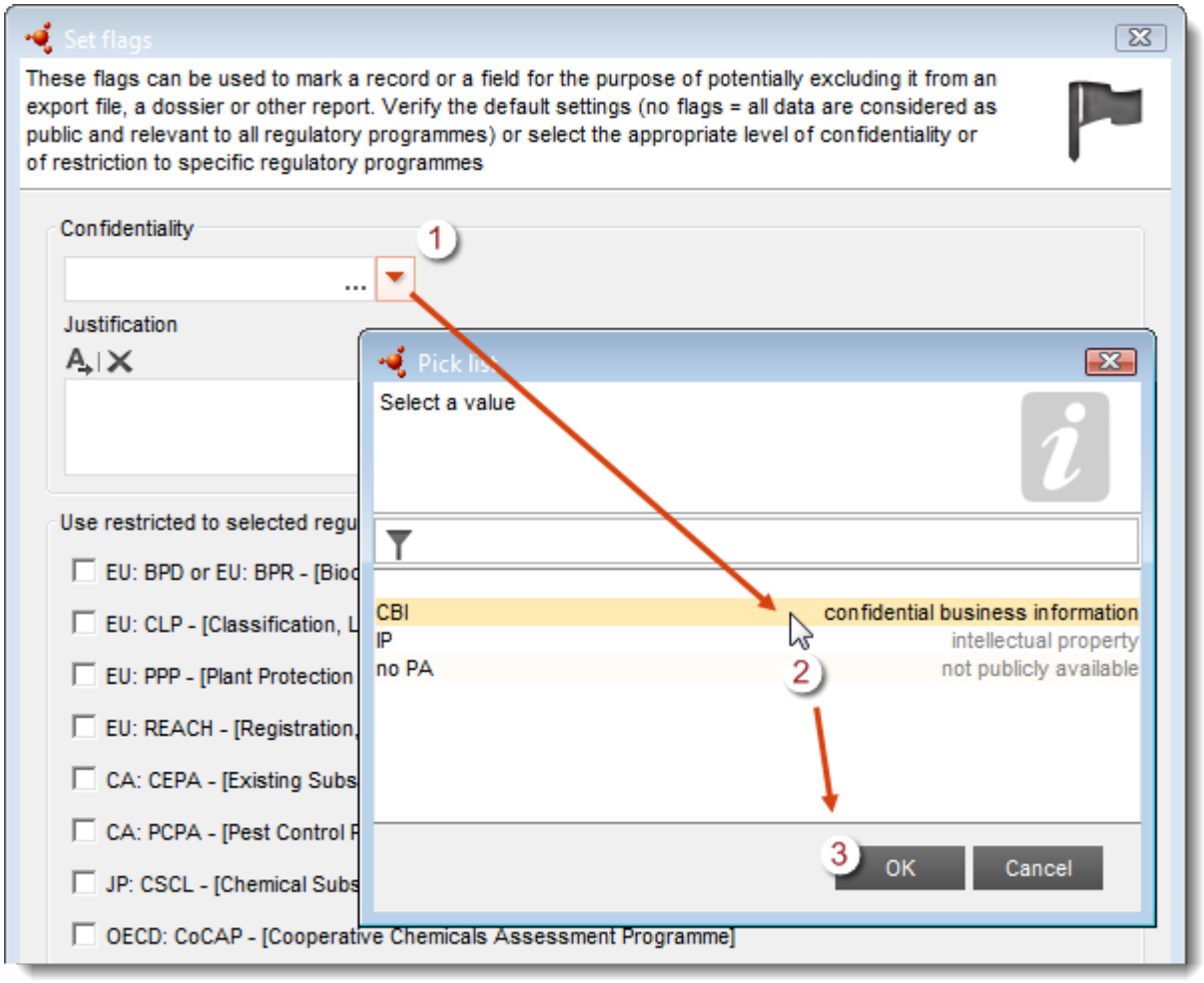
A free text template is a piece of text designed to help the user to enter all the required information into a field that can contain any text value. It provides a model text which must be edited to fit in with the particular circumstances of the user in that context.

To open a free text template, click on the icon that shows the letter A with an arrow at its lower right, . To copy the text from the template to the field, click on the button labelled *Insert*. The text should now be edited as required.

1.3.2. Flag

Individual fields and groups of fields can be labelled with a flag. By default, no flags are set. A single flag can indicate both confidentiality and/or an association with a particular regulatory programme. Flags can be used to filter data when placing it in a *Dossier*, exporting or printing. The field to which a flag refers is indicated either in the name of the flag, or is the field immediately below the flag icon. The flag is a field in itself that can be opened and data entered, as shown below.

Figure 3: Set confidentiality in a flag

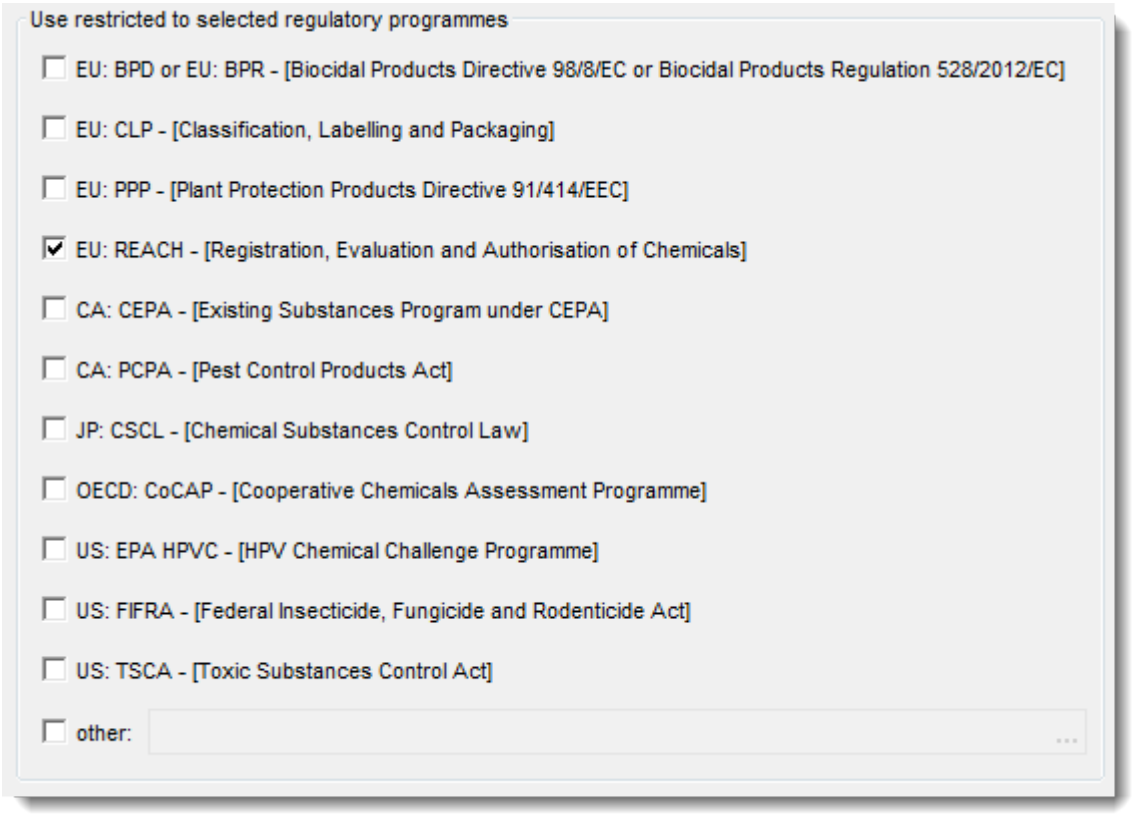


To add confidentiality to a flag, click on the downward pointing arrow to open the pick list (1), select the type of information in the field (2), an then click OK (3).

If a justification of the confidentiality is required, enter it into the field *Justification*, which is a free text field that has a free-text template. Suggestions as to what to enter are provided in free text template. To open the free text template, click on the icon that shows the letter A with an arrow at the bottom right, A. To copy the text from the template to the field, click on the button labelled *Insert*. The text should now be edited as required.

To set an association with a regulatory programme, tick one or more of the boxes, as shown below.

Figure 4: Set a flag for association with a regulatory programme



The possible states of a flag each have their own icon as shown below.

Table 2: The icons for the states of a flag

Icon	State
	No flag is set.
	A flag is set but confidentiality is not involved.
	A flag is set that involves confidentiality.

If a flag is set, a code is shown after it to indicate its type. The codes for confidentiality are CBI (*Confidential business information*), IP (*Intellectual property*) or No PA (*Not publicly available*). The code for association with a regulatory programme is the code shown in the interface in capital letters before the hyphen, for example EU: REACH. In the example shown below, there is a flag set that indicates the field contains confidential business information and is associated with the REACH legislation of the EU.

Figure 5: A flag applied to a field

1.4. Main menus

The menus provide access to various functions and parts of the interface. In some cases, the access to the same function is also provided from elsewhere in the interface, such as *right-click* on selected documents. If an icon is shown in a very pale grey, almost white, either the function is not relevant in the current context, or the current *User* does not have permission to access it.

1.4.1. File

The file menu provides access to a variety of functions, most of which can also be accessed from elsewhere. The administration functions can be accessed from only here.

1.4.1.1. New

This function is used to create a new software object of one of the types specific to IUCLID. These include *Legal entity*, *Site*, *Substance*, *Template*, *Mixture/Product*, *Category*, *Reference substance*, *Contact*, *Literature reference*, *Annotation*, and *Test Materials*. The same function can be accessed per entity by right-clicking on its icon on the home page, and also by clicking on the icon , in the header of the search results.

1.4.1.2. Save

This function saves the changes to the database that were made since the last save action. When data is saved successfully, a message is displayed with a green information icon.

1.4.1.3. Import

This feature is used to import data into IUCLID 6 that has been exported from either IUCLID 5.6 or IUCLID 6. It is a convenient way of moving data from one system to another. It may also be launched from the home page. The feature is described in detail in section *16 Import*.

1.4.1.4. Bulk export

In the first field, *Number of bulk exported documents allowed*; an upper limit may be placed on the number of documents that can be exported at once. For example, this can be used to avoid running out of storage space mid-way through an export process.

The second field, *Max number of bulk exported documents per directory*, may be used to set an upper limit to the number of files output to any one folder. When the limit is reached, IUCLID 6 creates a new folder automatically and then continues exporting to the new folder. This feature was introduced because some computer file systems become very slow when thousands of files are placed in the same folder, irrespective of the size of the files.

1.4.1.5. Background jobs

Background jobs are described in section *1.7.3 Background jobs*. They can also be accessed from the circular icon in the lower right corner of the interface.

1.4.1.6. Log in

This opens a pop-up window from which a *User* can log in, as shown below. It is accessible only when no *User* is logged in and user management is enabled. For more information, see section *15 User management.*

Figure 6: The log in window

1.4.1.7. Log out

Logging out leaves the application running with the main window open. A *User* can then log in as described in the previous section. This is relevant only whilst a *User* is logged in and user management is enabled. For more information, see section *15 User management.*

1.4.1.8. Exit

This shuts down the interface. For the desktop type of installation, the application itself is also shut down. For the server type of installation, the instance of the local client is shut down, but the application running on the server is unaffected.

1.4.2. Edit

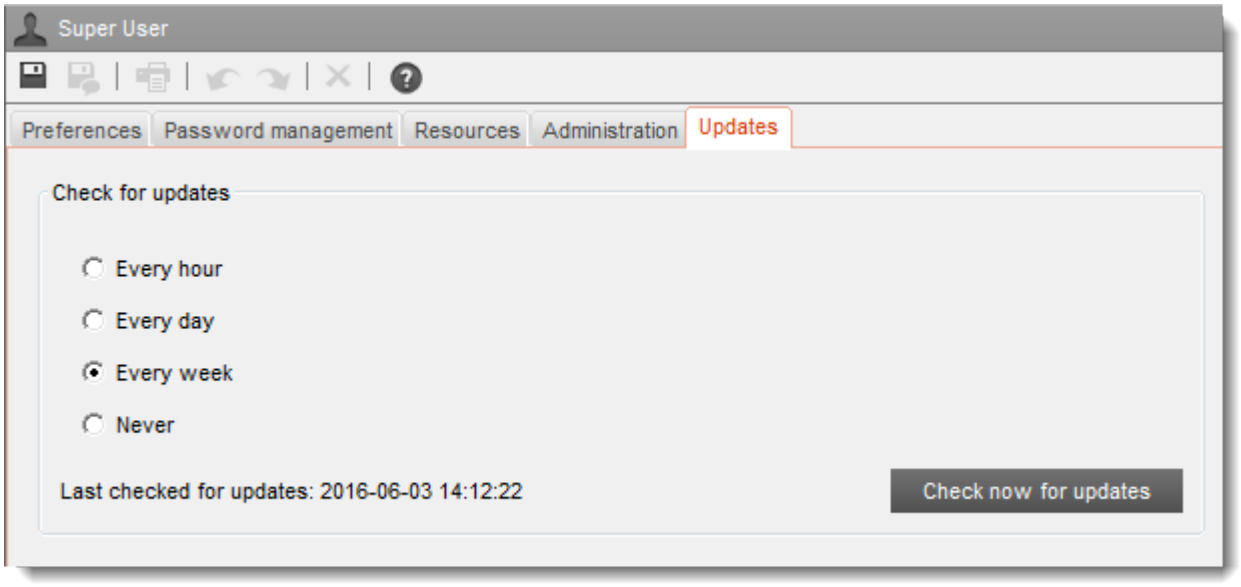
This menu contains the standard editing functions: *cut*, *copy* and *paste*. The standard shortcuts are available, for example CTRL+V for *paste*.

1.4.3. User

For an installation of IUCLID 6 Desktop made using default values, where User management is disabled, this menu contains only the item *My account*. From there, the User can manage values for the default User named SuperUser. For example, the working Legal entity can be changed from here. For a more detailed description of the fields, see the section on User management.

For an installation of IUCLID 6 where User management has been enabled, this menu contains shortcuts to the creation and management of *Users* and *Roles*. In addition, if Instance Based Security (IBS) has been enabled there is also access to *Groups*. There are also links to specialist user management tools, as described in sections *0 The feature Check for updates* may be used to instruct IUCLID 6 to send periodic automated requests to the IUCLID 6 web site to check whether a newer version of IUCLID 6 or its plugins is available. When IUCLID 6 detects that a newer version is available, it will notify the *User* in the message window. If an attempt to make a check gives an error message, check the internet connection and proxy settings on the host computer.

To check immediately whether the installation of IUCLID 6 or its plugins contain the most recent version, click on the button *Check now for updates*, shown in the figure below.



If an update is available, go to the downloads section of the IUCLID 6 web site, select the option for the appropriate *Updater tool* for the system, and then follow the instructions.

Note that update process updates both the application and its plugins. There are no separate updates to be done for plugins.

Export users, *15.1.2.7 Download empty users csv*, and *15.1.2.8 Import users*.

For more information about *Users*, *Roles*, *Groups*, and IBS see section *15 User management*.

1.4.4. *Admin* / System administration

This allows various settings to be adjusted that affect the behaviour of the whole system. The option is accessible only whilst the home page is displayed.

1.4.4.1. General

The query limit is the maximum number of documents returned by a single search in the navigation pane. An upper limit can be applied to prevent the system from running out of resources, for example memory, if a search returns too many results.

1.4.4.2. Security policy

These settings relate to the authentication of *Users*, as described in section 15.1.2.2 Password management, and in section 15.1.2.4.1 General. These functions are relevant only if user management is in use. The fields have self-explanatory labels.

The field *Instance Based Security* is an indicator of whether this feature is activated. The value of the field cannot be change via the interface. Instructions on how to turn this feature on and off are given in the document, IUCLID 6 Server installation manual that is available from the IUCLID 6 website. The field is not shown in IUCLID 6 Desktop.

1.4.4.3. Export

This section contains fields designed to avoid situations in which IUCLID 6 and its processes run out of sufficient IT resources. The field *Max number of bulk exported documents per directory* exists because some file systems become unusably slow if the number of files in a directory goes above a certain limit. This effect does not depend on file size.

1.4.4.4. Import

This field is designed to avoid situations in which IUCLID 6 and its processes run out of sufficient IT resources.

1.4.5. Help

This menu gives access to the help system of IUCLID 6 and information about the system itself.

1.4.5.1. Help

Help, opens the help system of IUCLID 6 at the most recently viewed page. The first time the help is viewed after start-up of the application, a default page is shown.

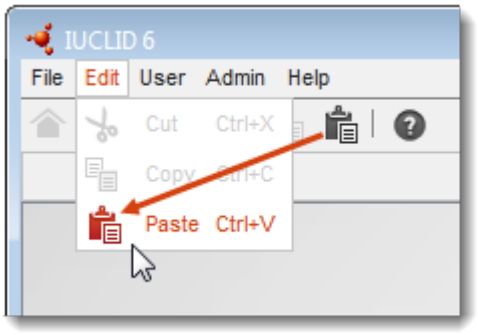
1.4.5.2. About

About opens a window that contains technical and legal information about IUCLID 6, and the specific instance of the software. For example, the version number of the application is shown at the bottom left of the first window.

1.5. Menu toolbar - upper

For user convenience, this menu contains links to frequently used functions that are also available via the main menu. An example is shown below in which the duplication of the link to *paste* is highlighted.

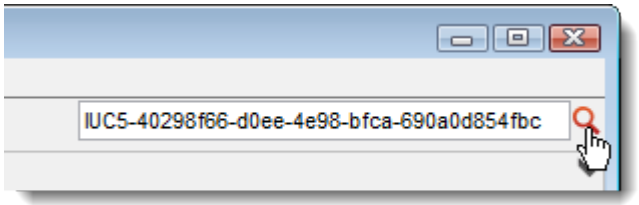
Figure 7: Upper menu toolbar



1.5.1. Search by UUID

To search for any document by its Universal Unique Identifier (UUID), paste the UUID into the field shown in the example below, and then either click the magnifying glass icon, or press the key, *Enter*.

Figure 8: Search by UUID, showing an example value



The search results are shown in the navigation pane. This is often the quickest way to get to a document, if the UUID is easily accessible.

Bear in mind that there can be more than one search result per UUID. For example, a *Substance dataset* may give a result for itself, and each of the copies of it that exist in *Dossiers*.

1.6. Message area

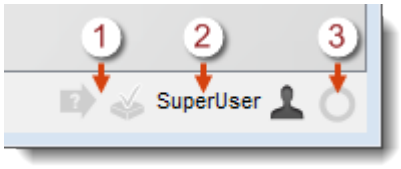
This part of the interface is used to display messages from the system, for example to state that a new document has been created successfully. If an error is displayed that you cannot explain, and you think should be reported to the providers of the software, see section 22 Getting additional help.

There can be more than one message displayed here at a time. To see more of the messages, expand the height of the message area by clicking on the downward pointing black arrow at the far right of the message area. Similarly, to collapse the area, click the upward pointing arrow.

1.7. Menu toolbar - lower

In the lower right-hand corner of the interface, the following functions are available, as shown in the figure below.

Figure 9: The lower menu toolbar



1.7.1. Plugins

An icon is shown for each of the plugins currently available in the system (see 1 above). If an instance of the plugin is running, its icon is shown in dark grey and provides an active link to the instance.

1.7.2. Current User

The second field (see 2 above)) shows the name of the currently active *User*. The access to data and functionalities are determined by the rights of the active *User*. SuperUser has complete access to data and administrative functions.

1.7.3. Background jobs

Background jobs are tasks that IUCLID 6 performs in the background to allow a user to continue using the interface whilst the task is being done. Some tasks, for example exporting a large amount of data, can take too long to expect a user to wait whilst they complete.

The state of background jobs is indicated by a circular icon in the lower right-hand corner of the interface. If the icon is orange and rotating, at least one job is under way. If the icon is orange and flashing, all jobs have finished, and there is a least one record of a job in the console. To open the *Background jobs* console, either select the menu item *File / Background jobs*, or click on the icon in the lower toolbar.

The background job console contains a record for each background job, with the most recently started job shown at the top. If a job is still in progress, there is an option to cancel it ✕. The record shows the type of job, a progress bar, and for finished jobs, a statement of whether the job succeeded or failed.

The meanings of the icons are given in the following table:

Table 3: The icons in the background jobs console

Icon	Meaning
✕	Cancel a running job.
⊗	Clear, or close, the record of a completed job. It cannot be re-opened.
	View the sub-jobs of a job. Not all types of jobs have sub-jobs.
	View a report for a job or a sub-job.
	Download data that was exported in the job. The data should already have been saved externally once, but this allows the save to be repeated, and to a different destination if required. An exception to that is the download of *User* data, which can be done only from the background job.
i	The job was completed successfully.
⊗	A problem was encountered during the job. See the report for details.

The button *Cancel all* cancels all the jobs that are still running.

The button *Clear finished* closes the records for the jobs that have completed. The records cannot be re-opened.

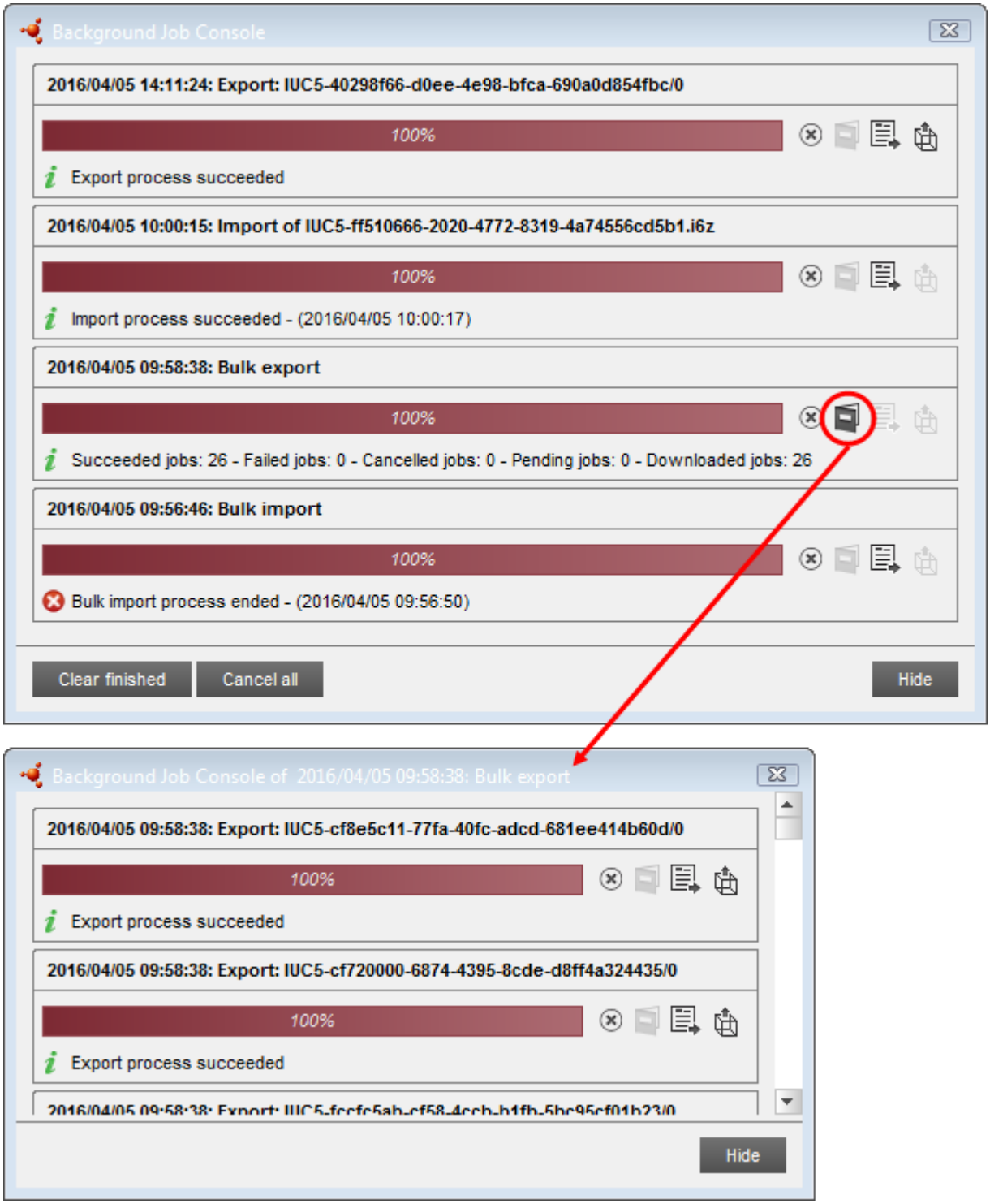
The button, *Hide* closes the background job console without affecting its contents or the jobs.

Example

An example is shown below in which there are four job records comprising, an export of a single entity, an import, a bulk export, and a bulk import. The first three jobs were successful, as indicated by the green icon, *i* , but in the fourth record, the red icon, ⊗, indicates that a problem occurred. In this example, the User would probably click on the report icon, , to see what the problem was.

The record for the second entry, the bulk export, has 26 sub-jobs, whose records can be accessed individually by clicking on the icon for open document, , that is circled in red below.

Figure 10: Example of records in the background job console



1.7.3.1. Background jobs for export

Exporting from the background job console is allowed only per sub-job. This can be seen in the example shown above where the export icon for the main job is disabled, but it is enabled for the

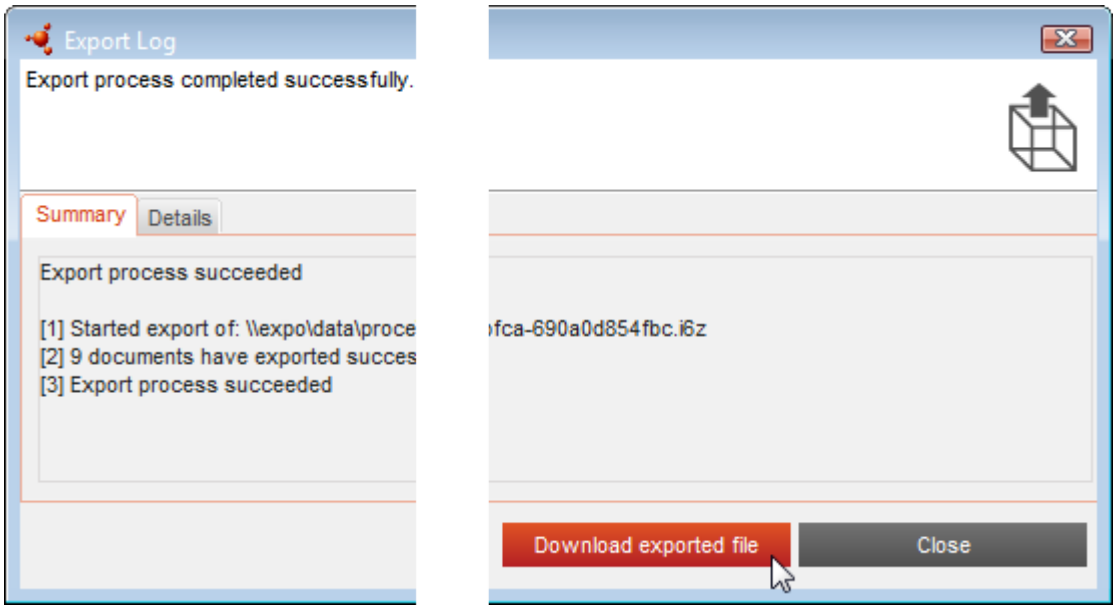
sub-jobs. The data should already have been saved externally once while the background job ran, but this allows the save to be repeated, and to a different destination if required.

1.7.3.2. Reports for background jobs

To obtain information about what happened in the job, click of the report icon  . This opens a pop-up window that contains a detailed list of events that occurred during the job.

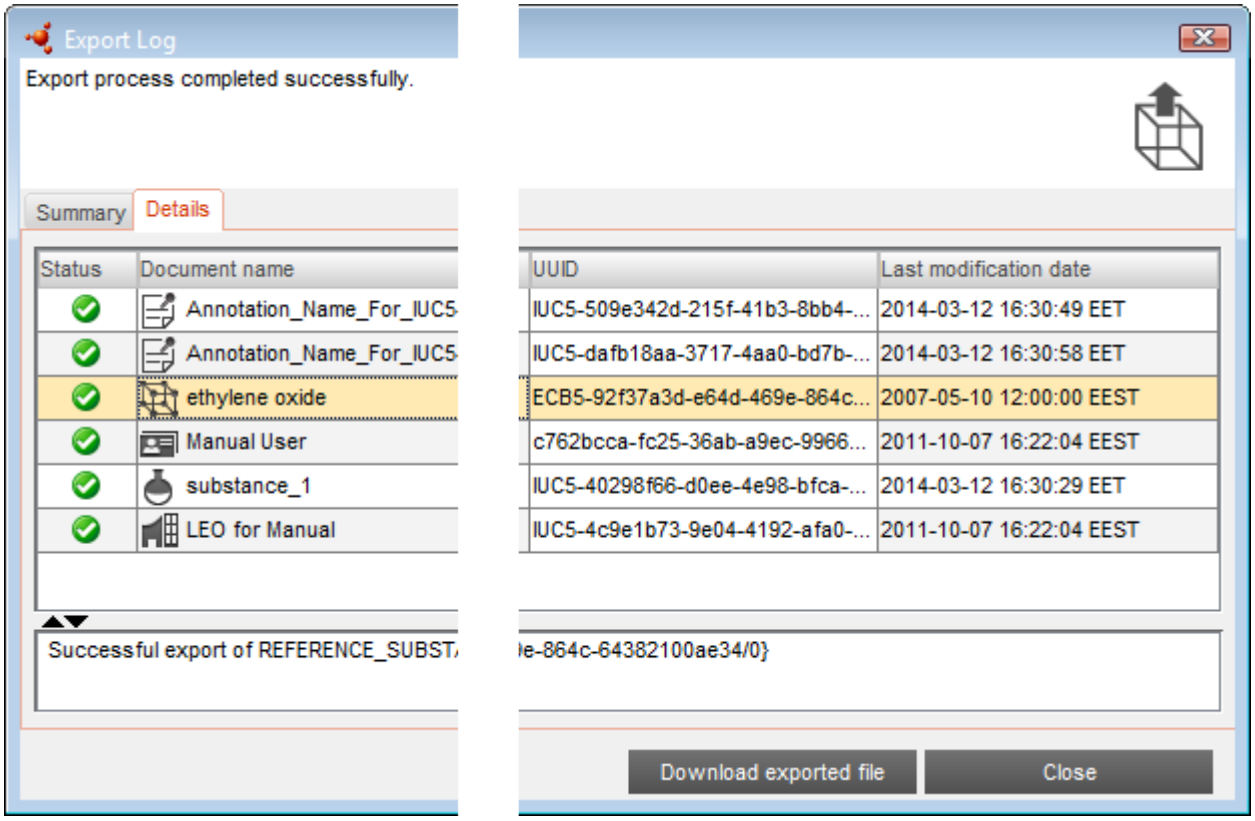
The pop-up window for an export process opens at a tab labelled *Summary*, but it also has a tab labelled *Details*. The tab *Summary* contains a list of steps of what happened, and a link from which all the data from the job can be downloaded at once, by clicking on the button, as shown in the example below. The data should already have been saved externally once, but this allows the save to be repeated, and for the destination to be selected.

Figure 11: The summary of a background job



The tab *Details* contains a list of the individual entities that were included in the export. The download button here functions in the same way as that under *Summary*.

Figure 12: The details of a background job



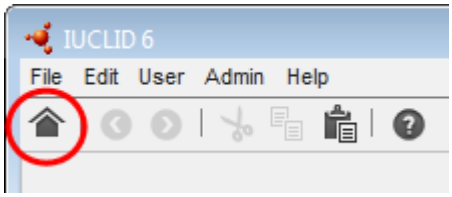
1.7.3.3. Clearing background jobs

Do not clear a record of a job until you are sure that you no longer need the information it contains. Once cleared, or removed, the information is no longer available via the interface.

1.8. Home page

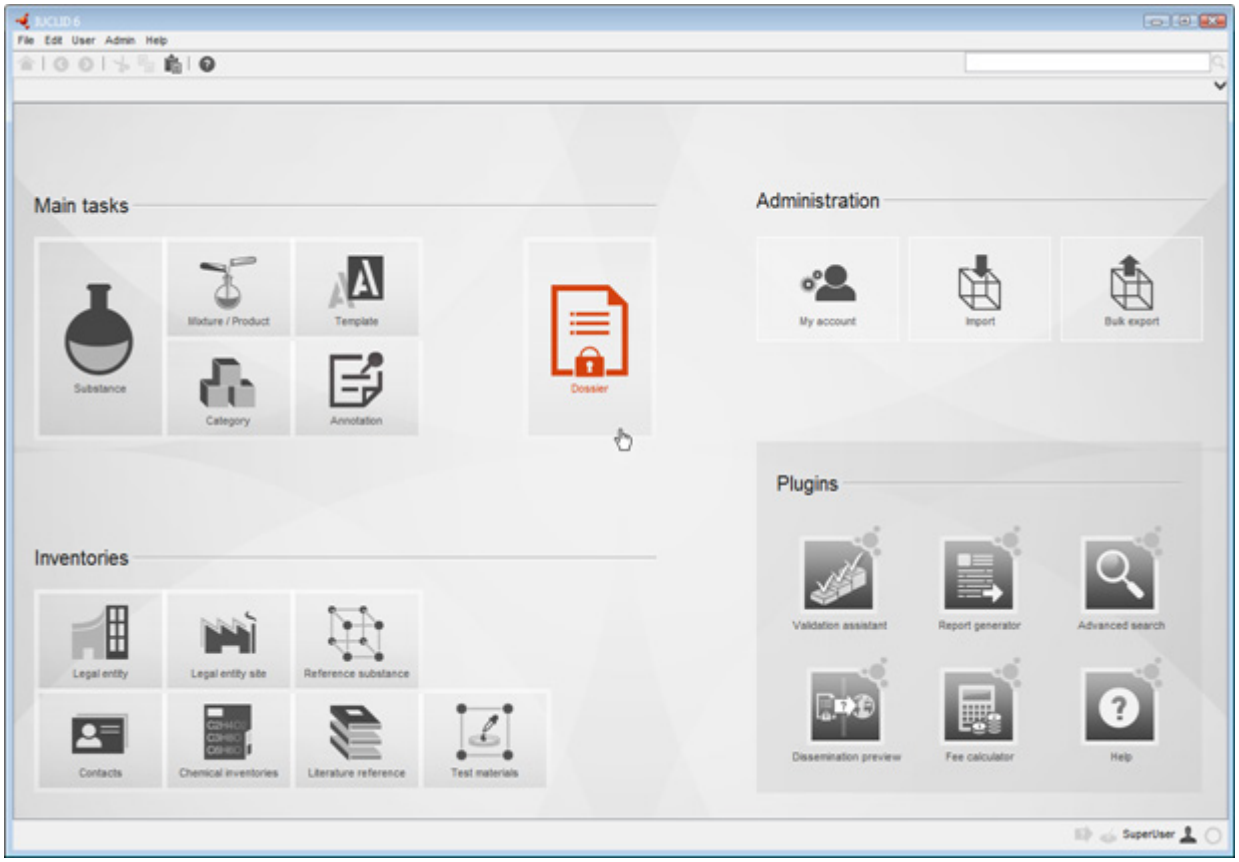
The home page is shown by default either when starting a desktop version of IUCLID 6, or when logging in to a server version. The home page can be viewed either by clicking on the house icon that is situated in the menu toolbar as shown below, or from the main menu Go / Home.

Figure 13: The icon for the home page



An example of the home page is shown below in a reduced size.

Figure 14: The home page shown at 50% of full size with the cursor hovering over Dossier



To display it at any time, click on the house icon in the menu toolbar. The home page contains panels that provide access to functions related to either a specific type of entity, or function of IUCLID 6. The term *entity*, as described in Table 1, is used to mean a particular type of data object that is specific to IUCLID, for example: *Substance* and *Legal entity*. Each panel contains an icon for either an entity or a function. Placing the cursor anywhere over a panel activates it, causing its icon to change colour. Whilst activated, primary click opens its window. For entities, right-click shows the option *New* as shown in the example below for *Substance dataset*.

Figure 15: Right-click on a panel on the home page to see its menu

Key for Figure 15:

1. The cursor is not over the panel;
2. The cursor is over the panel, activating it and causing the icon to change colour;
3. Secondary click (right-click) shows a menu of functions. In this example, for *Substance*, there is only the function to create a new *Substance*.
4. Select the function by hovering the cursor over it, and then primary click to carry it out

The panels are grouped together in four areas, to indicate that each group has something in common. The panel for *Dossier* has been placed centrally and made bigger than the others, to reflect its central role in regulatory tasks. The entities and functions behind the panels are explained in their own separate sections of this manual. The reasoning behind the groupings of the panels is given below.

Main tasks contains links to entities in which a user enters data such as toxicological data, physicochemical data and information on uses that are specific to their own needs and circumstances. This data may be subject to change, for example during an evaluation process under a particular regulation.

Tools and administration contains links to functions that are less to do with manipulating data, and more to do with who has access to what, and how data may be moved in and out of IUCLID 6.

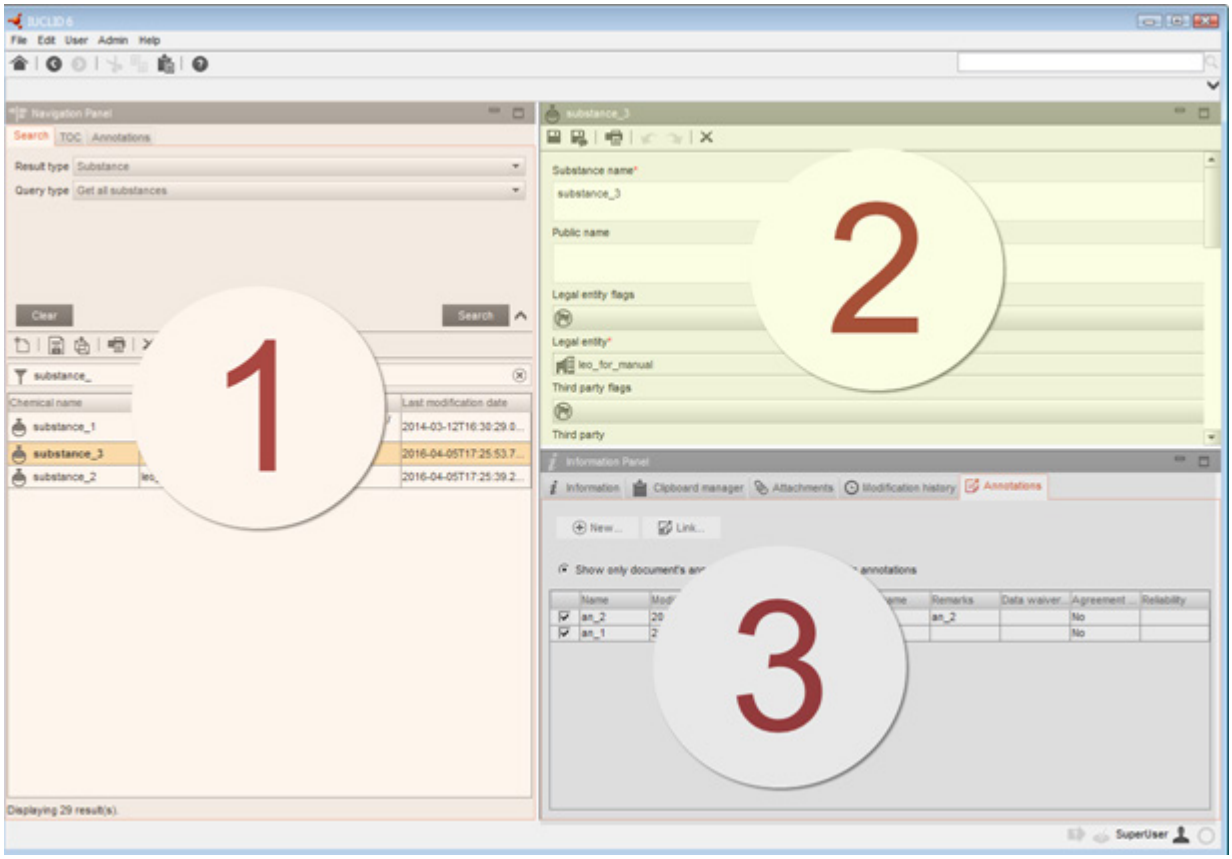
Inventories contains links to entities that are used to store information that typically does not change over time, and may be of relevance to different persons whose use of IUCLID 6 might differ significantly. For example, a *Reference substance* might be a small common molecule that is referred to under widely differing circumstances. The information in *Reference substances* is not usually subject to change, although they can be edited.

Plugins contains links to functionalities that have been deliberately kept out of the functions built in to IUCLID because not all users need them, and the separateness makes rapid development

possible without having to upgrade all of IUCLID. See the IUCLID 6 web site for more information about plugins.

The functions accessed via the groupings *Main tasks* and *Inventories*; as well as *User management*, are shown on a page divided into three panels: *Navigation*, *Data* and *Information*, as shown the figure below. The relative sizes of the panels within the main window can be changed by clicking and dragging on their boundaries.

Figure 16: The panels: Navigation (1), Data (2), and Information (3)



The panels *Navigation*, *Data*, and *Information*, are described in the following sections.

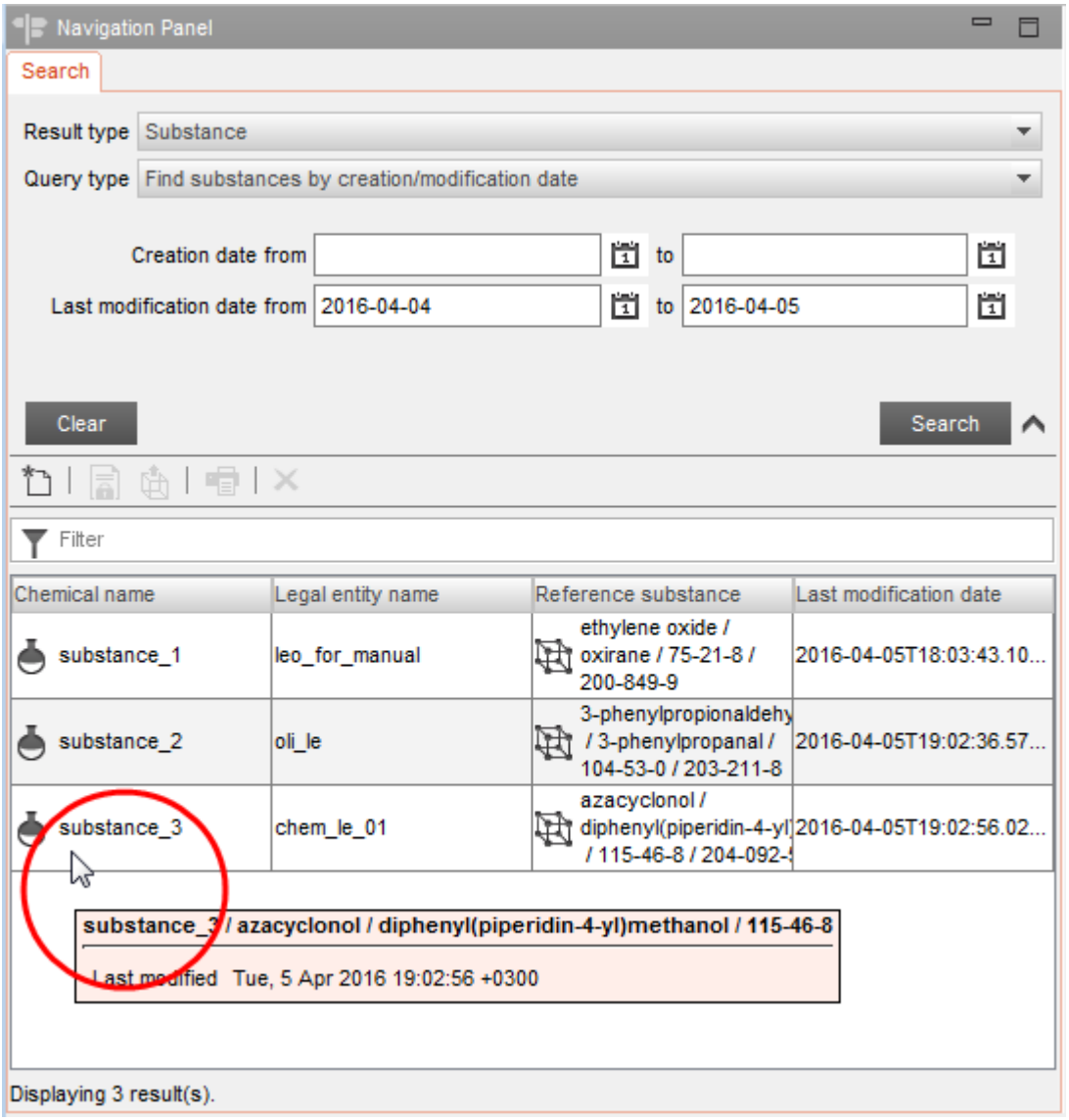
1.9. Navigation panel

The navigation panel is used to select a specific document and/or part of it either to perform some function on it, or to read data therein. Where relevant, multiple selections are possible. By default, when opening the navigation panel by clicking in the home page, IUCLID 6 tries to list all the documents of the chosen type of entity. By default, IUCLID 6 returns the first 500 it finds. Changing that limit is described in section 1.4.4.1 General. The selection of documents shown in the table can be adjusted using the search function described below. To access a specific part of a document, use the *Table of content* TOC function as described below.

1.9.1. Searching in the navigation panel

The navigation panel contains a general search functionality that can be used to find any type of entity. For some types of entity, in addition to searching, the navigation panel can contain addition panes. In this case, searching has its own dedicated tab. This is true for Dossier, Template, Mixture/Product and Substance. For example, the latter three have tabs for *TOC* (Table of Content) and *Annotations*. Additional tabs are shown only once a relevant entity has been selected from the search results. An example of a search is shown below.

Figure 17: Search for a substance by modification date



To perform a search, enter the required search criteria into the fields at the top of the panel, and then click on the button *Search*. The results are shown in a table under the criteria. Data in all the search criteria can be removed in one go by clicking on the button *Clear*. The asterisk character can be used as a wild card for one or more characters. For example, the criterion `meth*` returns all entries that begin with `meth`.

Hovering over the name of entry produces a tool tip which displays the name and a relevant identifier. In the example shown above, the identifier is the name of a Reference substance. The entries in the list of search results can be selected, and then various functions carried out on them either by right-clicking on them, or via the icons just below the button *Clear*. For example, clicking on the icon for a new document,  , creates a new document of whatever type is shown in the search results. Multiple selections are possible using the standard methods, although not all functions can be carried out on a multiple selection. To open a document so that the data and information panels show values specific to it, select the document in the list, and then either double-click on the selected entry, or right-click to open the menu, and then select *Open*.

The part of the panel that in which search criteria are displayed can be collapsed and expanded by clicking on the black arrow at the right of the criteria.

The number of search results that can be displayed at once has been capped at 500 to avoid overloading the search function. If there are more than 500 results a warning message is given. It is safer to refine the search criteria, than to assume the 500 results are taken from the database in any particular order.

1.9.1.1. Result Type

Result type is used to change the type of entity that is found and displayed in the table of results. This is equivalent to going to the home page, and then clicking on the icon for the type of entity for which you want to search.

1.9.1.2. Query type

Query type offers various different kinds of search that depend on the type of entity that will be found. The fields presented depend on the type of entity and the type of search. For example, searching for *Dossiers* can be done by impurity; in which case, fields are presented in which chemical identifiers can be entered for the impurity.

1.9.1.3. Ownership

Ownership is shown as a criterion only if instance based security (IBS) is on, as described in section 15.2.2.5 IBS management.

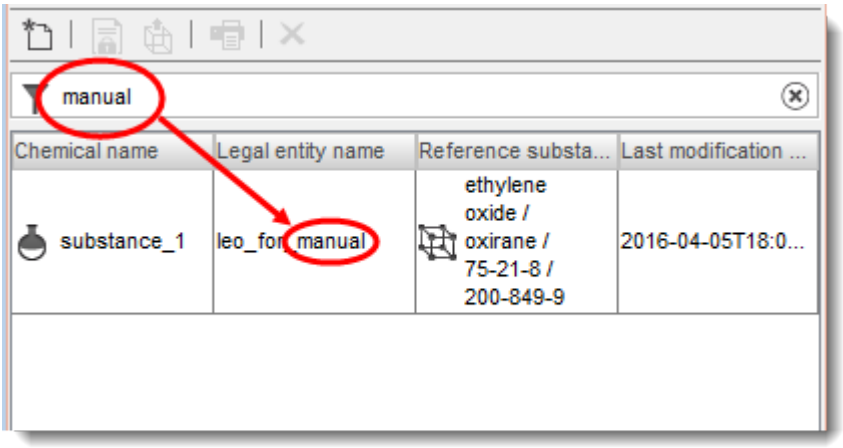
1.9.1.4. Group

Group is shown as a criterion only if instance based security (IBS) is on, as described in section 15.2.2.5 IBS management.

1.9.1.5. Filter the search results

Filter is a field into which a text search term can be entered that is applied immediately to the entries in the table. It is identified by a filter funnel icon as shown in the example below.

Figure 18: Filter search results



A search result is shown if it contains the search term anywhere in the fields in the list. In the example above, filtering is done for the word "manual". Spaces are interpreted literally. It is not sensitive to case.

The search term can be cleared by clicking on the icon with a cross that is located at the right of the field.

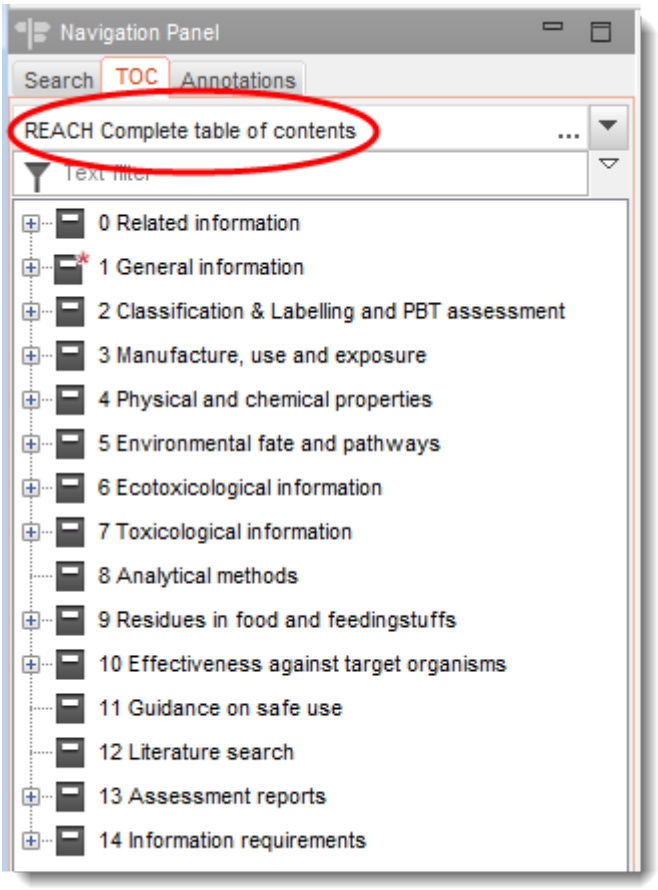
1.9.2. TOC (Table of Content) tab in the navigation panel

The tab labelled TOC (Table of Content) is shown for entities of type *Substance*, *Mixture/Product* and *Template*, but only when such an entity is open in the data panel. The TOC has three main functions as follows:

1. Provides access to specific documents in an entity;
2. Shows the structure of the documents in an entity in a particular regulatory context;
3. Indicates whether a document is mandatory for a particular type of data submission made for regulatory purposes. This is done using a red asterisk on the icon of a document.

The way in which the TOC is displayed can be set to suit a particular regulatory context, and/or type of data submission made for regulatory purposes, which includes a view for each type of Dossier. The name of the current view is stated in the field just below the tabs. The default option is *REACH Complete table of contents*, as shown below.

Figure 19: The default view for the TOC: REACH Complete table of contents



REACH Complete table of contents, shows all the documents that have any relevance to the REACH regulation, in the structure used for Dossiers submitted under REACH. This view refers to no specific type of Dossier so the only document that is marked as mandatory is *General information / Identification*. To change the type of view in the TOC, click on the solid black arrowhead icon at the right of the name of the view, and then select one of the options, as shown in the example below.

Figure 20: Change the view in the TOC

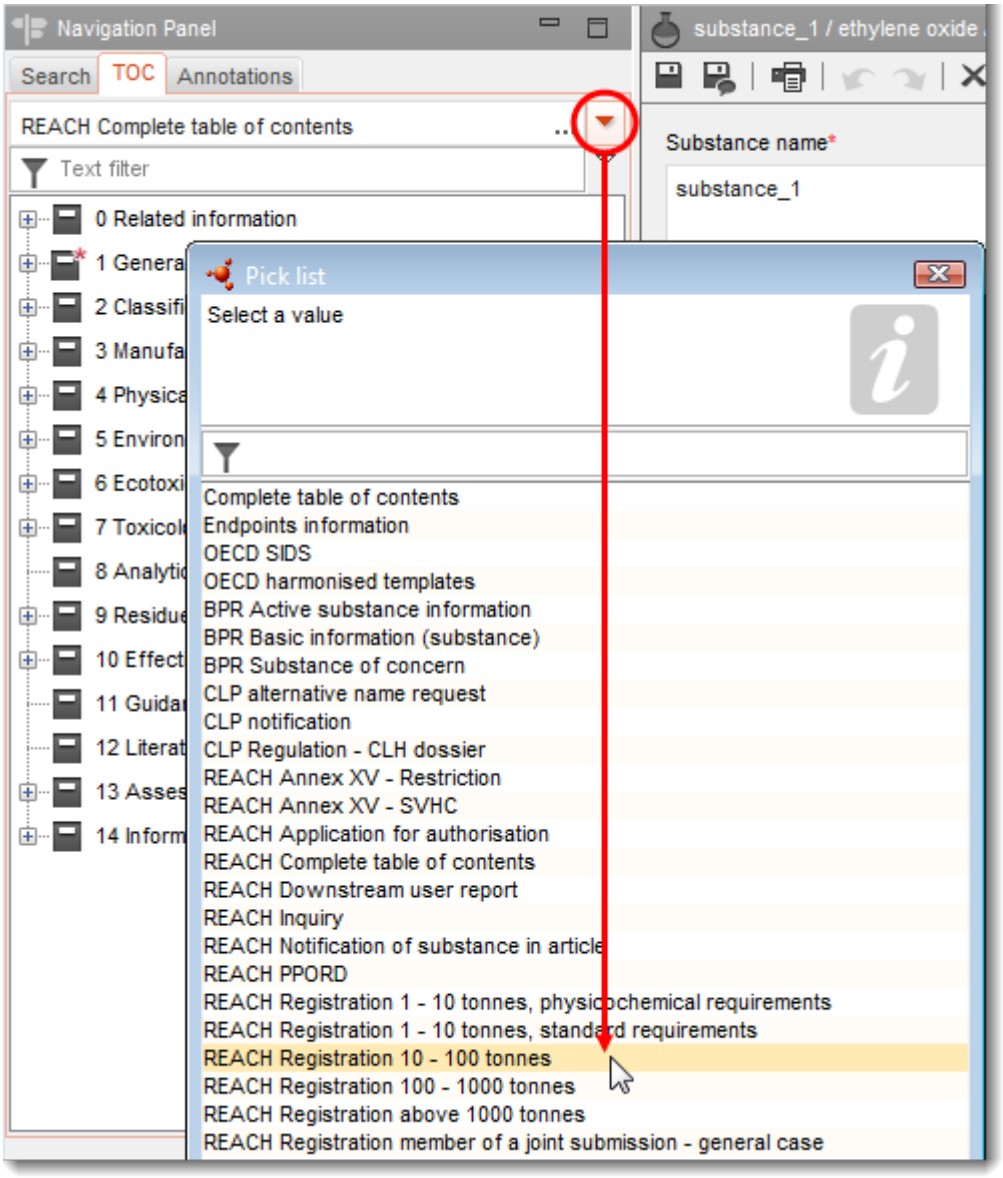
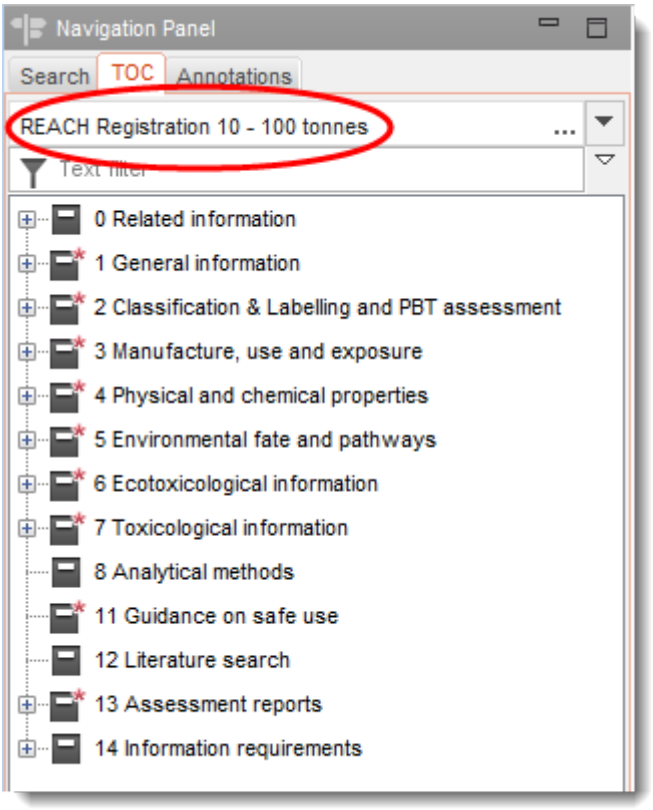


Figure 21: The TOC view: REACH Registration 10 - 100 tonnes

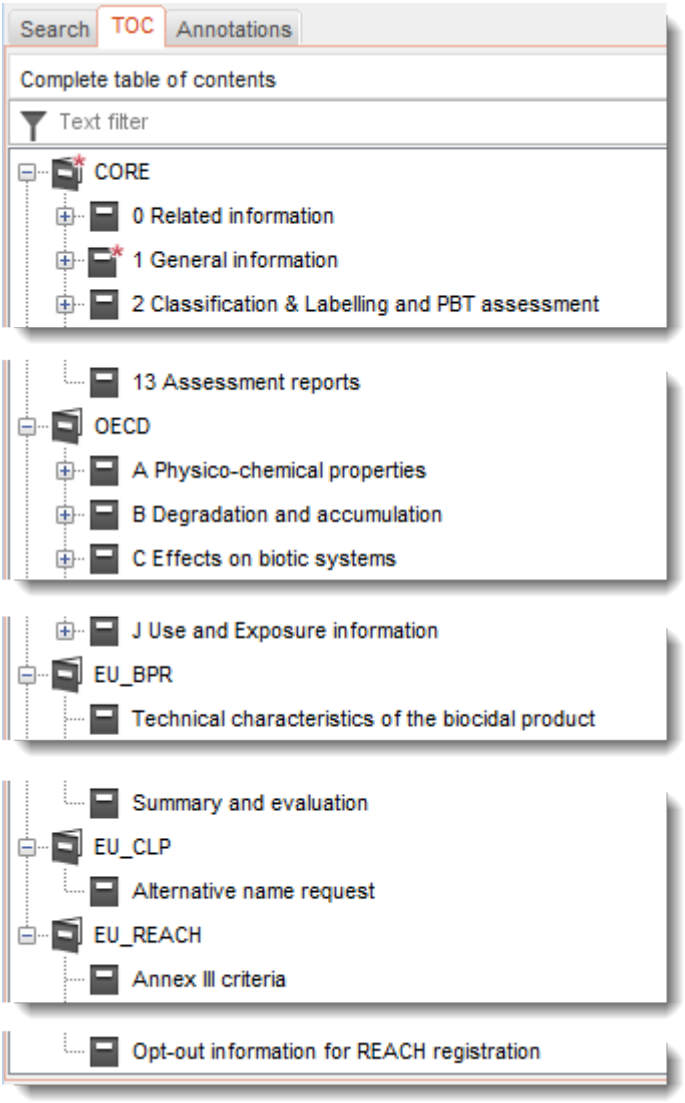


The view selected in the example above is *REACH Registration 10 - 100 tonnes*. Note how that compared to *REACH Complete table of contents*, sections 9 and 10 are no longer shown, and more sections are marked as mandatory.

Whilst entering data intended for submission in a particular type of Dossier, it is recommended to keep the TOC view set to that Dossier type.

The TOC view *Complete table of contents* is different from the others. It is shown in the figure below with each of the top layer sections opened to reveal the structure underneath.

Figure 22: Structure of the TOC view: Complete table of contents



In the TOC view *Complete table of contents*, sections have been separated out from each other and displayed in sections determined by their origin. Sections not specific to a legislation are displayed in a section referred to as *CORE*, and those from the OECD harmonised templates are in a section named OECD. In addition, IUCLID 6 is supplied with the following EU_BPR, EU_CLP and EU_REACH.

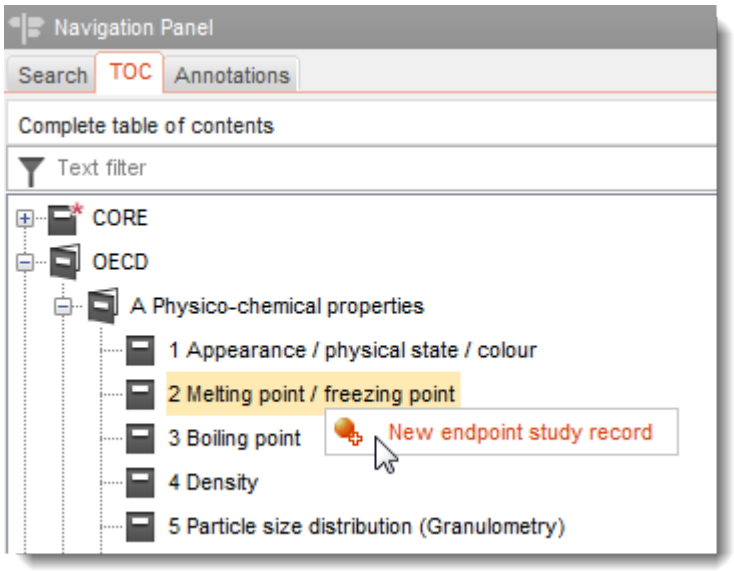
This means that under a legislation specific TOC view such as *REACH Registration above 1000 tonnes*, documents could have originated from either CORE, OECD, or EU_REACH. In addition, some documents can be shown together in the same section under TOC view for REACH, where under the TOC view *Complete table of contents*, those same documents are shown in separate sections.

For example, for a submission type of *REACH Registration 10 – 100 tonnes*, if a *Site* is added to section *3.3 Sites*, it appears under *complete table of contents* in *CORE / section 3.3 Sites*. Similarly, for a submission type of *REACH Registration 10 – 100 tonnes*, if an endpoint study summary is added to section *6.1.1 Short-term toxicity to fish*, it appears under OECD in the harmonised template *C Effects on biotic systems, section 41 Short-term toxicity to fish*.

1.9.2.1. Endpoint study record

An *endpoint study record* provides a template with predefined fields in which data is entered to describe a study carried out within the subject area defined by the title of the section, for example *Long-term toxicity to fish*. All entries under the OECD harmonised templates are *endpoint study records*.

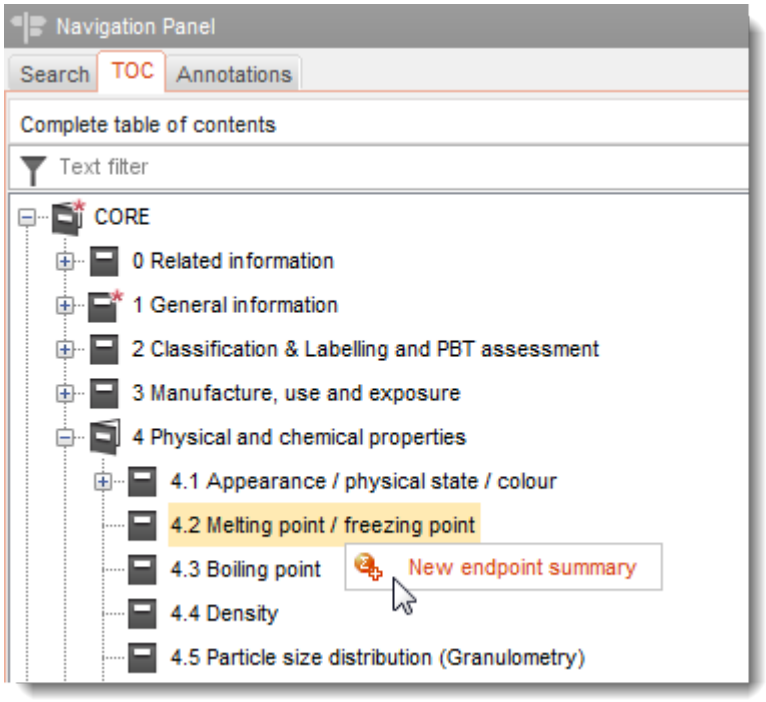
Figure 23: Creating an endpoint study record under OECD



1.9.2.2. Endpoint summary

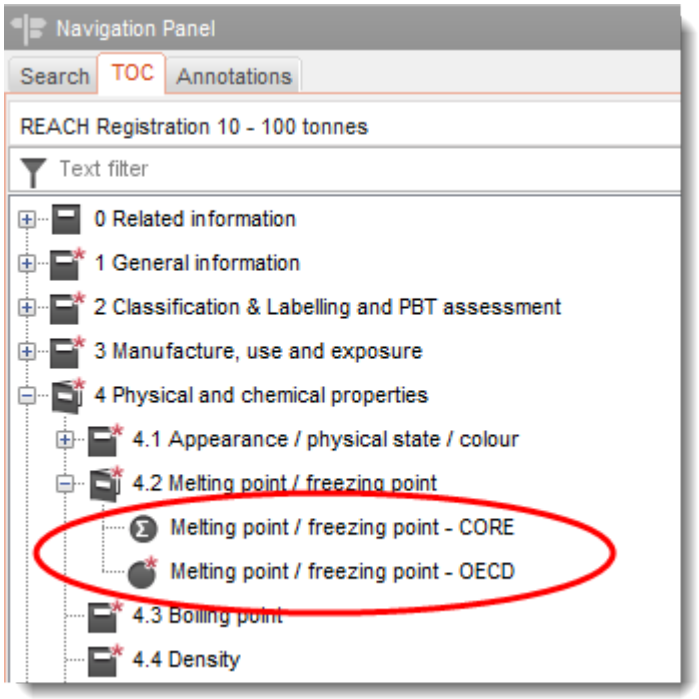
An *endpoint summary* provides a means of grouping *endpoint study records* and of providing further information about the grouping. An *endpoint summary* contains links to *endpoint study records* in the field *Link to relevant study records(s)*. To create a link, click on the button labelled *Add*.

Figure 24: Creating an endpoint summary in CORE



If an endpoint study record is created under OECD, and an endpoint summary is created under CORE for the same section, when that section is viewed for a particular legislation, both are shown. For the previous two examples above of Melting point, under REACH the view could look something that in the figure below.

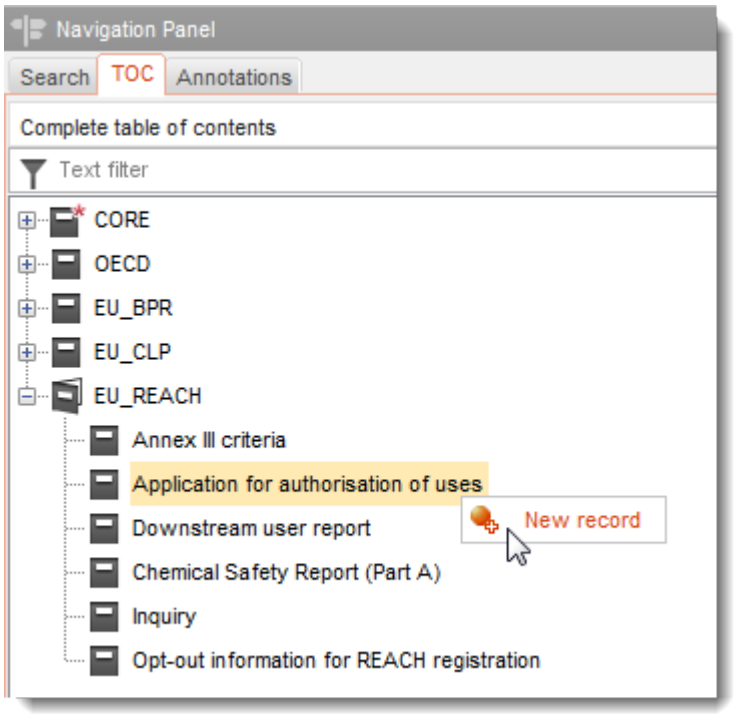
Figure 25: An endpoint summary and an endpoint study record shown together under a specific legislation



1.9.2.3. Record

If a *record* contains data that cannot be described as an *endpoint study*, it is referred to just as a record.

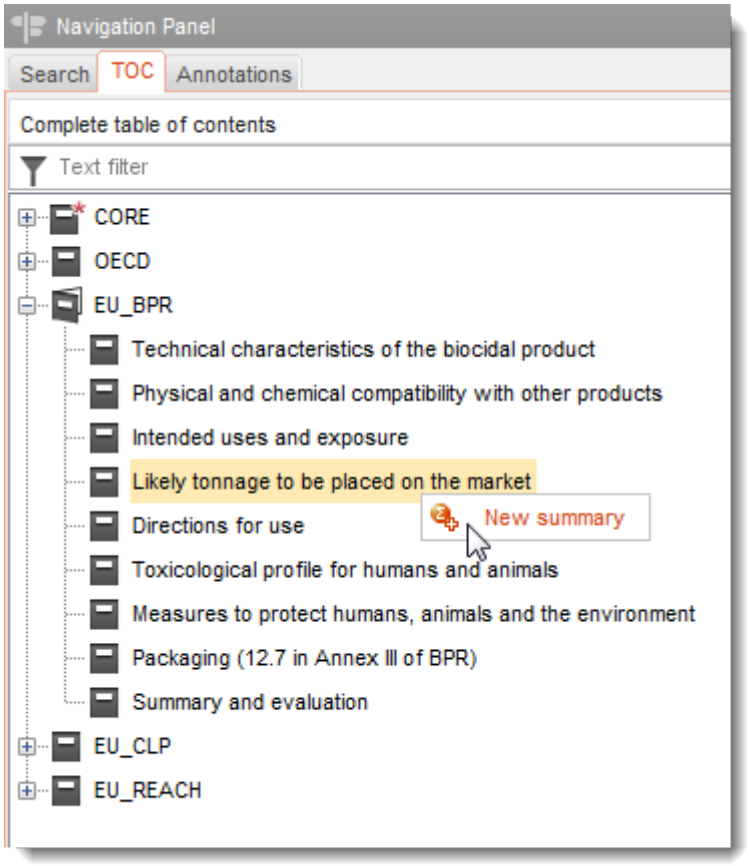
Figure 26: Creating a record under EU_REACH



1.9.2.4. Summary

A *summary* as opposed to an *endpoint summary* refers to only *records*, not *endpoint study records*.

Figure 27: Creating a summary under EU_BPR



1.9.2.5. Fixed record

A *fixed record* is created in a section where there can be only one *record*.

1.9.2.6. Filter the TOC

Filter is a field into which a search term can be entered that is applied immediately to the TOC. Any node in the TOC that contains the search term anywhere in its name is shown. This includes all records and summaries. The TOC hierarchy is expanded as far as is required to show the matching node or nodes. Spaces are interpreted literally. It is not sensitive to case.

The search term can be cleared by clicking on the icon with a cross that is located at the right of the field.

The example below shows filtering for section titles:

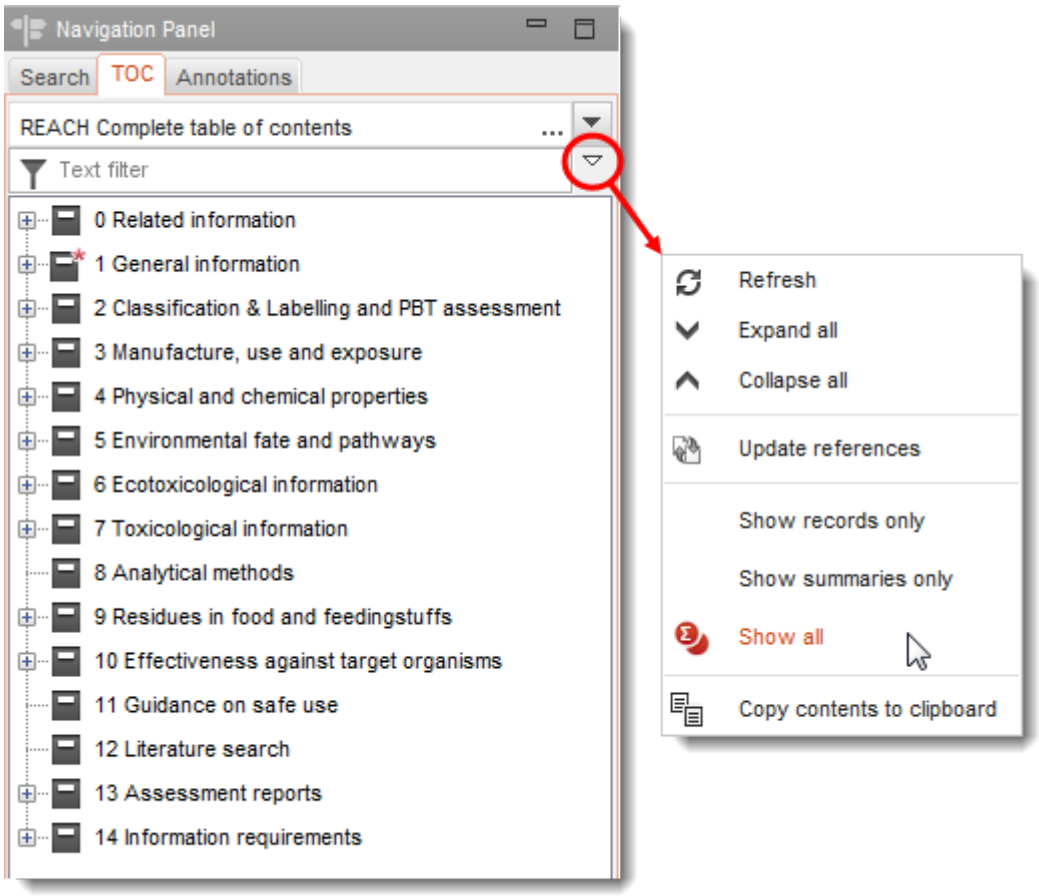
search term **biot** shows *OECD / C Effect on biotic systems / 56 Biotransformation and kinetics*

search term **bioti** shows *OECD / C Effect on biotic systems*

1.9.2.7. TOC functions menu

To the right of the filter window there is an icon in the form of a white-filled downward pointing arrow. Clicking on the icon opens a menu, as shown below.

Figure 28: Opening the TOC functions menu



1.9.2.7.1. Refresh

Refresh causes the TOC to be redrawn in accordance with the most recent data in the database.

1.9.2.7.2. Expand all

Expand all shows the complete tree structure of the TOC.

1.9.2.7.3. Collapse all

Collapse all shows only the first level of branches in the tree structure of the TOC.

1.9.2.7.4. Update references

Update references copies any changes in records and summaries to the document in which they appear as a reference. Such references are made using the function *paste reference* in the

clipboard manager, as described in section 1.11.2 Clipboard manager. If a record or a summary is a reference, its icon in the TOC has an arrow overlaid onto it.

1.9.2.7.5. Show only records

Show only records filters the TOC so that only *records* and *endpoint study records* are shown.

1.9.2.7.6. Show only summaries

Show only summaries filters the TOC so that only *summaries* and *endpoint summaries* are shown.

1.9.2.7.7. Show all

Show all shows removes any filter applied by *record* or *summary*.

1.9.2.7.8. Copy contents to clipboard

Copy contents to clipboard copies all the data in the TOC to the clipboard irrespective of what is currently displayed.

1.9.3. Annotations tab in the navigation window

The *Annotations* tab shows a list of all the *Annotations* that are associated with the selected document. Clicking on an entry in the list opens the *Annotation* in the data panel. This can also be done by clicking on the pane *Annotations* in the home page, searching for the annotation, and then double-clicking on its entry in the search results.

The annotations tab is shown for the entities of type *Substance*, *Mixture/Product*, *Template* and *Dossier*.

1.10. Data panel

The data panel is used to either read or edit the data in specific fields within a document. The document must first be selected in the navigation panel and then opened. The edit mode that existed in IUCLID 5 does not exist in IUCLID 6.

In most cases, the fields present in IUCLID 5 have been migrated to IUCLID 6 unchanged, in which case, the guidance for how to use them has not changed.

1.11. Information panel

The values and functions in the information panel are specific to the currently open document. These include a statement of the technical identifiers of the document, information about data associated with the document, and a history of modifications made to the document. In a change from IUCLID 5, the information panel also contains the clipboard functionality.

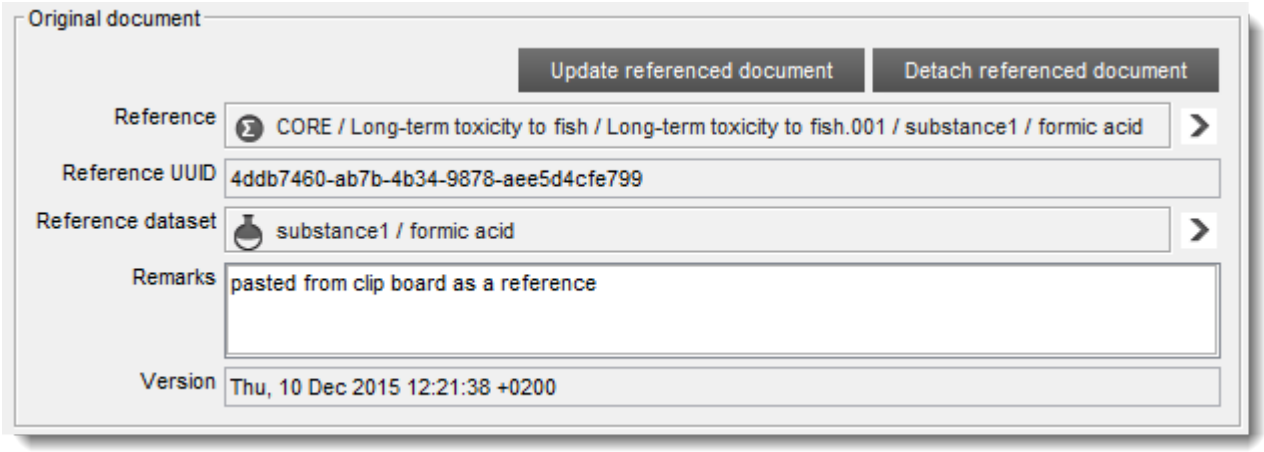
1.11.1. Information

Information contains a statement of the type of the document and its Universal Unique Identifier (UUID). If the document is in a *Dossier*, the UUID of the *Dossier* is given.

1.11.1.1. Original document

Original document is shown if the open document is either a record or summary that is a reference. The reference can be either updated or removed by clicking on the relevant button. If it is removed, the referring record or summary becomes a static copy of the record or summary to which it referred. It contains the data obtained during the most recent update. An example is shown below.

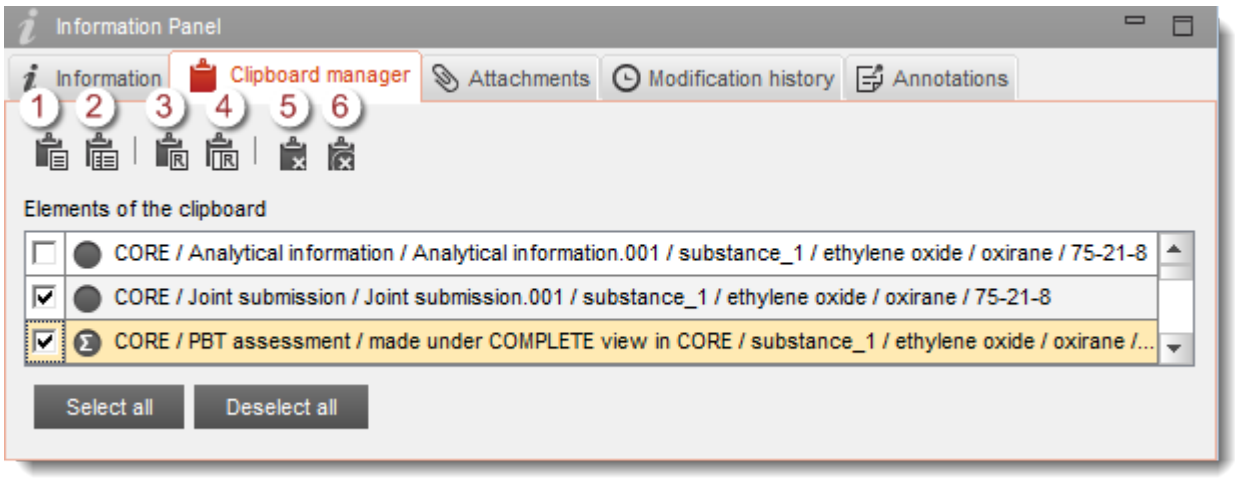
Figure 29: Original document for a reference



1.11.2. Clipboard manager

The clipboard can contain entries for *records*, *endpoint study records*, *summaries* and *endpoint summaries* that have been copied by right-clicking on their entries in a table of contents (TOC). An example is shown below.

Figure 30: The clipboard manager



Key for Figure 30

1. Paste selected
2. Paste all
3. Paste selected as a reference
4. Paste all as a reference
5. Delete selected
6. Delete all

Once on the clipboard, an entry can be pasted into a document either as one-off event, or as a reference. In the TOC for a *Substance*, *Mixture/Product* or *Template* an entry pasted as a reference appears with an arrow on its icon. References can be updated either all in one go within the referring document, or individually per record or summary that is a reference. An individual update per record or summary is done from the information tab in the information panel, as described in section 1.11.1 Information.

1.11.3. Attachments

This is where the relationship between the currently open document and its attachments is managed. Attachments are individual computer files created from outside IUCLID. Attachments can be added, opened, deleted, and remarks can be recorded.

1.11.4. Modification history

Modification history shows a read-only list of events associated with the currently open document. The fields are *date*, *author*, *legal entity*, *remarks*. The author is the name of the *User*.

1.11.5. Annotations

This is where the relationship between the currently open document and its *Annotations* is managed. *Annotations* can be associated with entities of type *Substance*, *Mixture/Product*, *Template* and *Dossier*. The button *New* is used to create a new *Annotation* that is automatically associated with the currently open document. The button *Link* is used to associate an existing *Annotation*. To do that, click on *Link* to open a search window. Search for the *Annotation*, select it, and then click the button *Assign*. Multiple selections are possible using the standard methods.

1.11.6. References

This tab is shown only if the currently open document is an *Annotation*. It provides a list of the documents associated with the *Annotation*. An association can be removed by selecting a document from the list, and then clicking on the button *Unlink*.

2. Substance

A *Substance* is an entity in IUCLID that is used to store information about something that, in a regulatory context, is considered a single chemical substance.

The fields in a *Substance* are designed to allow the recording of a broad range of different types of information relevant to the regulation of chemical substances. The fields are organised in a table of content (TOC). The general functionality of a TOC in IUCLID 6 is described in section *1.9.2 TOC (Table of Content) tab in the navigation* .

The identity of the *Substance* is defined in section *1 General information*. In section *1.1 Identification*, there are two mandatory fields *Substance name* and *Legal entity*. To make a link to a *Legal entity*, click on the link icon in the field *Legal entity*, select a *Legal entity*, and then click *Assign*. In *section 1.1 Identification*, the identity of the most important constituent of the *Substance* can be identified by linking to a *Reference substance*. To make a link to a *Reference substance*, click on the link icon in the field *Reference substance*, search for and then select a *Reference substance*, and then click *Assign*. The search window also allows a new a *Reference substance* to be created.

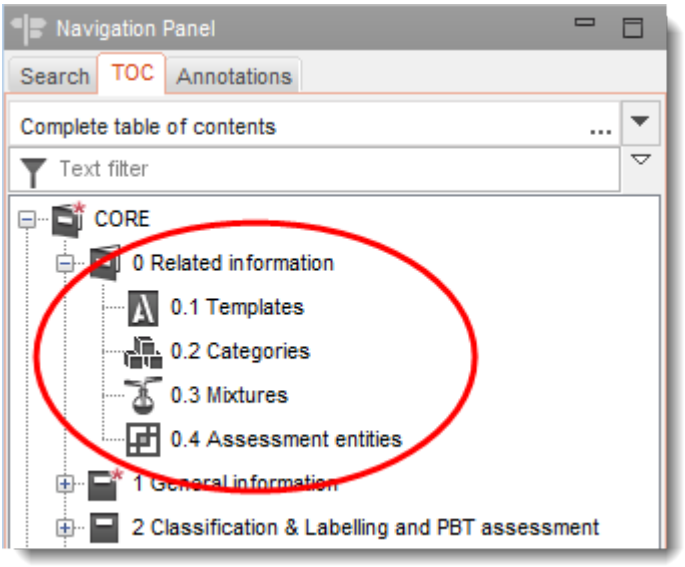
More detail can be provided about the *Substance* identity in section *1.2 Composition*, where one or more compositions can be defined. A composition may contain the identities of *constituents*, *additives* and *impurities*, and their relative proportions. To define the identity of a *Substance* properly for a specific legislation, and to know how to enter sufficient data into the *Substance* entity, see the guidance for that legislation, such as the manuals provided on the ECHA website at the following link.

http://echa.europa.eu/manuals

2.1. Related information for a Substance

In Section *0 Related information* for a *Substance* there are subsections that show how the particular *Substance* relates to other specific entities of type *Template*, *Category*, *Mixture/Product* and *Assessment entity*. The location in the TOC is shown below.

Figure 31: The complete TOC for a Substance showing the sections in Related information



Templates indicates which *Templates* are attached to the *Substance*, as described in section *4 Template*. *Categories* indicates in which *Categories* the *Substance* has been placed, as described in section *5 Category*. *Mixtures* indicates in which *Mixture/Products* the *Substance* plays a role, as described in section *3 Mixture/Product*. *Assessment entities* contains information on how the *Substance* is involved in the assessment process, as described in the next section.

2.2. The Assessment entity

An *Assessment entity* can be thought of as a wrapper for a set of substance property data (across endpoints) that is used for assessment purposes. It enables the definition of consistent sets of properties that are relevant to the assessment of specific compositions/forms of the substance (placed on the market or generated upon use).

The Assessment entity aims to provide a tool to assist users in documenting complex assessment cases in IUCLID. When the assessment is straightforward, there is no need to define Assessment entities.

Each Assessment entity consists of a name, a composition and a list of related endpoint summaries. All endpoint study records that are relevant for the summary of a specific endpoint, are to be actively linked by the assessor to the summary itself.

2.2.1. Introduction to Assessment entity in IUCLID

When clicking on the *0.4 Assessment entity*, the *Assessment entity* overall pane opens. In the field Approach to fate/hazard assessment, a description of the set(s) of properties of the substance used for the assessment considering the chemical behaviour of the substance in the different foreseen uses, can be provided. Such description provides the overall reasoning where Assessment entities are created.

A specific field to provide a description on the approach to fate/hazard assessment for the public is also available.

In the same overall pane, the Assessment entities table shows the full list of Assessment entities available for the substance. This table is automatically populated as soon as an Assessment entity is defined in section 0.4 of the Substance. The functionality go to link target navigates to the selected Assessment entity and displays the related information.

2.2.2. How to create an Assessment entity

An *Assessment entity* can be created from within the TOC of a *Substance* by right-clicking on section 0.4, then selecting *New*, followed by a type of *Assessment entity*. The options are:

- Registered substance as such
- Specific composition/form of the registered substance
- (group of) constituent in the registered substance
- Transformation of the registered substance

The following fields are displayed for the various types of *Assessment entity*.

2.2.2.1. Name of the Assessment entity

The user should indicate the name of the *Assessment entity*. As this name will not be displayed in the tree view, it is suggested to re-name the *Assessment entity* in the tree view accordingly.

2.2.2.2. Relation to the registered substance

This depends on the type of *Assessment entity*. It is read-only.

2.2.2.3. Assessment entity composition

In this table, the user defines the composition of the *Assessment entity*, to support the understanding of the *Assessment entity* definition. Depending on the type of *Assessment entity*, the user creates link to one of the following:

- an available composition in section 1.2 [*Specific composition/form of the registered substance*];

- a list of *Reference substances* that are part of the compositions in section 1.2 [*(group of) constituent in the registered substance*];

- one of the *Reference substances* available in IUCLID [*transformation of the registered substance*]

2.2.2.4. Compositions/forms covered by the Assessment entity

A link to compositions reported in section 1.2 can be made to indicate that the *Assessment entity* is expected to be used for the assessment of those compositions. Such a link is useful for the understanding of the assessment approach.(see the Manual on How to prepare Registration and PPORD Dossiers).

2.2.2.5. Additional information

Report specific information not already stated in the overall explanations on why Assessment entity has been created (in the field *Approach to fate/hazard assessment*). For example one could use this field to explain the reasoning for grouping constituents as part of a (group of) constituents.

2.2.2.6. Endpoint summary linked

To enable transparency and sorting of the information in the IUCLID dataset, all study records and endpoint summaries relevant to an *Assessment entity* should be linked to it. This will for example enable them to be sorted in the view of the IUCLID data set, and to report them in a sorted way in the CSR when using the *Report generator*. From this table, the user can link all endpoint summaries that are relevant for the *Assessment entity*. An explanation of the relevancy of one or several endpoint summary(-ies) for the *Assessment entity* can be provided, when needed, in the field *Notes* when linking it to the *Assessment entity*. In case one or several summaries have a different explanation, a new repeatable block can be added. In each endpoint summary linked, users are invited to provide the link to all study records relevant for the summary itself. In this way, the *Assessment entity* is indirectly linked to the endpoint studies.

2.2.2.7. Reaction schema

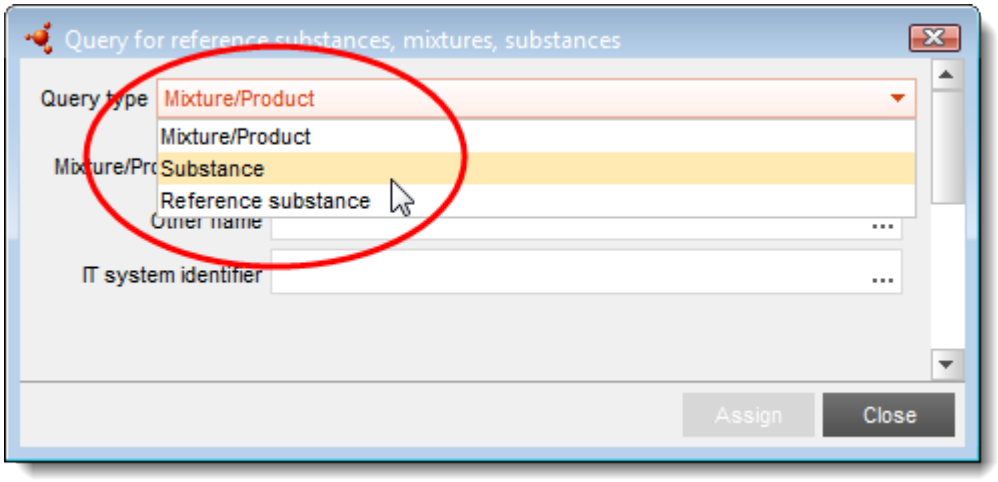
Upload the image of the reaction schema when needed [for *Transformation of the registered substance*].

3. Mixture/Product

A *Mixture/Product* is an entity in IUCLID that is used to store information either about something that, in a regulatory context, is considered a mixture or, under the biocides legislation BPR, a product.

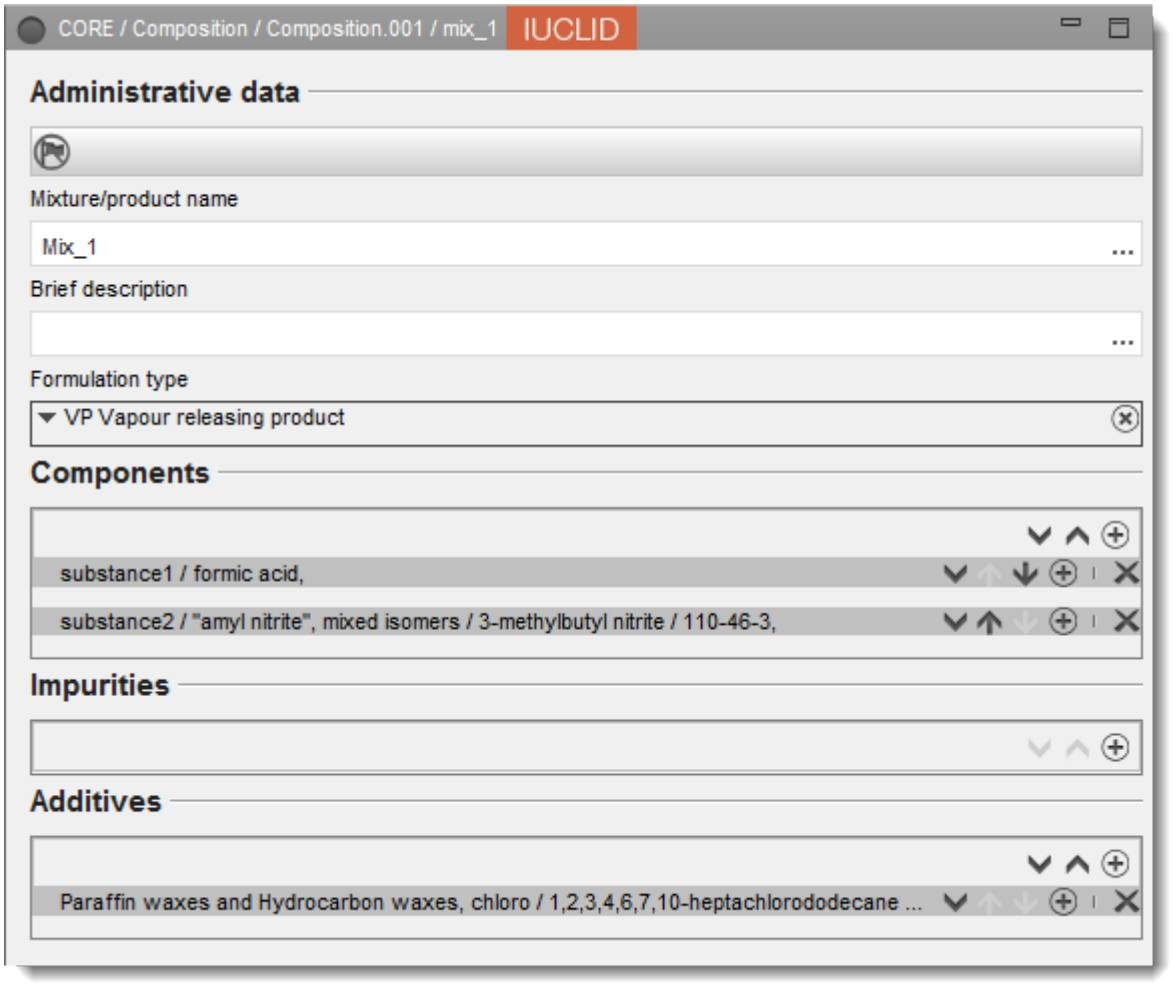
The structure of the entity *Mixture/Product* is similar to that for *Substance*, which is described in section *2 Substance*, but there are important differences in section *1.2 Composition*. There is an additional field named *Formulation type* which is relevant to *Products*. In addition, the *Mixture/Product* can contain *components* instead of *constituents*. There can be multiple *components*, *impurities* and *additives*, all of which can refer not just to a *Reference substance*, but also to either a *Substance* or a *Mixture/Product*. Thus, where a link is made to define the identity of a *component*, *impurity* or *additive*, the type of entity must be selected as shown in the figure below.

Figure 32: Select the type of entity referred to in the composition of a Mixture/Product



Multiple *components*, *impurities* and *additives*, are added in repeatable blocks. An example is shown below in which there are two components, both of which are a Substance. There are no *impurities* and there is one *additive*.

Figure 33: An example of a composition for a Mixture/Product



3.1. Related information for a Mixture/Product

In Section *0 Related information* for a *Mixture/Product* there is a subsection that shows which *Templates* are attached directly to the specific *Mixture/Product*, as described in section *4 Template*.

4. Template

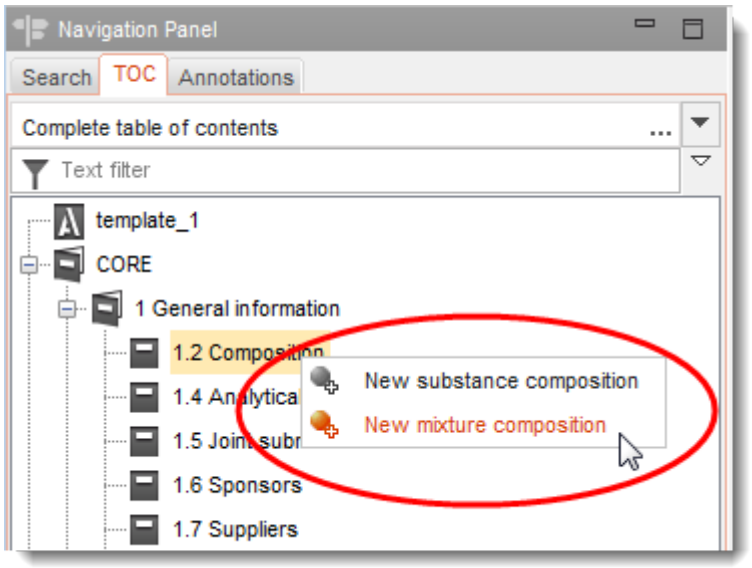
A *Template* is an entity that allows data from multiple sections to be inserted into a *Substance* or *Mixture/Product* entity all at once without having to manually recreate all the sections individually and re-enter data.

A *Template* has two mandatory fields, *Template name* and *Legal entity*. To make a link to a *Legal entity*, click on the link icon in the field *Legal entity*, select a *Legal entity*, and then click *Assign*. The structure of a *Template* is similar to that of a *Substance*, but it does not contain *section 0*, and sub-sections *1.1 Identity* and *1.3 Identifiers* in CORE because they are supplied by the entity to which the *Template* is attached.

4.1. Composition in Template

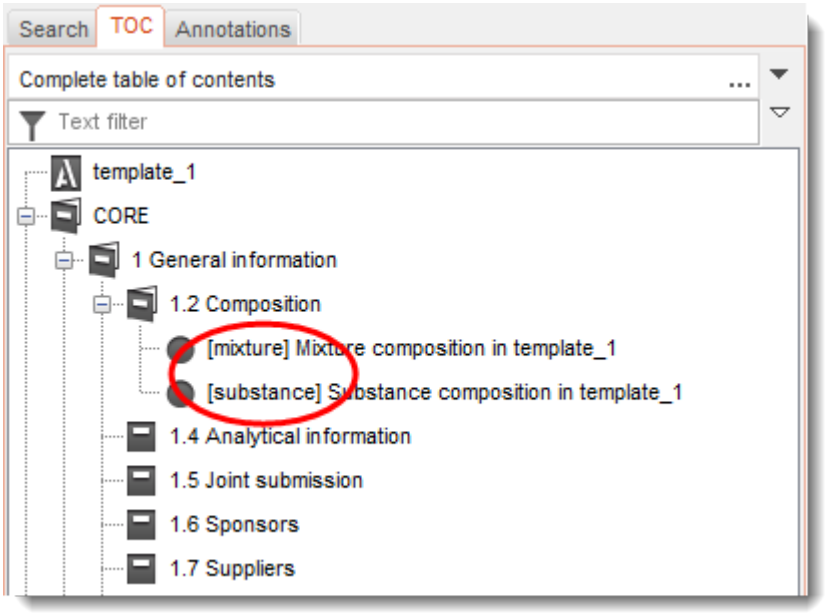
Section *1.2 Composition* is different for *Substance* and *Mixture/Product*. Whilst editing a *Template*, if the TOC view is set to *Complete table of contents*, it is possible to create either type of *Composition*, as shown below:

Figure 34: Create a composition in a Template

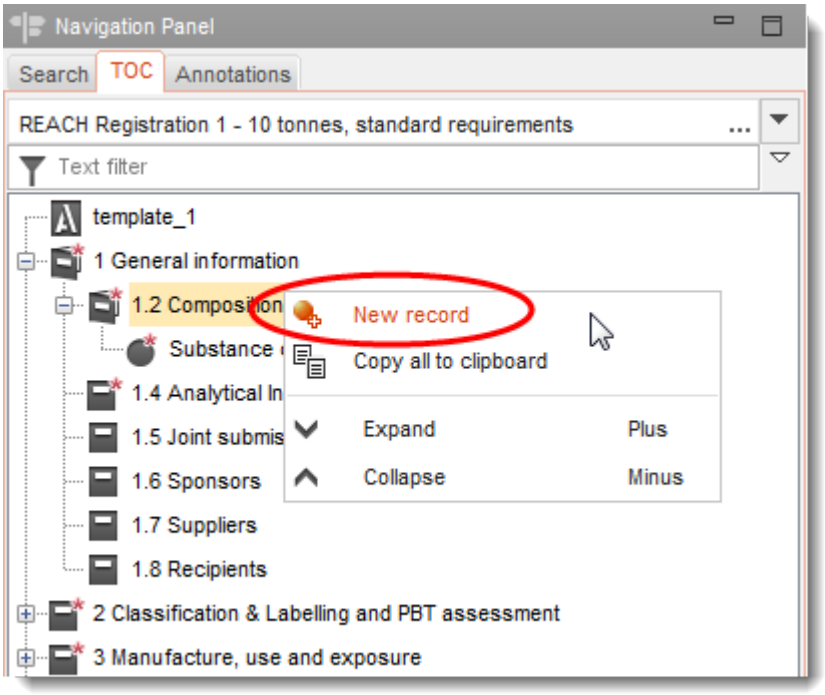


The names of the *Compositions* are prepended with their type, as shown in the example below:

Figure 35: Compositions in a Template for Substance and Mixture/Product



If the TOC view is specific to REACH, only Compositions for a Substance can be created. In that case, when a new Composition is created, the option shown is for a new record, as shown below:

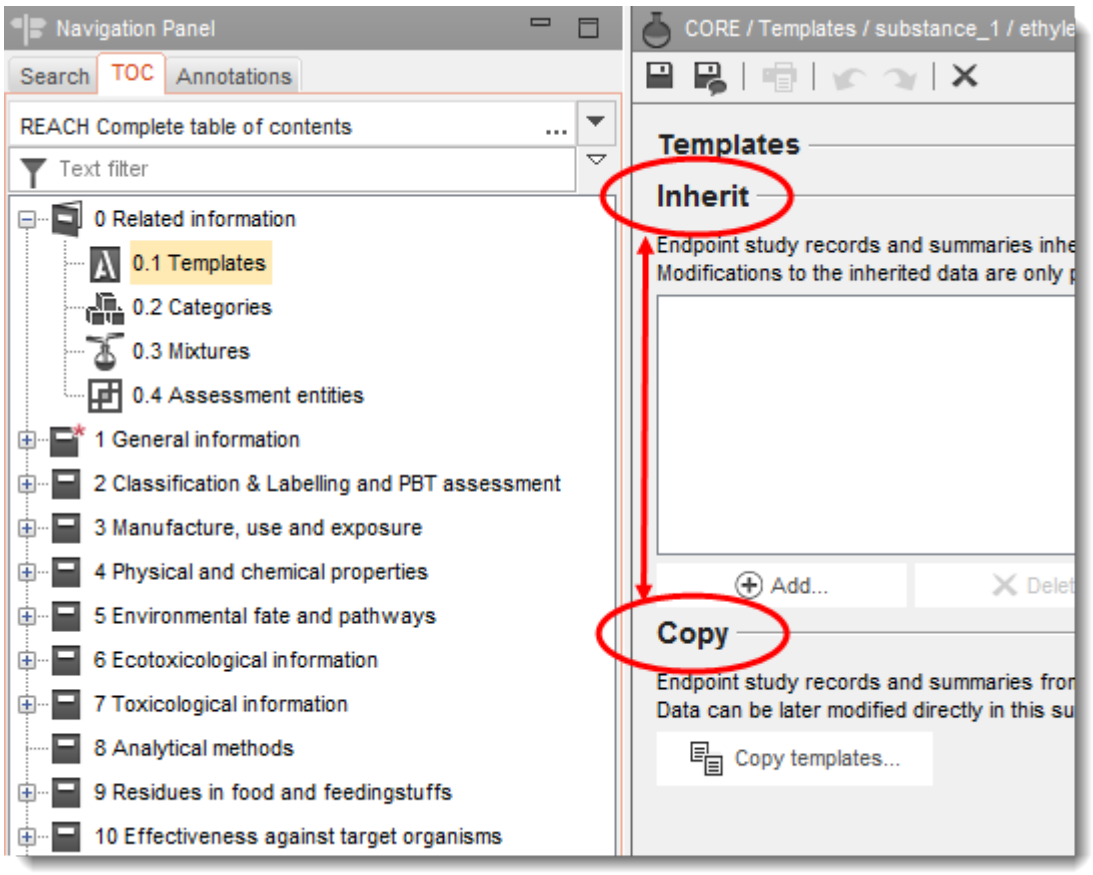


When a *Template* is attached to a *Substance* or a *Mixture/Product*, only a *Composition* of the correct type is accessible.

4.2. Attaching a Template to a Substance or a Mixture/Product

To attach a *Template*, open the *Substance* or *Mixture/Product*, open it at section *0 Related information* and then double click on *Templates*. This opens the *Templates* management window for that *Substance* or *Mixture/Product*, as shown in the example below for a *Substance*.

Figure 36: Attach a Template as copy or inherit



A *Template* can be attached in one of two different ways, *inherit* or *copy*.

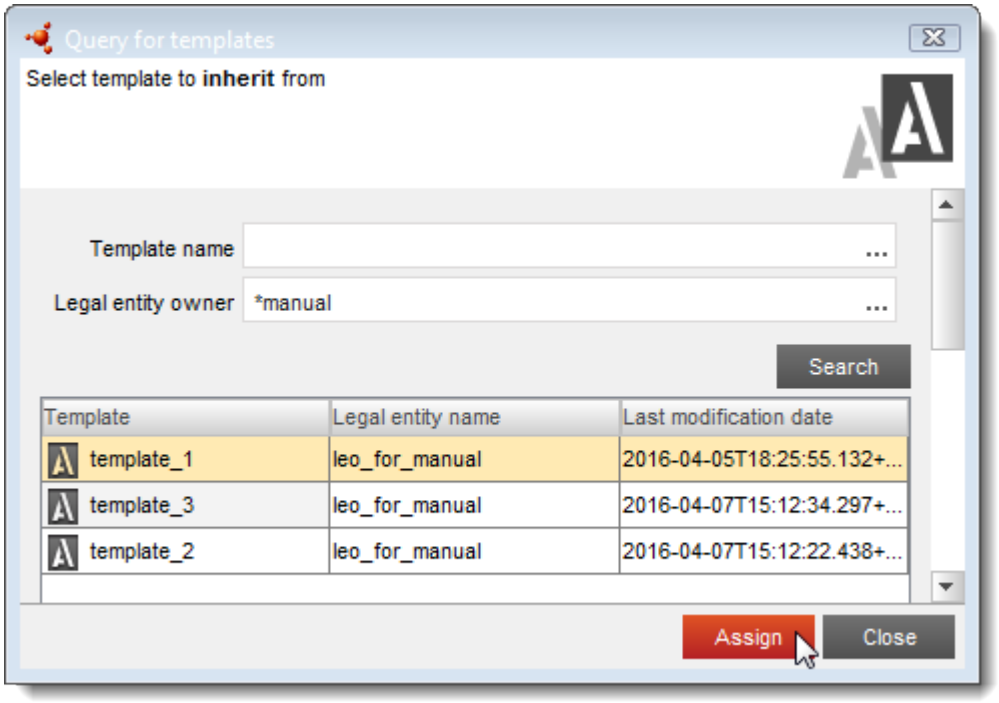
Inherit creates a dynamic link from the *Substance* or *Mixture/Product* to the *Template*. The data can be modified only from within the *Template*, not from the *Substance* or *Mixture/Product* to which the *Template* is attached. Modifications made in the *Template* are available immediately in the *Substance* or *Mixture/Product*.

Copy adds a copy of the documents in the *Template* to the *Substance* or *Mixture/Product*. There is no link. A document copied in this way can be modified in the *Substance* or *Mixture/Product* to which it was copied. Even if the *Template* is completely deleted, the data in the *Substance* or *Mixture/Product* is unaffected.

The functionality of *Template* differs in IUCLID 6 compared to IUCLID 5 in that the *Template* itself is neither of type *inherit* nor type *copy*. The distinction between the behaviours *inherit* and *copy* is applied only to the link between the *Template* and the *Substance* or *Mixture/Product*. Thus, the same *Template* can be inherited in one reference, and copied elsewhere.

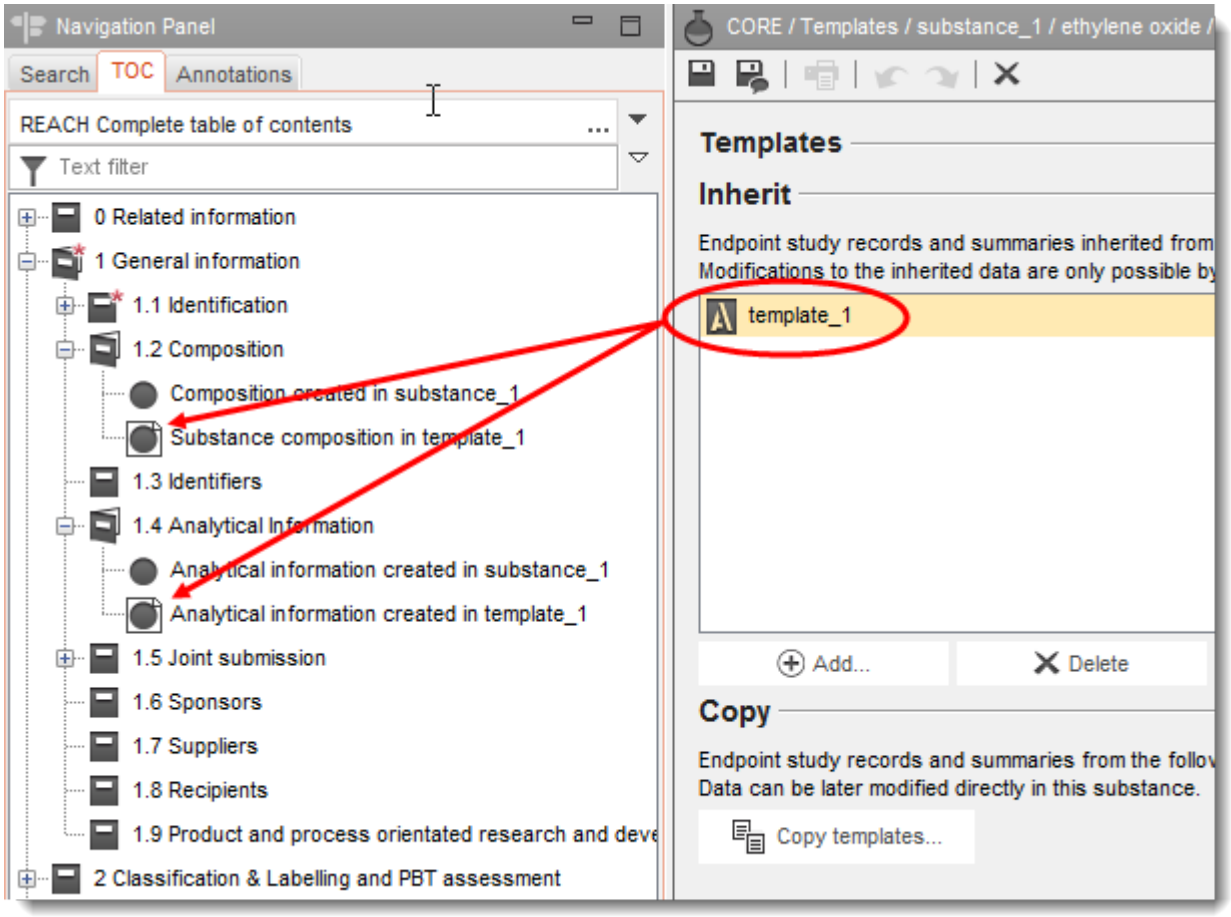
When you have decided between using *inherit* or *copy*, in the *Template* management window, click on either *Add* or, *Copy templates*. In the example shown above, the pointer is hovering over the function *Add* ready to create a dynamic link to the currently open *Substance*. Clicking on *Add*, opens a pop-up window in which a *Template* can be searched for and assigned. In the example shown below, all the *Templates* whose Legal entity name ends in "manual" have been found using the wild card "*". The *Template* named `template_1` is about to be assigned.

Figure 37: Select a Template from which to inherit

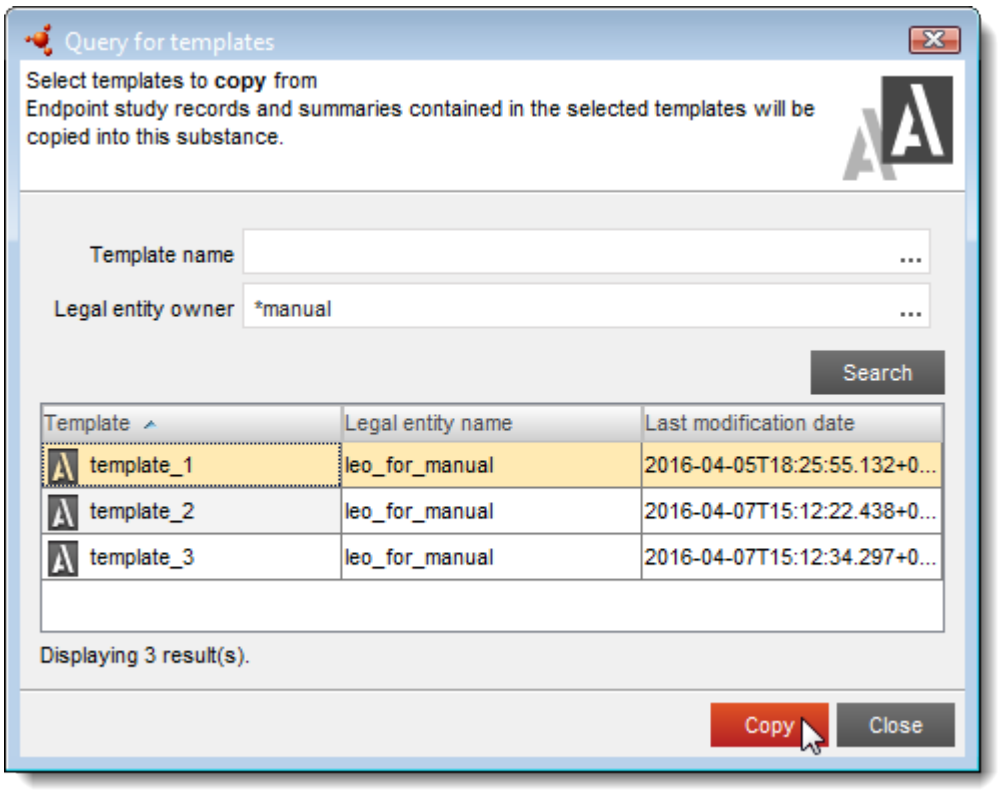


After assignment, the *Template* is added to the list of *Templates* that were attached using *inherit*. *Templates* on the list can be re-ordered and deleted from the list. Deletion from the list does not affect the *Template* itself; it just removes the data provided by the *Template* from the *Substance* or *Mixture/Product*. Documents provided by a *Template* are added to the TOC alongside existing documents, and marked out by an icon that has a folder surrounding the standard icon, as shown below.

Figure 38: Documents in a Substance inherited from a Template

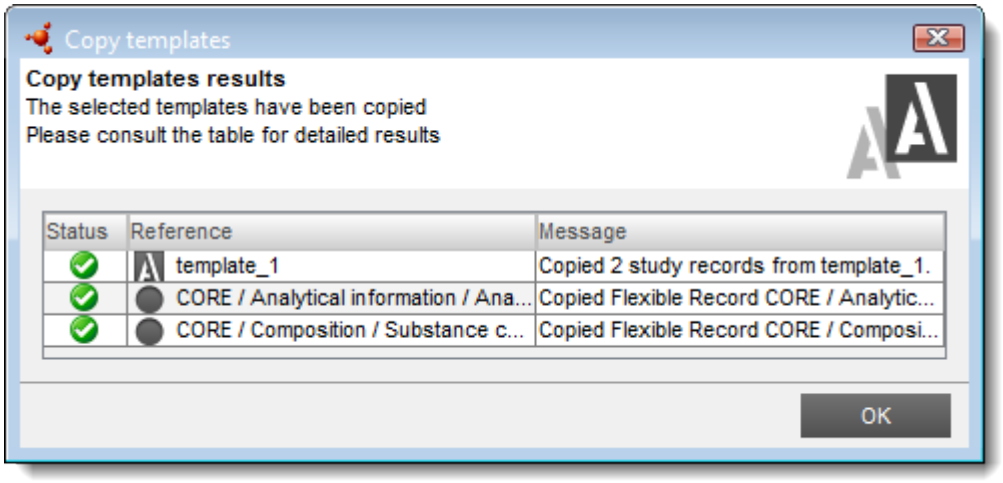


To copy documents from a *Template*, click on *Copy templates* in the *Template* management window. This opens a pop-up window in which a *Template* can be searched for and assigned. In the example shown below, all the *Templates* whose Legal entity name ends in "manual" have been found using the wild card "*". The *Template* named `template_1` is about to be copied.



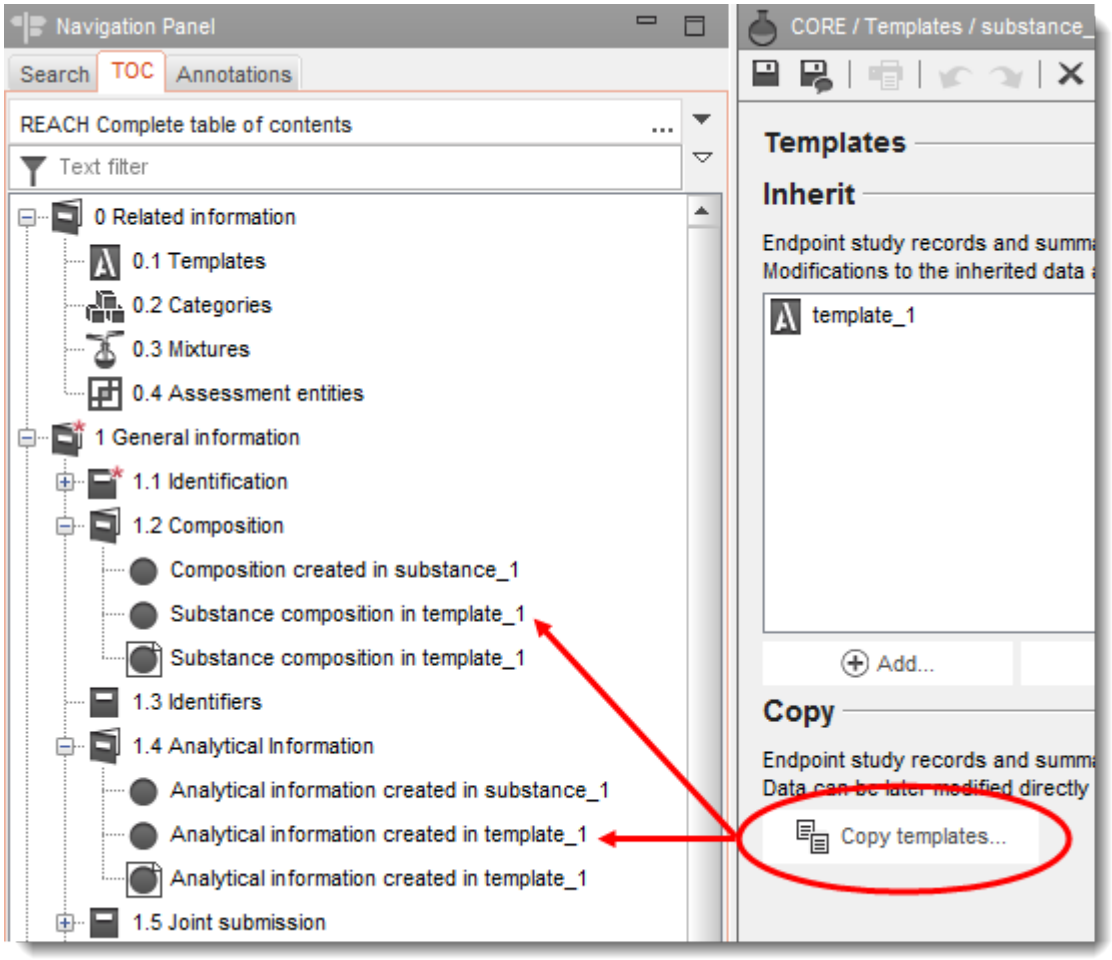
After clicking on *Copy*, a report is displayed of which documents were copied, as shown below.

Figure 39: Report on the documents copied from a Template



The documents copied from the *Template* are added to the TOC alongside existing documents. The document icon is the standard icon because there is no link to the data from the *Template*, and the data can be modified. Documents copied and inherited from a *Template*, and created from within a Substance, are shown in the example below.

Figure 40: Documents copied from a Template to a Substance



All the documents from a *Template* are copied. There is no way to make a limited selection during the copy process. If a *Template* is copied more than once to the same *Substance* or *Mixture/Product*, new extra copies of the documents are added to the TOC without over-writing data.

5. Category

A *Category* is an entity that allows a chemical category to be described within IUCLID 6. This section is divided into two parts. First, there is in introduction to the concept of chemical category, and then there is a description of how IUCLID 6 can be used to represent and analyse data in a chemical category.

5.1. Chemical category

A chemical category is a group of chemicals whose physicochemical and toxicological properties are likely to be similar, or to follow a regular pattern because of structural similarity. These structural similarities may create a predictable pattern in any or all of the following parameters: physicochemical properties, environmental fate and environmental effects, and human health effects. The similarities may be based on the following:

1. a common functional group (e.g. aldehyde, epoxide, ester, metal ion, etc.); or
2. the likelihood of common precursors and/or breakdown products, via physical or biological processes, which result in structurally similar chemicals (e.g. the 'metabolic pathway approach' of examining related chemicals such as acid/ester/salt); and,
3. an incremental and constant change across the category (e.g. a chain-length category).

A chemical category is defined by a list of chemicals (the category members) and by a set of properties and/or effects for which experimental and or estimated data are available or can be generated (the category endpoints). A chemical category can be represented in the form of a matrix.

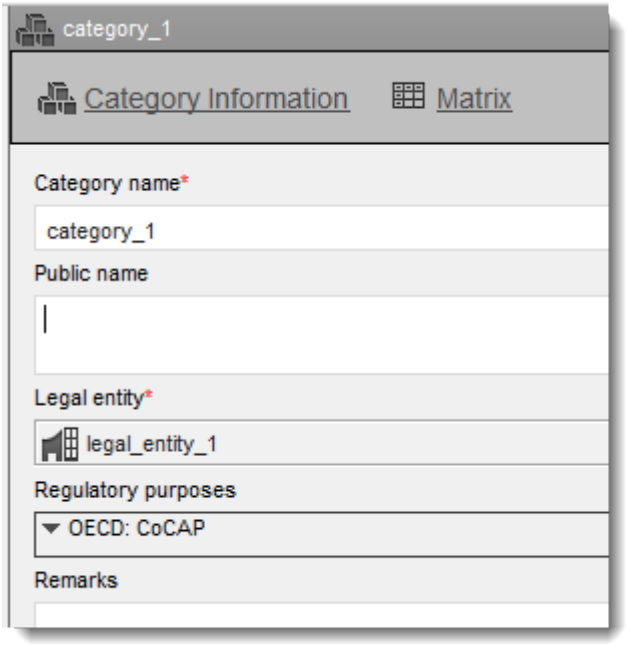
Data gaps in a chemical category can be filled by using various approaches, including simple read-across, trend analysis (interpolation and extrapolation) and computational methods based on SARs, QSARs or QAARs.

5.2. Category entity

A *Category* entity contains a description of the rationale behind the chemical category, and a group of *Substance* entities that contain data about the members of the chemical category. A *Category* entity provides a functionality known as the *category matrix*. This displays links to all documents across the member *Substances* per section. The *matrix* makes it easier to see which *Substance* entities contain relevant documents, and aids navigation between them.

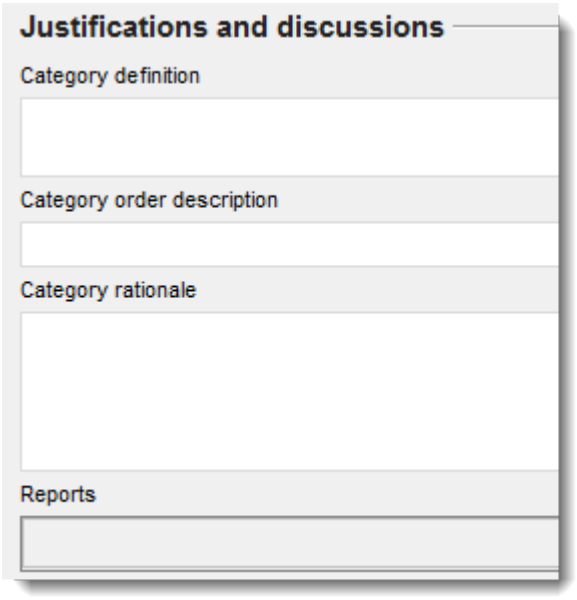
A *Category* entity must have a name, and be associated with a *Legal entity*. There is an option to indicate the regulatory purpose of the category, as shown below.

Figure 41: The mandatory fields in a Category



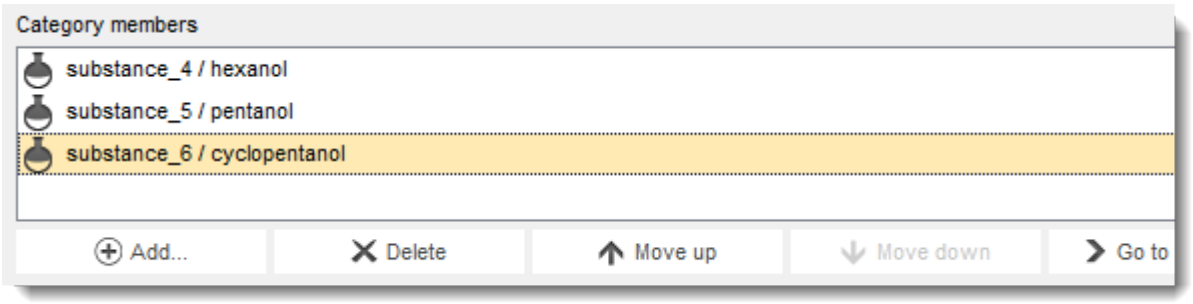
Information about the category and is rationale can be entered into the field at the bottom of the page, as shown below.

Figure 42: Justifications and discussions for a Category



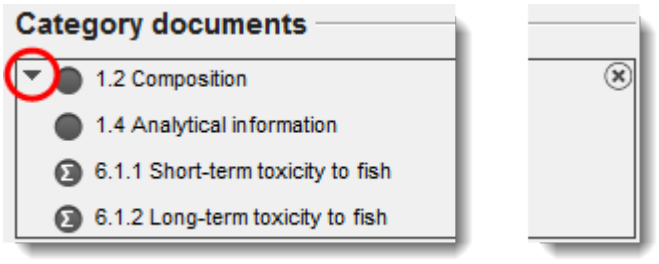
The members of a *Category* are managed in a table as shown below. A member can be any *Substance* to which the *User* has access.

Figure 43: Managing the members of a Category



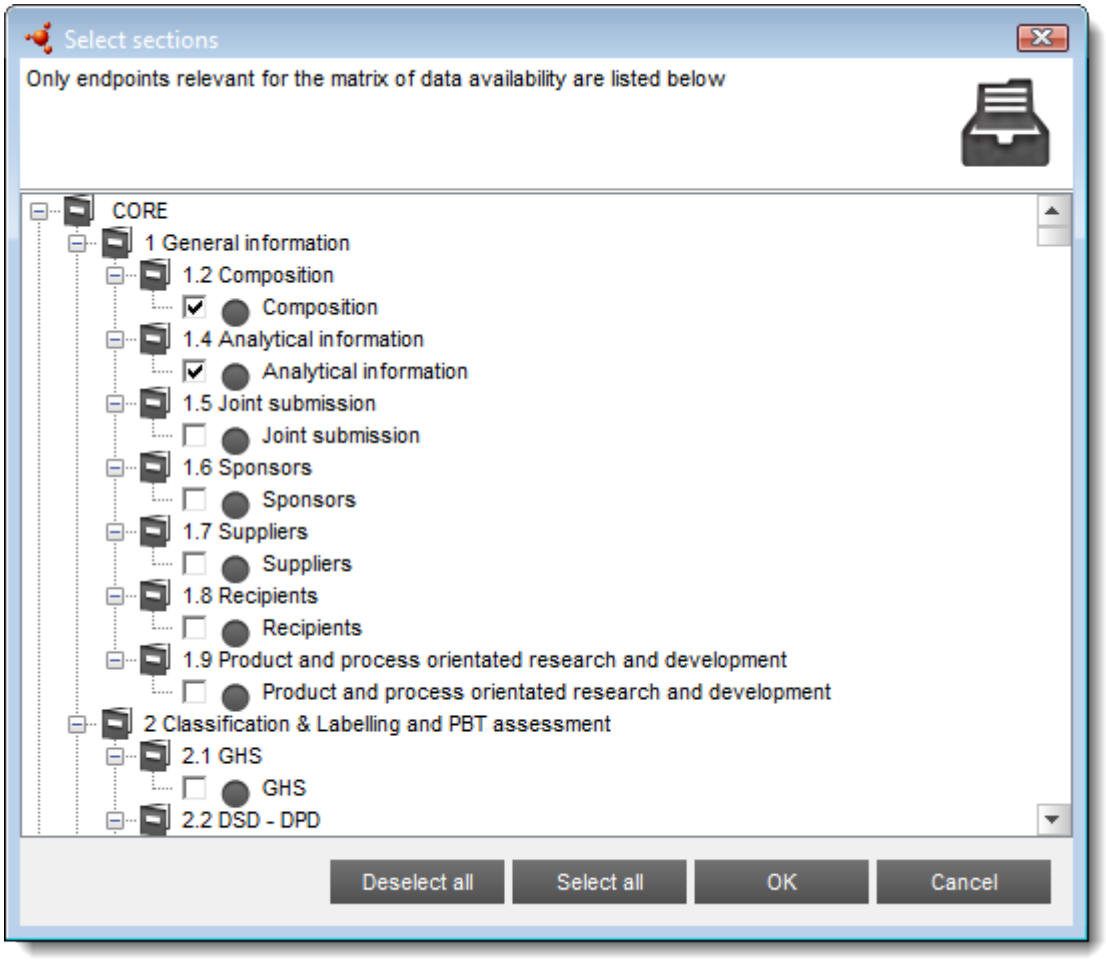
The category matrix shows the documents in the sections selected in the field shown below. Click on the downward facing arrow to open the selector.

Figure 44: The sections available in the matrix view for a Category



The selector for sections is shown below.

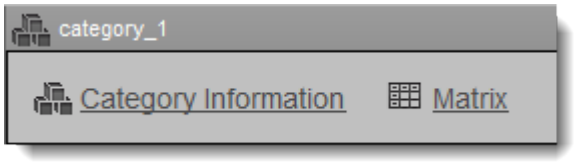
Figure 45: Determine which sections are shown in the matrix view for a Category



When you have made your selection, click on *OK*. The selection can be edited later if required.

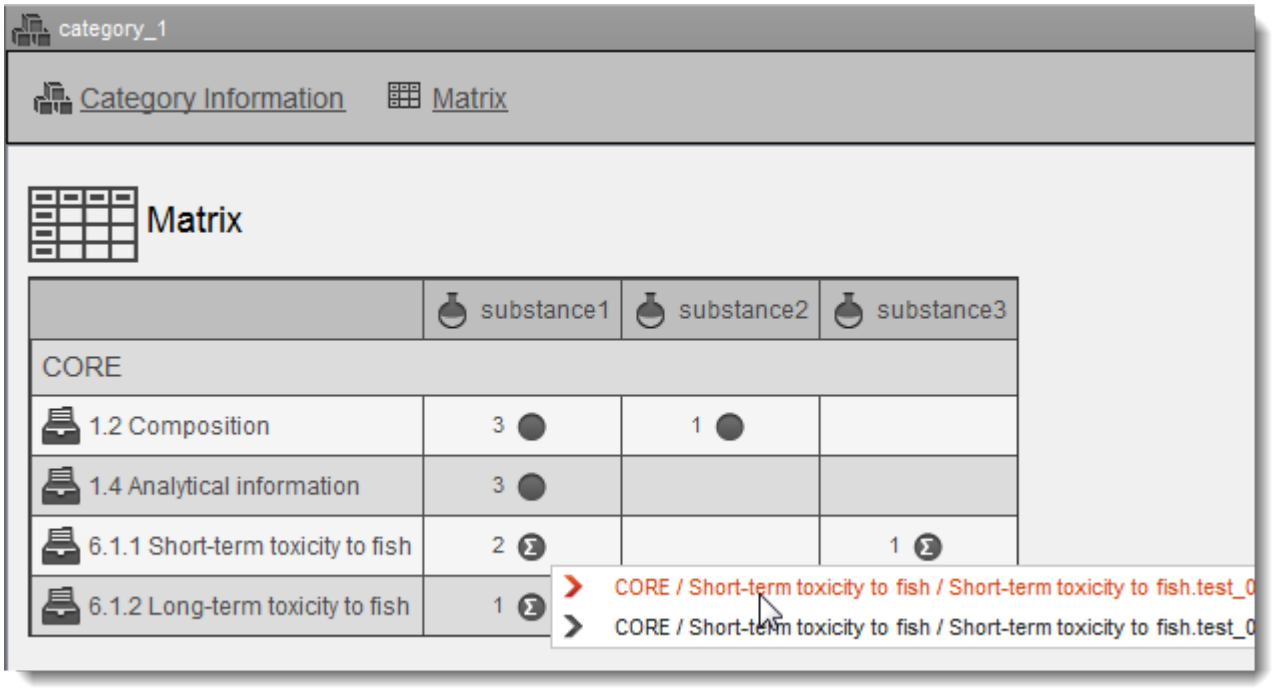
To open the category matrix click on the link *Matrix* in the header of the *Data* panel, as shown below. It is possible to toggle between the matrix and the category management window using the links shown below.

Figure 46: Toggle between the matrix and the category management window



An example of the main page of the matrix is shown below.

Figure 47: The main page of the matrix

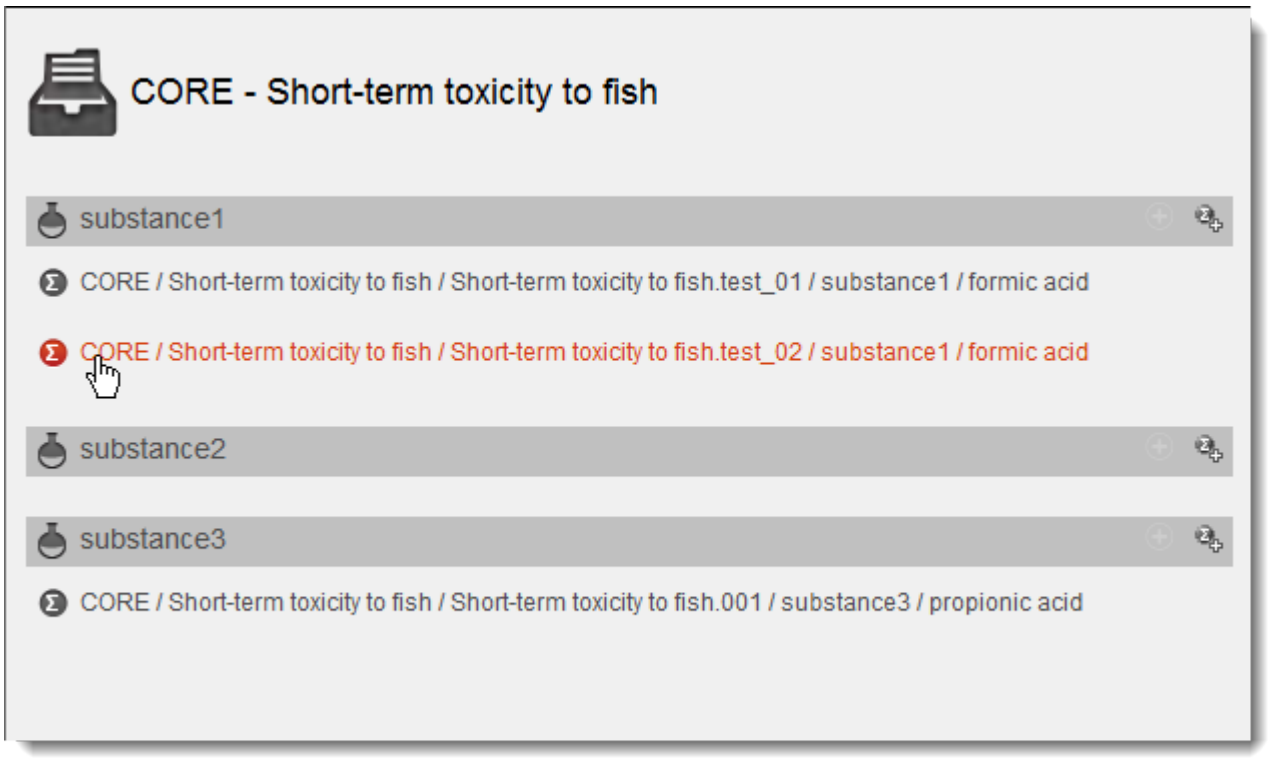


The matrix shows the selected sections as rows and provides a column for each member *Substance*. Where there is at least one document, an icon indicates whether it is study record or a study summary, and whether it is a referenced document. The icons at the top right of the matrix interface are used to filter the type of document shown. The number of documents in that section in that *Substance* is indicated before the icon. Clicking on the icon opens a drop-down menu from which a document can be selected. A selected document is shown in the data panel. To get back to the *Category*, click on the back button in the upper menu toolbar.

Clicking on the *Substance* name opens the *Substance* in the *Data* window.

To show all the documents for a particular section across all the *Substances*, click on the name of the section. This opens a view like the one shown below.

Figure 48: The documents in a Category for a particular section



A new summary can added from here by clicking on the add summary button .

Category differs in IUCLID 6 compared to IUCLID 5 in that a *Template* cannot be attached directly to a *Category*. However, a *Template* can be attached to a *Substance* that is in a *Category*.

6. Annotation

An *Annotation* is a type of entity in IUCLID 6 that is used as a container for information that relates to the evaluation of data in a particular regulatory context, for example, by a regulatory body. It allows the data to be stored in a structured manner, so it is not just an attachment. There are two tabs in the interface, as described below.

6.1. Basic data

Enter a name for the annotation and the organisation carrying out the work. The field *Annotation status* may be used to record whether the annotation is still being worked on or whether it has been finalised. An evaluation may be uploaded as an attached file to the field *Attached regulatory authorities' evaluation*.

6.2. Dataset data

This tab contains fields into which details about the evaluation process may be recorded. The field *Remarks*, is a free text field that has a free-text template. Suggestions as to what to enter are provided in free text template. To open the free text template, click on the icon that shows the letter

A with an arrow at the bottom right, . To copy the text from the template to the field, click on the button labelled *Insert*. The text should now be edited to contain the relevant data.

7. Dossier

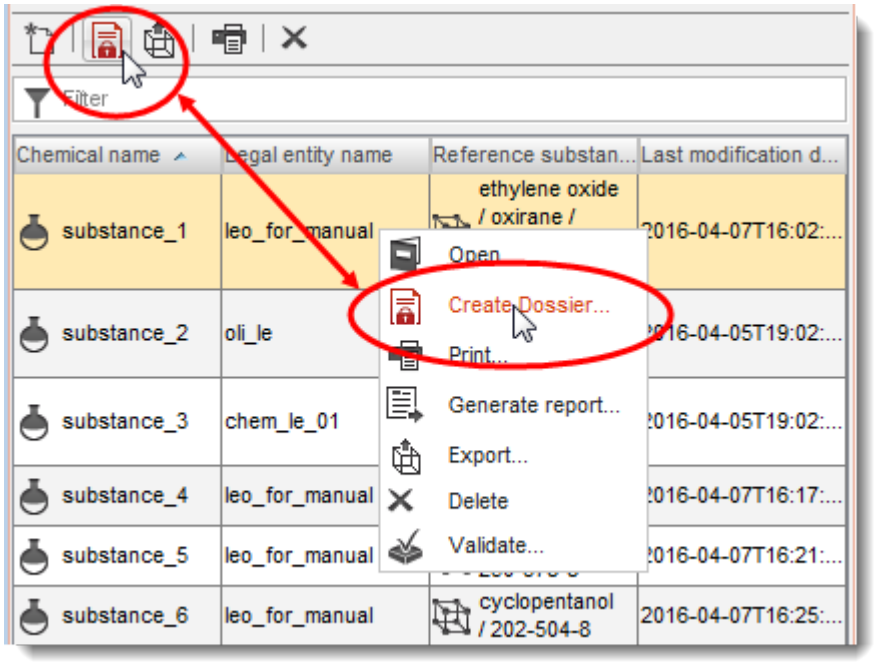
A *Dossier* is a write-protected copy of the data stored in a *Substance* or *Mixture/Product*. Typically, a *Dossier* is used to submit data to a regulatory authority to satisfy a legal obligation arising from a legislation, for example REACH.

7.1. Dossier creation

Before creating a *Dossier*, ensure that at least all the required data is in the *Substance* or *Mixture/Product* from which the *Dossier* will be created. During the creation of a *Dossier*, data from the *Substance* or *Mixture/Product* that is not required can be excluded. Therefore, there is no need to remove unrequired data from the *Substance* or *Mixture/Product* before starting *Dossier* creation. Remember that a *Dossier* cannot be modified, so if changes are required, the *Dossier* must be re-created. A *Dossier* is created using a dedicated wizard. Whilst the wizard is running, no other functionalities are accessible in the IUCLID interface, so data cannot be modified.

To start the wizard, select the record of the *Substance* or *Mixture/Product* in the search results of the *Navigation* panel, and then either click on the *Dossier* icon, or right-click and then select *Create Dossier*, as shown in the figure below.

Figure 49: Starting the Dossier creation wizard

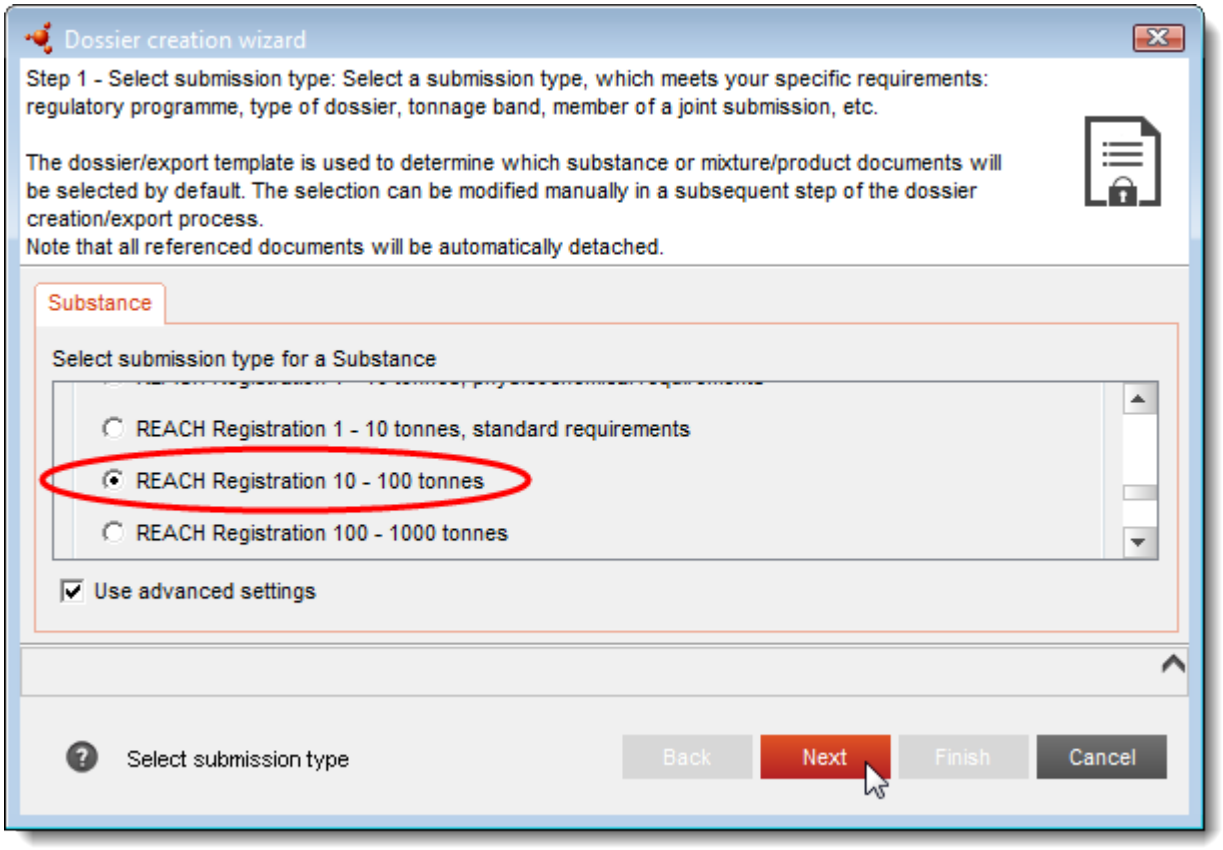


The wizard opens in a pop-up window. In the header of the window there are some instructions on how to fill-out the wizard. In the footer, there is an indicator of the current step in the process. If there is a problem with the data entered, a message is shown in the footer.

7.1.1. Selecting the Dossier type

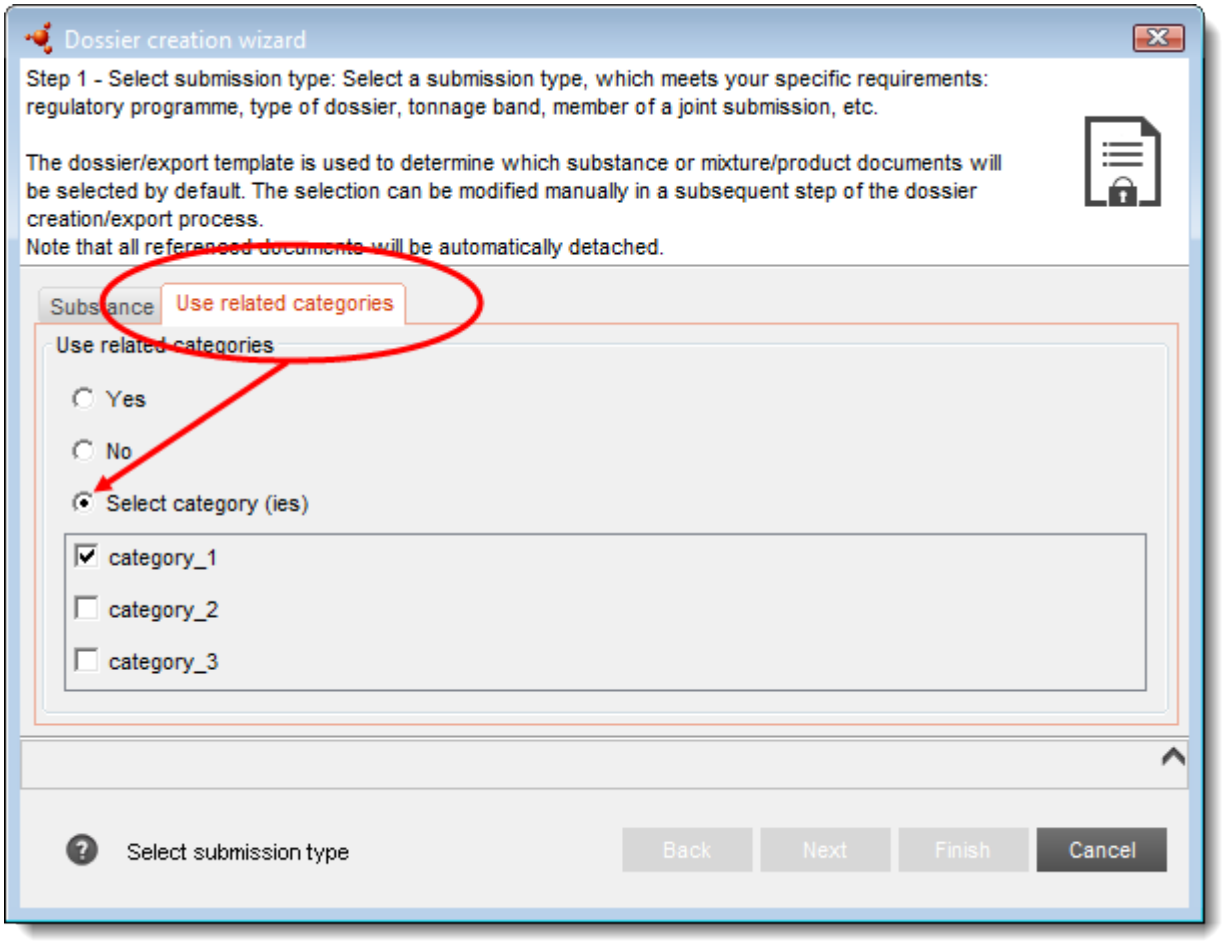
On the first page of the wizard, select the type of *Dossier*. The types correspond to the views that can be applied to the TOC of *Substances* and *Mixture/Products*. If you are not sure which one to select, see guidance specific to the legislation for which the *Dossier* is intended. An example is shown below where the type of Dossier selected is *REACH Registration 10 - 100 tonnes*.

Figure 50: Select the type of Dossier



If the *Substance* or *Mixture/Product* from which the *Dossier* is being created is referred to by a *Category* entity, the first page of the wizard has a tab labelled *Use related categories*, under which the inclusion of *Category* entities in the *Dossier* is controlled. The default option *Yes*, includes all the *Category* entities that refer to the *Substance* or *Mixture/Product*. In addition, either a subset, or none of *Categories* can be selected. An example is shown below in which only the *Category* entity named category_1 is included in the *Dossier*.

Figure 51: Including a Category in a Dossier



The option *Use advanced settings* provides options that allow data to be selectively included and excluded from the Dossier. It also allows the User to check exactly what will be in the Dossier. For example, fields flagged as confidential can be excluded. If all the available data required for the Dossier type is to be placed in the *Dossier*, the box can be left unticked.

To proceed with the wizard, click on the button labelled *Next*.

If the option *Use advanced settings* were left unticked, the next page of the wizard to be shown is that described in section *7.1.3 Administrative data to be placed in the Dossier header*. If the option *Use advanced settings* were ticked the description of the wizard follows on directly from here.

7.1.2. Choosing the Data that is placed in the Dossier

The filtering rules that are set in the following fields are applied cumulatively such that if any rule excludes a type of document or a field, it is excluded from the *Dossier*.

7.1.2.1. Include legal entity

Either exclude or include the *Legal entity* that is attached to the *Substance* or *Mixture/Product*. The default is exclude, which is the opposite of all the other fields.

7.1.2.2. Detail level of document fields

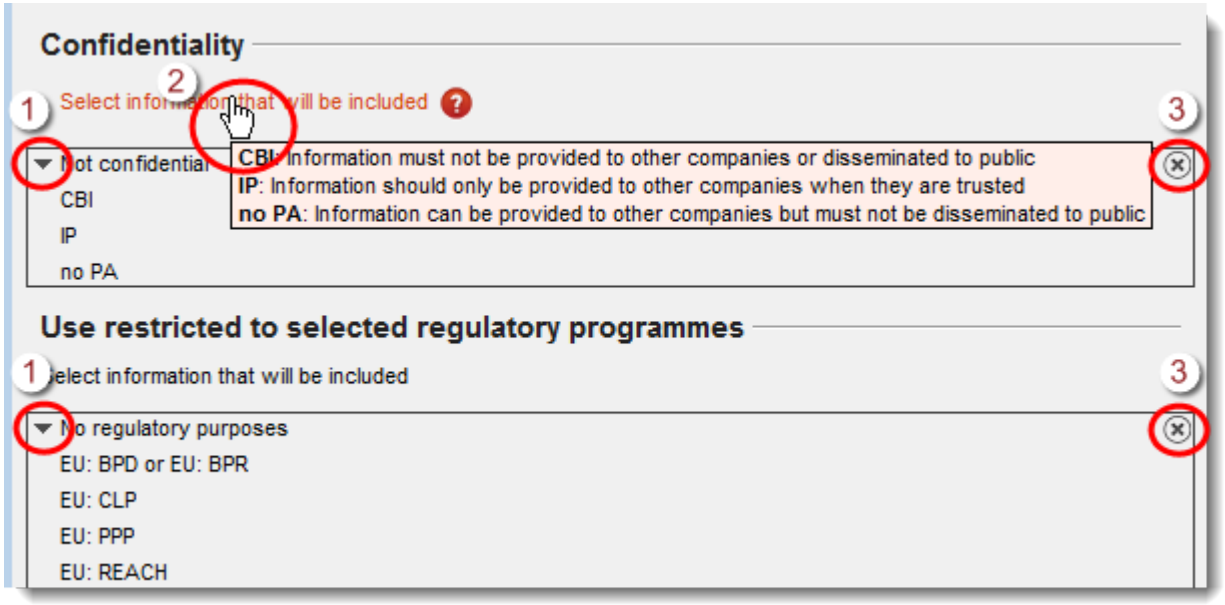
Unticking the box labelled *Detailed fields*, excludes some fields from the *Dossier*.

To exclude confidential fields by type, untick the box labelled *Confidential fields*. The type of confidentiality is set in the next section.

7.1.2.3. Confidentiality and Use restricted to selected regulatory programmes

The fields *Confidentiality* and *Use restricted to selected regulatory programmes* both relate to flags, which are described in section 1.3.2 Flag. The figure below provides a summary of how the interface behaves for these fields.

Figure 52: Automatically exclude fields from a Dossier



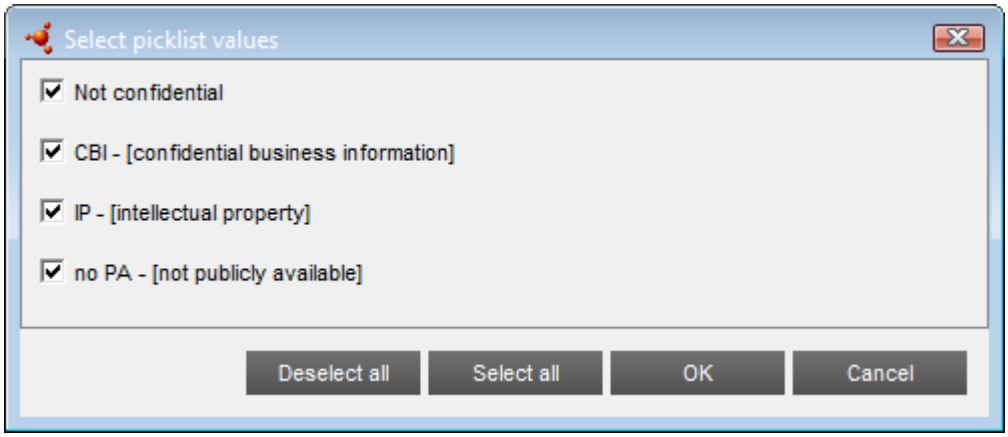
Key for Figure 52

1. Open the pick lists shown in the figures below
2. Get some tips on what the abbreviations used here mean.
3. Untick all the options in one go, and collapse the field.

Clicking on the black triangle opens a pick-list. Unticking a box automatically excludes the fields that are flagged with that particular type of *confidentiality*, or *regulatory programme.*

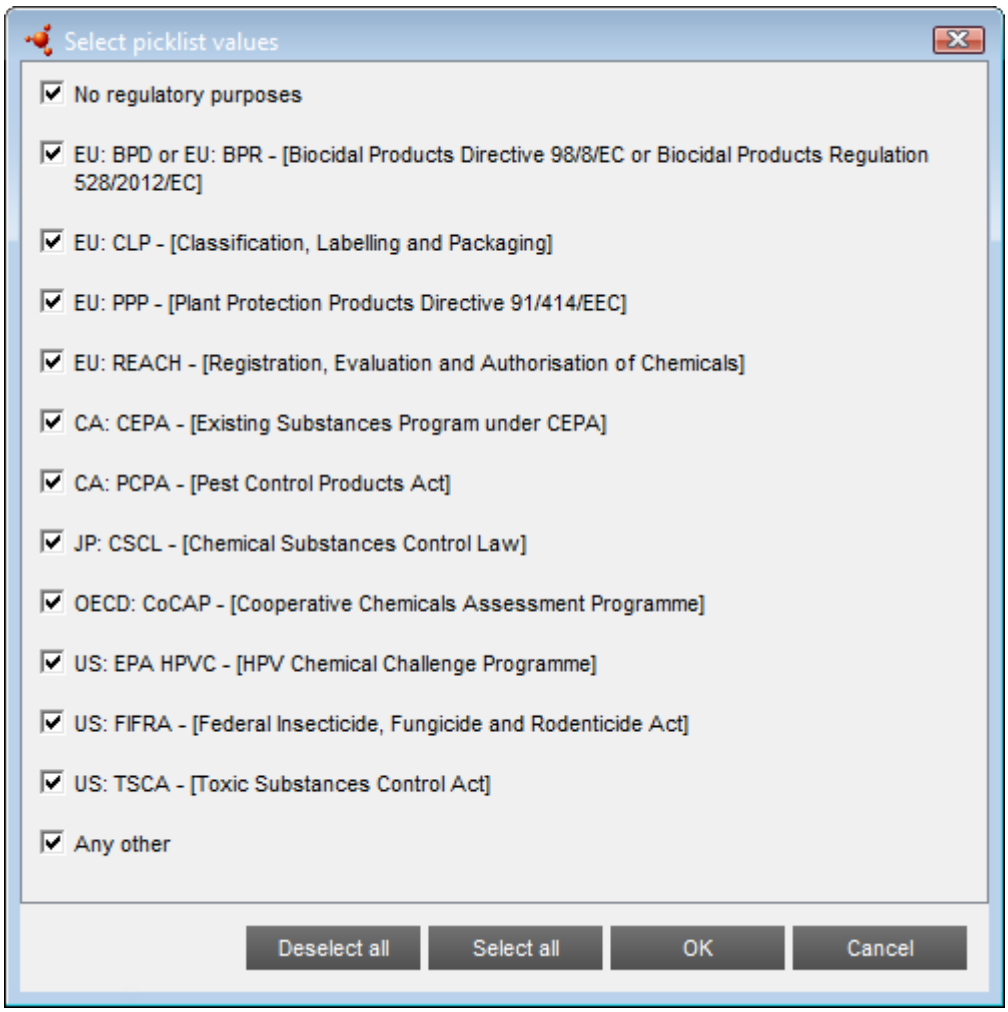
The pick-list for confidentiality flags is shown in the figure below. For example, if the box for CBI were unticked, all fields flagged as CBI would be automatically excluded from the Dossier.

Figure 53: Automatic exclusion of fields from a Dossier according to the values of confidentiality flags



The pick-list for regulatory flags is shown in the figure below. For example, if the box for EU: CLP were unticked, all fields flagged with EU: CLP would be automatically excluded from the Dossier.

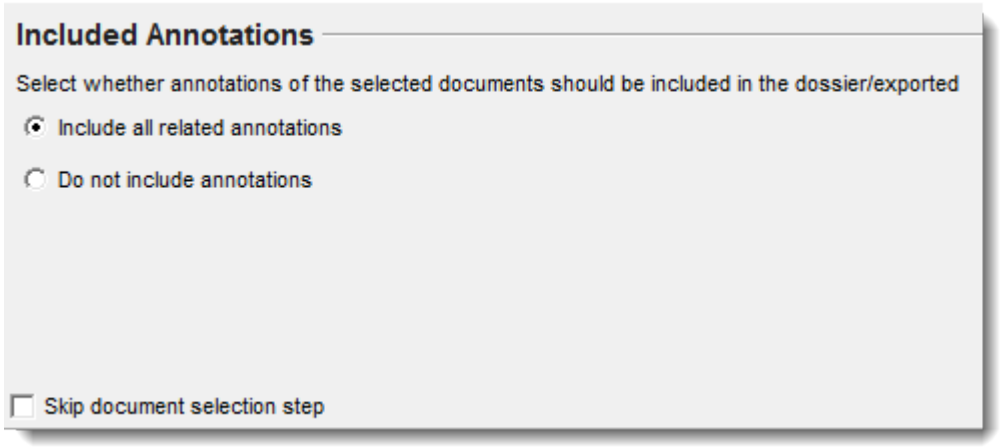
Figure 54: Automatic exclusion of fields from a Dossier according to the values of regulatory flags



7.1.2.4. Include Annotations

This step in the wizard allows *Annotation* entities to be excluded. The default is to include them all, as shown below.

Figure 55: Exclusion of Annotation entities

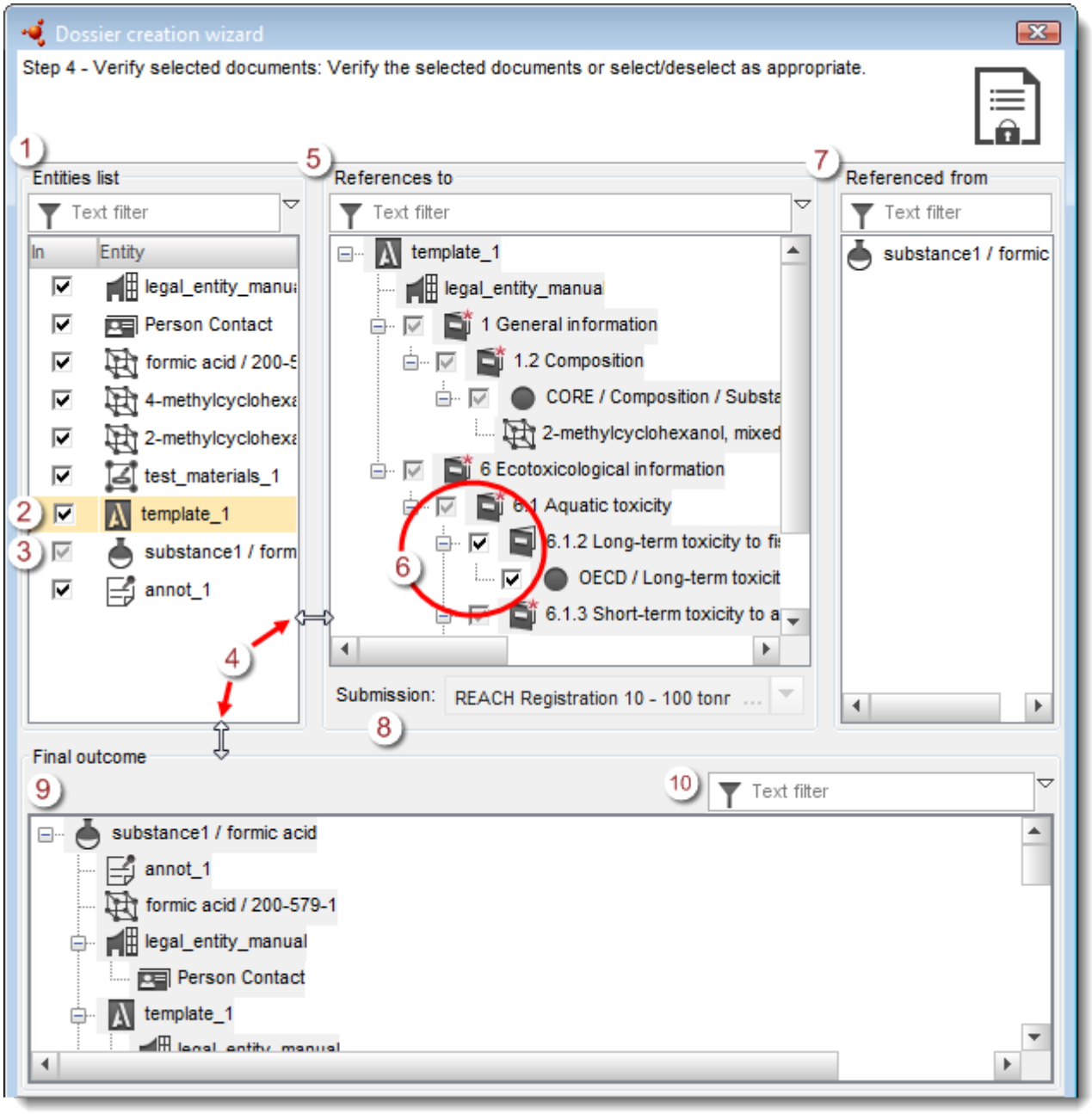


At the bottom left of the wizard page is an option to skip the next step of the wizard.

7.1.2.5. Verify selected documents

This step of the wizard is used to manually exclude documents from the *Dossier*, and to check which documents will be included. An annotated example is shown in the figure below.

Figure 56: Manual selection of documents in a Dossier

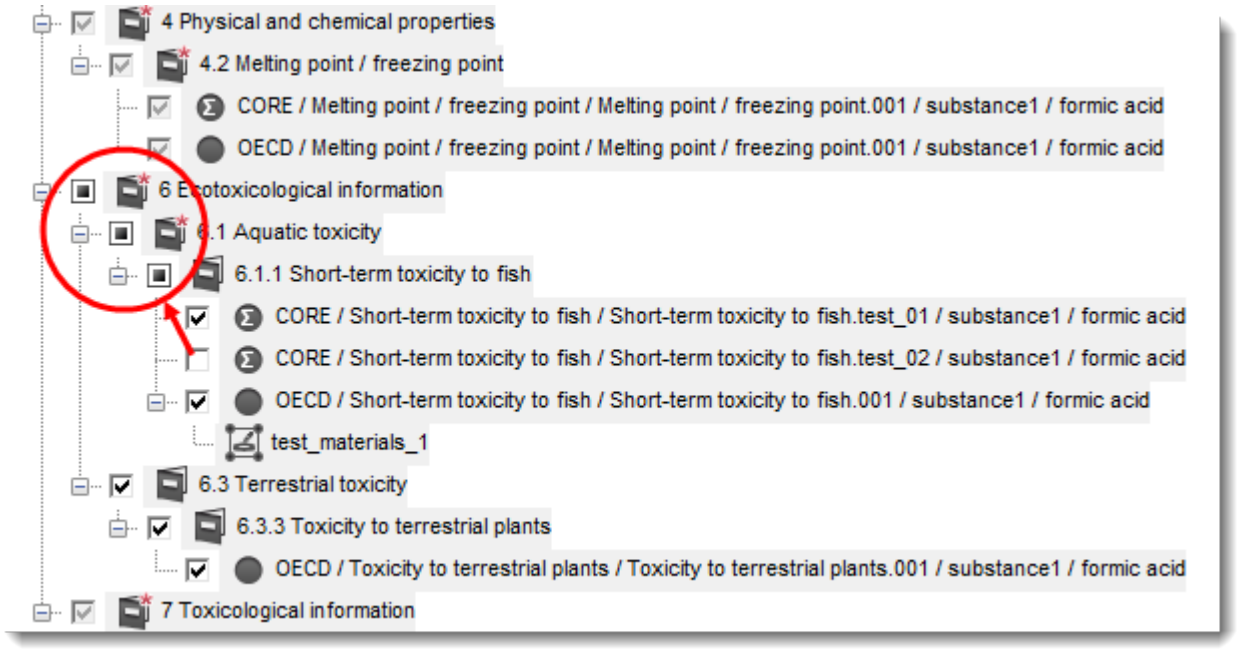


Key for Figure 56

1. On the left, there is a list of all the entities due for inclusion in the *Dossier*.
2. Selecting an entity in the list causes information about the entity and its documents to be shown in the middle and right-hand upper panes.
3. Unticking an entity from the pane on the upper left causes it to be excluded from the *Dossier*. However, the entity from which the *Dossier* is being created cannot be excluded. This explains why in the example shown above, the tick box for the *Substance* is greyed-out.
4. To resize a pane, hover the cursor over its boundary until a double-headed arrow appears, and then click and drag.

5. The upper middle pane contains a tree view of the entity currently selected in the upper left pane.
6. Within the entity tree view in the upper middle pane, some sections and documents can be excluded by unticking their boxes, but some cannot. This is because IUCLID is applying the rules for which sections are mandatory, in accordance with the type of *Dossier* selected in step 1 of the wizard. Mandatory sections cannot be excluded. The examples shown include documents in both mandatory and not mandatory sections. A section from which a document has been excluded is shown in the tree with a different icon for its node, as shown below.

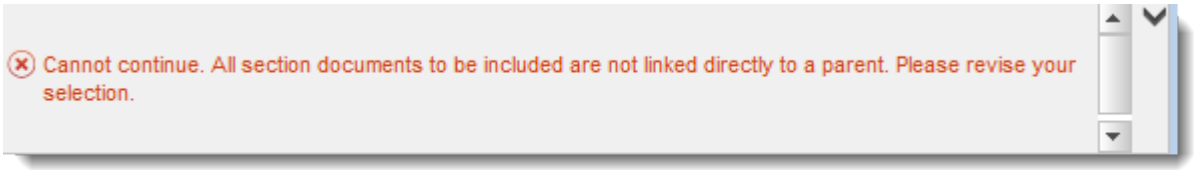
Figure 57: Section with excluded documents in Dossier creation



7. The right-hand upper pane shows documents that refer to the selected entity.
8. The type of *Dossier* is stated here, under the upper middle pane.
9. The expected final outcome of what the *Dossier* will contain, is shown in the lower pane.
10. The content of each pane can be filtered by entering text into the box next to the funnel icon.

If an entity is excluded that is essential for the *Dossier* to be created, a warning of the type below is shown.

Figure 58: Error message on exclusion of an essential entity from a Dossier

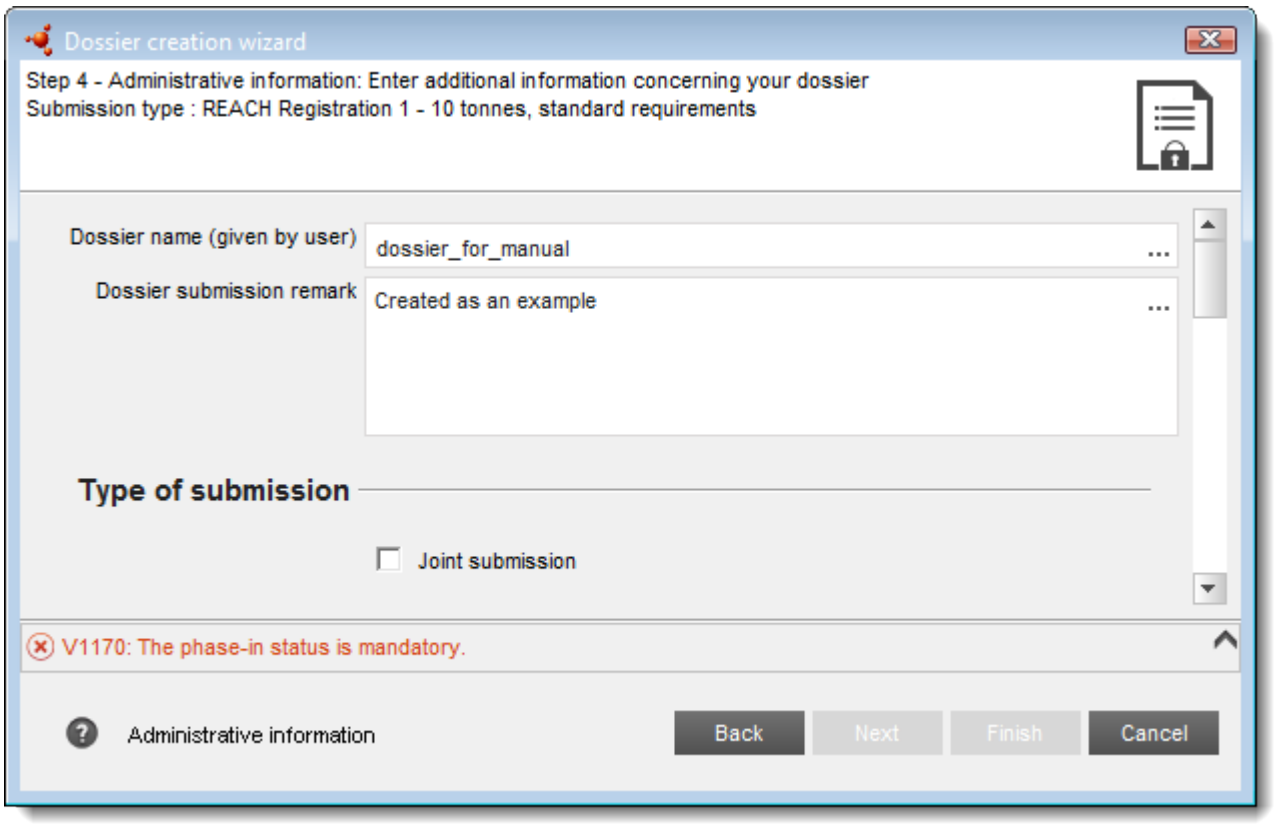


After making any exclusions of documents required, go to the next step of the wizard where administrative information is entered.

7.1.3. Administrative data to be placed in the Dossier header

This information entered on this page will be placed in the header of the *Dossier*. All types of *Dossier* have the fields *Dossier name* and *Submission remark*. The field *Dossier name* is an optional field in the *Dossier* header. For instructions on what values to enter, see the guidance for the particular legislation. If a field contains an erroneous value, it is coloured in pink, and some help as to what the problem is stated in the footer of the wizard page. An example is shown below in which the value for a mandatory field has not yet been entered.

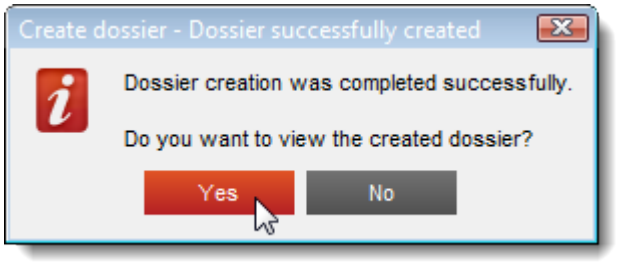
Figure 59: Administrative data to be placed in the Dossier header



7.1.4. Final step in Dossier creation

When all the mandatory fields have been filled, the button labelled *Finish* becomes active. Click on it to start the process of creating the Dossier. When the *Dossier* has been created correctly, the following message is shown.

Figure 60: Dossier created successfully

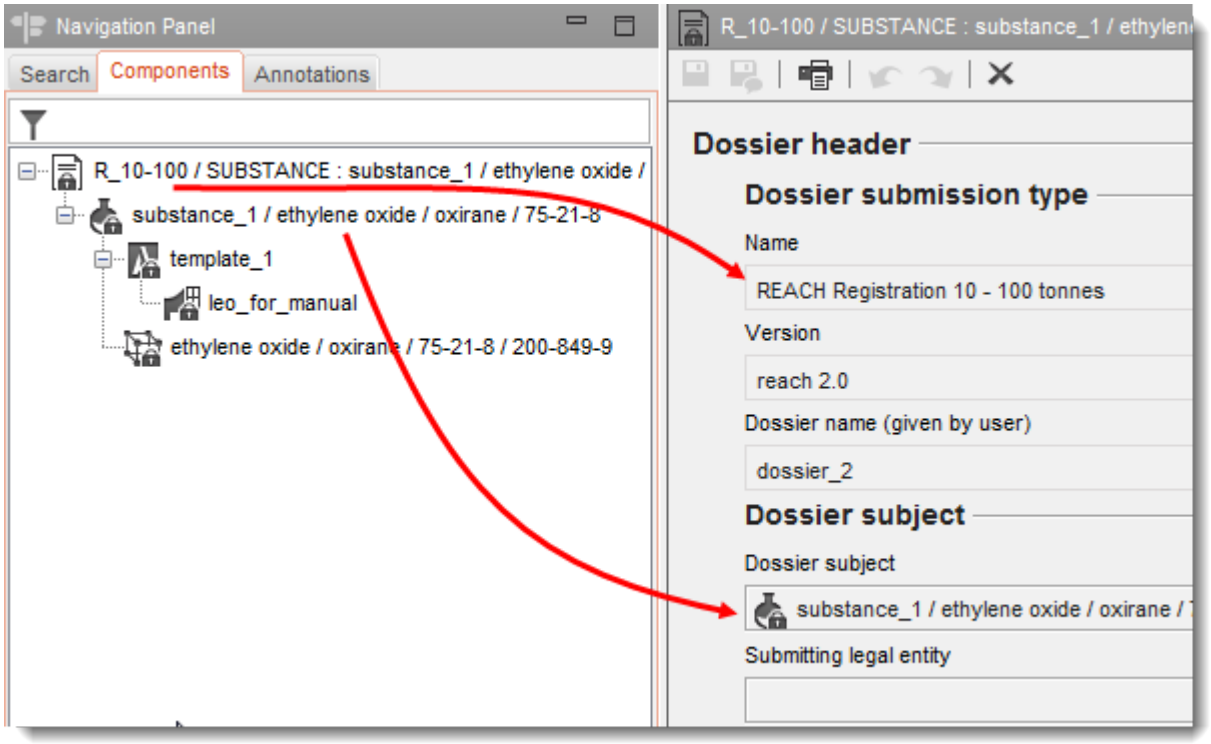


Click on *Yes* and then check that the *Dossier* has been created as expected. The structure of a *Dossier* is described in the next section.

7.2. The structure of a Dossier

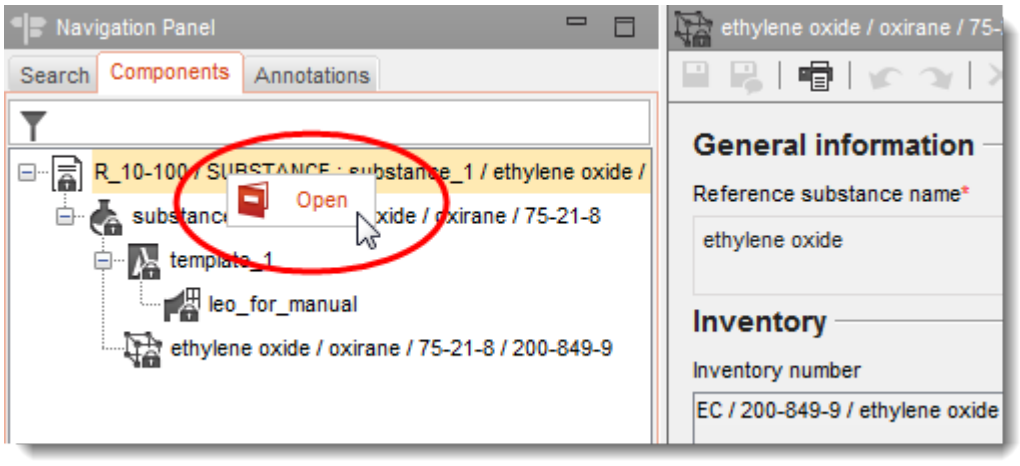
A *Dossier* is an entity that contains a read-only copy of data from a *Substance* or *Mixture/Product*, plus header information, and in some cases category information. On opening a *Dossier* from the list of search results in the *Navigation* panel, a tab appears labelled *Components*. Under this tab, there is a tree view of the entities in the *Dossier*. The copy of an entity in a *Dossier* has an image of a lock superposed on to its icon to indicate that it is read-only. The original entity is still accessible, but there is no link between it and the copy in the *Dossier*. By default, the tree view is fully collapsed showing only the *Substance* or *Mixture/Product* from which the *Dossier* was created, and any *Legal entity* that may have been included in the *Dossier*. Check that the *Dossier header* contains all the information that was entered into the *Dossier* creation wizard. The example in the figure below indicates where the *Dossier* type and the subject of the *Dossier* are located in the *Dossier* header.

Figure 61: Top-level entities under the component tab and in the Dossier header



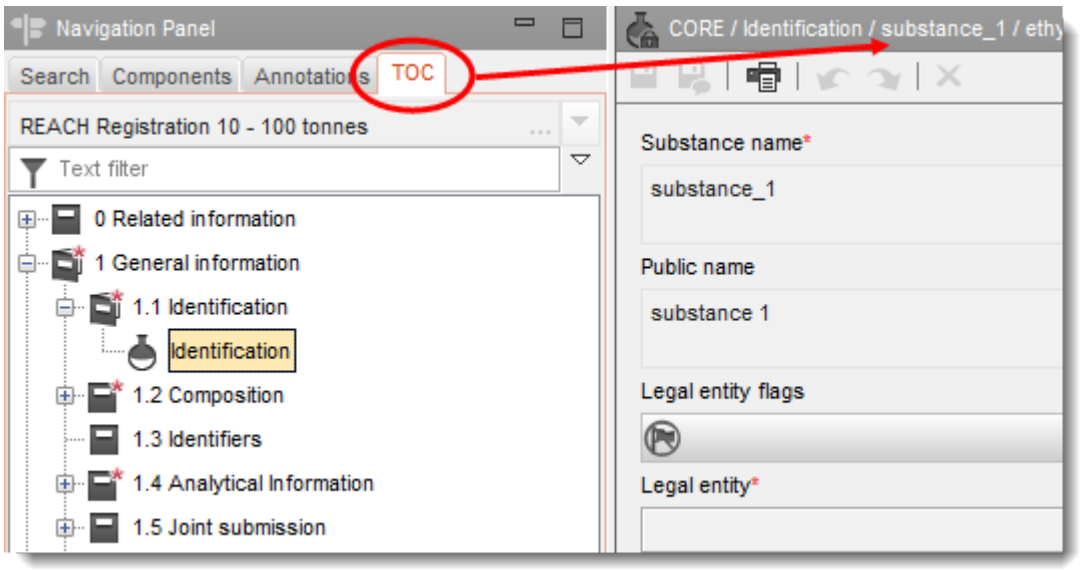
The tree view can be expanded to see which entities are in the *Dossier*. Opening an entity from the tree view displays it in the *Data* panel. To return to the *Dossier* header, open the top-level node in the tree view, as shown below.

Figure 62: How to display the Dossier header



Opening a *Substance* entity displays its TOC under a new tab. The TOC of the *Substance* can be browsed in the usual way, in read-only mode.

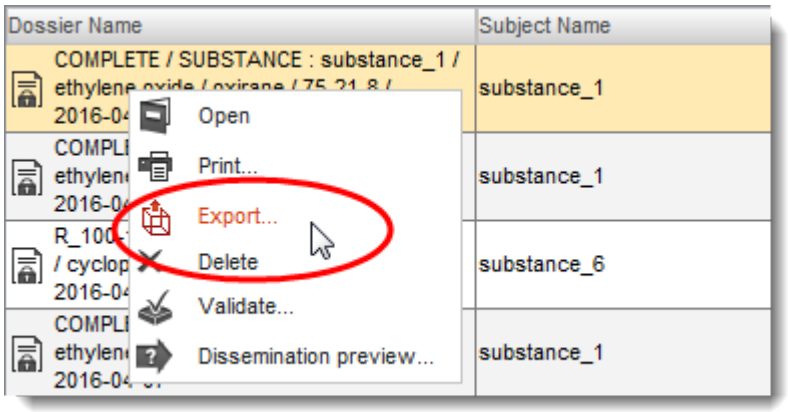
Figure 63: Viewing a Substance in a Dossier



7.3. Export a Dossier

If a *Dossier* is to be submitted to a regulatory authority, it must first be exported. To export a single *Dossier* to a file, right-click on its record in the search results shown in the *Navigation* panel. A simple wizard starts that allows the destination file to be defined.

Figure 64: Export a Dossier



8. Legal entity

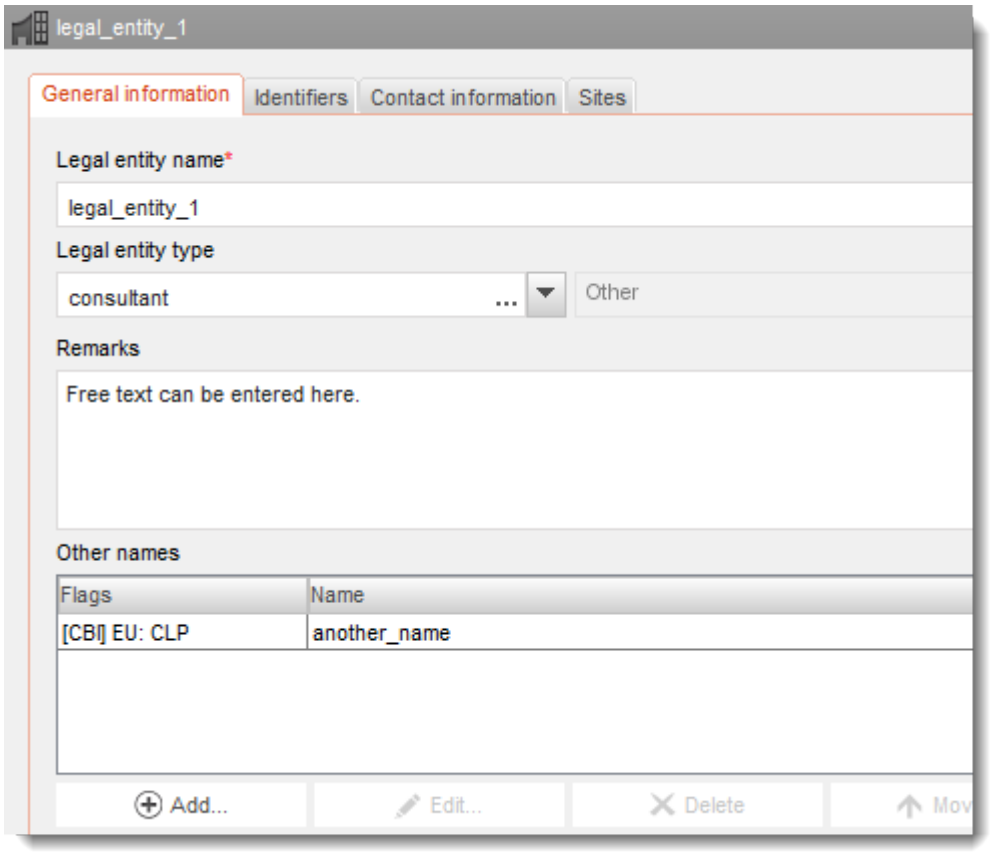
A *Legal entity* is an entity that is used to indicate the legal ownership of other entities. It can be associated with various entities, such as *Substance*. When a User creates an entity, by default, the working legal entity for the User is assigned to the entity. This can subsequently be changed to any of the *Legal entities* to which the User has access, not just the working one.

To change the working legal entity go to the function *My Account under the tab Administration*, which is accessible from the *Home page* in the pane *Administration*. The working *Legal entity* has

the text *(working)* after its name. To set a *Legal entity* as the working one, move it to the top of the list using the button *Move up*. If the Legal entity you want is not present, either import or create it. If you do not have the access rights in IUCLID 6 to do that, consult your system administrator, if applicable.

The data panel for *Legal entity* contains the following four tabs, as shown in the example below.

Figure 65: Data window for Legal entity



8.1. General information

The name of the *Legal entity* must be entered, but the other fields are optional. If an attempt is made to create a *Legal entity* with a name that already exists in the database, a warning is given. If the warning is dismissed, a *Legal entity* is created with the name, but with a unique UUID.

The type of the Legal entity and other names are for information purposes. Flags can be set for the *other names*.

8.2. Identifiers

The identifiers can be recorded of type *Legal entity*, *Regulatory programme*, and *Other IT system*. Each type contains a menu from which relevant sub-types of identifier can be selected. For example, *Legal entity* has an option for DUNS. A flag can be set for each identifier.

8.3. Contact information

An address can be defined for a contact of the *Legal entity* and a link can be made to the entity *Contact*.

8.4. Sites

This shows a list of the *Legal entity sites* that have been associated with the *Legal entity*. The association is made from within the *Legal entity site*. Clicking on a record in the list opens the data window for that *Legal entity site*.

9. Legal entity site

A *Legal entity site* is an entity that is used to associate a *Legal entity* and its associated entities with a physical location. This can have important legal implications, especially where the country is concerned. A *Legal entity site* must have a name and must be associated with a *Legal entity*. To make the association to a *Legal entity*, click on the link icon in the field *Legal entity owner*, select a *Legal entity*, and then click *Assign*.

More than one *Legal entity site* can be associated with the same *Legal entity*.

A contact address and IT identifiers can be added. Optionally, a flag can be set that refers to the whole *Legal entity site*.

10. Reference substance

A *Reference substance* is an entity that is used to define a particular molecular structure, or narrow range of molecular structures in such a way that the definition may be re-used. A *Reference substance* contains chemical identifiers and structural information. For example, there is typically a one to one relationship between *Reference substance* and EC number. A single *Reference substance* can be referred to from multiple entities wherever a chemical identity needs to be defined, for example in a constituent of a *Substance*.

To make a link to a *Reference substance* from some other entity, click on the link icon in the field *Reference substance*, search for and then select a *Reference substance*, and then click *Assign*. The search window also allows a new *Reference substance* to be created.

The use of *Reference substances* is efficient because some chemical substances appear frequently across multiple *Substances* and *Mixture/products*. In addition, *Reference substances* can be shared and exchanged among instances and users of IUCLID. A collection of *Reference substance* entities are available to download free of charge from the IUCLID 6 web site under the section *Support / Get Reference Substances*. If the required *Reference substance* is not available on the web site, or if you otherwise prefer, it is possible to create a *Reference substance* within IUCLID.

10.1. Inventory

A *Reference substance* must at least have a name defined. The name is often the same as an entry in an inventory such as the EC Inventory, but it does not have to be. To link the *Reference substance* to an entry in an inventory, click on the link icon in the field *inventory*, search for and then select an entry, and then click *Assign*. The arrow icon next to the link icon leads to the record of the inventory entry. To return to the *Reference substance* after clicking the arrow, click the *back* button. The cross icon removes the link. This is useful if you need to link to a different inventory entry than the current one.

If no link is made to an inventory, a reason and a justification can be supplied under *No inventory information available*.

10.2. Reference substance information

Reference substance information is a collection of fields that contain identifiers for the Reference substance and related substances. Identifiers are entered here in addition to any link to an inventory. In the field identifiers of related substances, a block may be created per related substance. Within the block there is a field Relation, where the relationship can be described.

A single flag can be applied to all of Reference substance information, for example for confidentiality.

10.3. Molecular and structural information

In Molecular and structural information, enter the molecular formula, the molecular weight, and upload an image that shows the structure in either JPEG, GIF, or PNG format. The field molecular formula accepts text but no characters in subscript, so for example ethane would be C2H4.

A single flag can be applied to all of Molecular and structural information, for example for confidentiality.

11. Contacts

A *Contact* is an entity that records the contact details for a particular person. It can also be used to record something about *a person's* role in a process, for example, as the competent person who is responsible for a safety data sheet (SDS). Links can be made from various other entities to a *Contact,* for example from a *Legal entity*.

Using *Contacts* removes the need to re-enter details where a particular person is involved across multiple processes and *Substances*. The built-in types of contact are *competent person responsible for the SDS*, *emergency contact*, *substance manager*, and *toxicologist*.

11.1.1. The migration of contact details from IUCLID 5 to IUCLID 6

The entity of type *Contact* does not exist in IUCLID 5. Instead, contact details are embedded within the entities of type *Substance*, *Mixture/Product* and *Legal entity*. When such entities are migrated from a IUCLID 5 database to a IUCLID 6 database using the *Migrator tool*, a new *Contact* is

created in IUCLID 6 for each set of contact information in IUCLID 5. The *Migrator tool* may be downloaded from the IUCLID 6 website.

12. Chemical inventories

Chemical inventories is used to provide access within IUCLID to inventories of information on chemical identity that originate from outside IUCLID. A *Reference substance* may be linked to an entry in a *Chemical inventory*, to provide information on chemical identity in a standard format.

The EC Inventory is delivered with IUCLID 6 Desktop but not with IUCLID 6 Server. When IUCLID 6 Desktop is first run after installation, the EC Inventory is imported in a background job. For more information about background jobs, see section *1.7.3 Background jobs*. The EC Inventory is available for download on the IUCLID 6 website.

The EC Inventory contains chemical identifiers such as EC numbers, CAS numbers and molecular formulae. The value of the field state is active for all the entries. Clicking on the icon for *Chemical inventories* on the IUCLID home page opens the navigation window and attempts to display all of the EC Inventory. However there are over 500 records, so with default settings, not all of them can be displayed at once. A *User* with system administrator rights can change this limit.

Chemical inventories cannot be created from within IUCLID, but they can be imported, after which they are read-only.

13. Literature reference

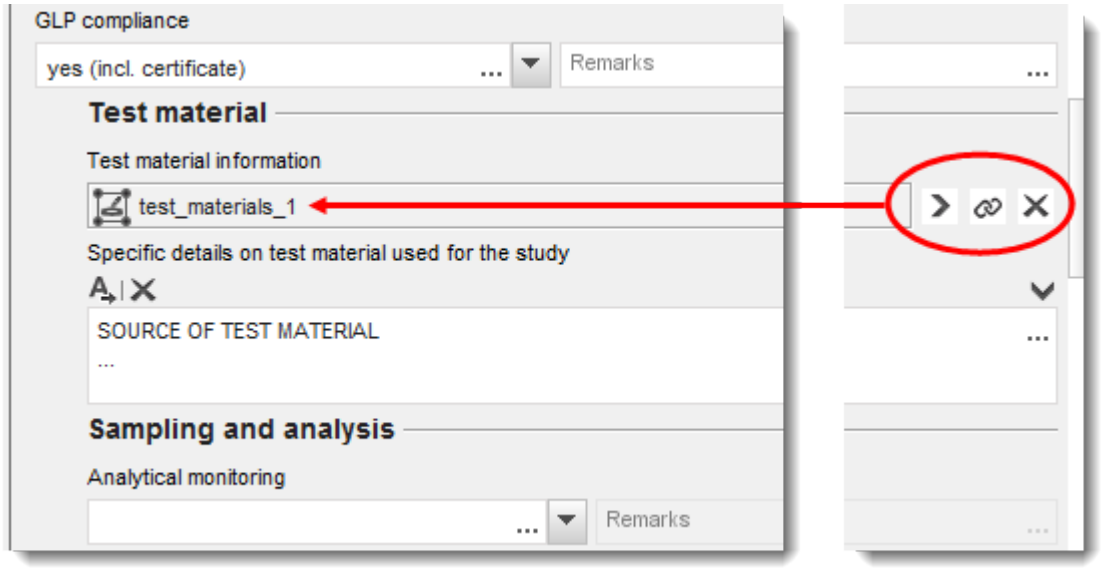
A *Literature reference* is an entity that identifies a particular document that contains information on a *Substance* or a *Mixture/Product*. The only mandatory field is the title, but there are also various other fields that allow a reader to find the document outside IUCLID. A link may be made to a *Literature reference* from an endpoint study record in a harmonised template. The link is made from the field *data source*.

As with all entities, each *Literature reference* has a unique UUID, which is shown in the information panel. This allows the entity to be found directly using the function *Search by UUID*.

14. Test materials

Test materials is an entity used to describe the material on which a physical test has been performed. A link can be made to a *Test material* entity from within an endpoint study record. An example is shown below.

Figure 66: A Test material entity referred to from within an endpoint study record



A *Test material* entity consists of a composition, similar to that used for a *Substance*, a description of the physical form, and some extra information that may be considered confidential, such as a batch number.

The composition can have components of type *constituent*, *impurity* or *additive*. The components are shown in a table that can be edited in the usual way. Each component should be linked to a *Reference substance* and given a concentration range. To make a link to a *Reference substance*, click on the link icon in the field *Reference substance*, search for and then select a *Reference substance*, and then click *Assign*. The search window also allows a new *Reference substance* to be created. If you click on the button *New* to create a *Reference substance*, after creating it, you will have to go back to the *Test materials* entity, and create the component of the composition from the beginning. The option *Go to link target* opens the *Reference substance* of the component selected in the table.

The field *Composition / purity: other information* is provided to record more qualitative information about the purity. The field *Test material form* is provided to record information about the physical state and characteristics of the material used in the test. Finally, there are two free-text fields where more details can be added. Suggestions as to what to enter are provided in free text templates. To open a free text template, click on the icon that shows the letter A with an arrow at the bottom right, . To copy the text from the template to the field, click on the button labelled *Insert*. On saving the *Test materials* entity, watch the message area above the navigation panel for a few seconds whilst the data is checked. If anything is found to be wrong with it, an information message will be shown. For example, if the message is "Concentration: At least one of the values are not set", check the components of the composition.

15. User management

User management provides a means of controlling access to data and functionalities within IUCLID 6. If IUCLID 6 is run on a server, *User management* allows a single IUCLID 6 database to be accessed by many different persons at the same time, each with personalised access. For

example, this allows a large organisation to centralise all its data in one database, and to provide access that is tailored to both the security and functional needs of the organisation.

If IUCLID 6 is run as a desktop application with only one person accessing it at a time, there may be no need to restrict access at all. For that reason, the desktop version of IUCLID 6 is delivered with *User management* disabled. On starting IUCLID 6, the log in window is not displayed because the log in is done automatically into a default *User* named SuperUser. The functions associated with *User management* are replaced by the function *My account*. However, it is possible to switch *User management* on and off via the menu, *Admin / System administration*. When data is migrated from IUCLID 5 to IUCLID 6, if the IUCLID 5 database contains any *User* other than *SuperUser*, *User management* is switched on in IUCLID 6. This is done on the assumption that a multi-user set up is required. If that is not the case *User management* can be switched off via the menu, *Admin / System administration*.

By default, *User management* contains only the types of data object *User* and *Role*. However, switching on Instance Based Security (IBS) provides the additional type of data object, *Group*, and with it, the related concepts of *ownership* and *sharing*. For an overview of IBS, see section 15.3 Instance based security (IBS).

User management is accessed either from the menu *Users*, or from a pane on the home page.

15.1. User

A *User* is a type of data object in IUCLID 6 that links the actions carried out in IUCLID 6 with an individual person or persons who use the software. A *User* has authentication details in the form of a username and password that must be entered to gain access to the *User*. The purpose of having *Users* is to provide different levels of access to data and functionality, to different people. This also allows a record to be kept of who has done what and when.

The username uniquely identifies the *User* throughout the interface. It is common to have a one to one relationship between a person using IUCLID 6 and a *User*, in which case only one person knows the authentication details of each *User*. For the desktop type of IUCLID 6 installation, only one user can be logged in at once, and they must do so from the same machine as that is used to run IUCLID 6. For the server type of IUCLID 6 installation, more than one user can be logged in at once, and IUCLID 6 does not have to be running on the same machine as any of the persons who access the software.

When someone creates or imports a document, the current *User* automatically gains ownership of the document. The access to the document for other *Users* depends on how the system has been set up. Ownership can be transferred between *Users*, but a document can be owned by only one *User* at a time. An important function of a *User* is to define the legal ownership of data via a *Legal entity*. For example when creating a *Dossier*, the ownership of the *Dossier* is defined by the *Legal entity* selected for the *User* at that time. A *User* can have more than one *Legal entity* attached to it, but can act on behalf of only one *Legal entity* at a time. The access a *User* has to functions and data within IUCLID 6 is controlled via *Roles*, and if instance based security is turned on, via *Groups*, as described in later sections.

If the installation of IUCLID 6 is in a multi-user environment, it is common practice to give each person who uses the software access to their own *User*, and to tailor it to the individual needs of the user via *Roles* and *Groups*.

15.1.1. Users supplied with IUCLID 6

A fresh installation of IUCLID 6 Desktop comes with only the *User* named *SuperUser* for which there is no need to log in. There is no need for authentication. On starting IUCLID 6 Desktop, the home page is shown.

A fresh installation of IUCLID 6 Server comes with two *Users*: *SuperUser* and *FullAccess*. Authentication details must be entered into a log in page.

15.1.1.1. SuperUser

The default password of *SuperUser* is *root*, but it can be changed during installation of a desktop type of installation made using the installer. On first logging in, it is recommended to change the password from the default value. *SuperUser* has complete access to functions of IUCLID 6 and the data therein.

By default, the rules that govern the authentication of the *User* SuperUser are the same as those for all the other *Users*. This means that it is possible for the *User* SuperUser to become locked as described in section *User management / Administration / General 15.1.2.4.1*. The locking of SuperUser can be prevented by setting a system parameter, as described in the document *Installation Instructions for IUCLID 6 Server*, which is available on the IUCLID 6 website.

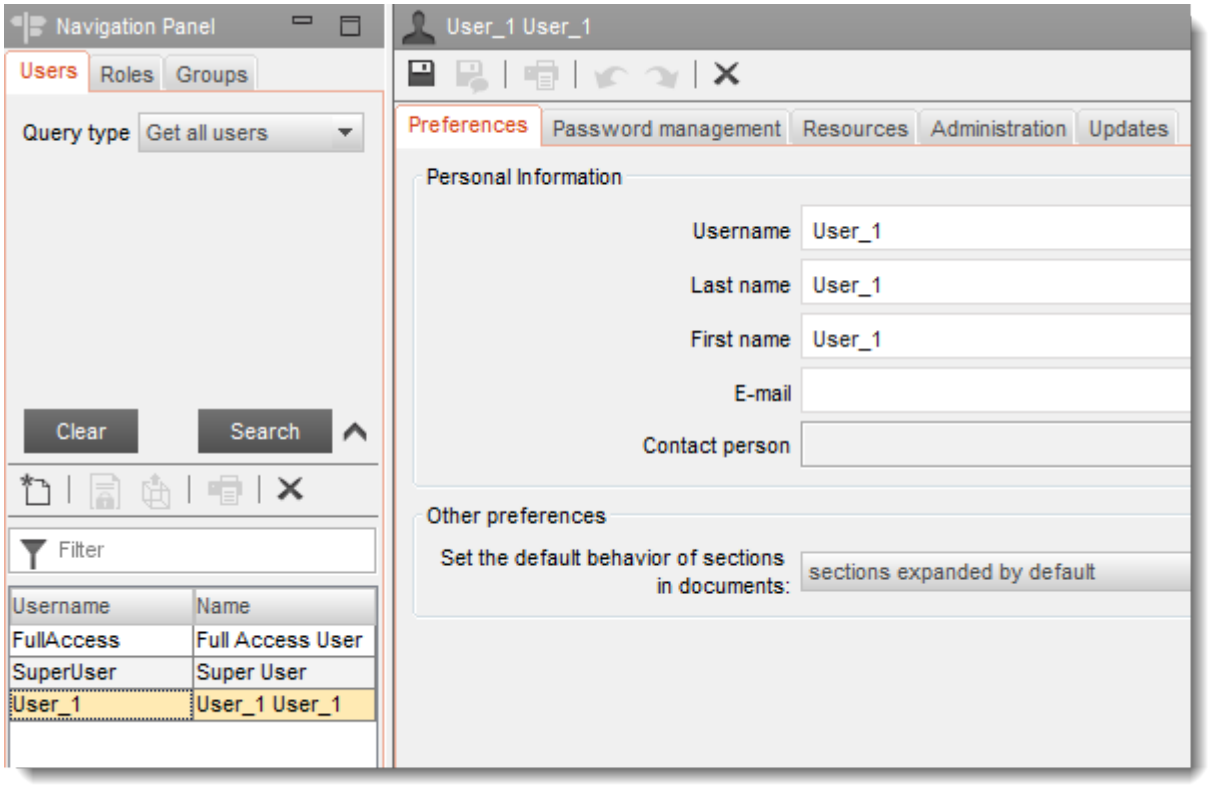
15.1.1.2. FullAccess

The user named *FullAccess* has full access to documents within the IUCLID 6 database, but no access to administrative functions such as *User management*. If you want to log in as this *User,* you will first have to set its password. *SuperUser* can do that.

15.1.2. User management

User management can be performed by a *User* that has the rights provided by the built-in *Role* of *User Manager*. The relevant rights in a *Role* are described in section 15.2.2.4 User management. An example of the user management window is shown in the figure below, where a record for a *User* is highlighted in the *Navigation panel*, and its details are shown in the *Data panel*. Note that in this example, there is a tab for *Group*, which means that instance based security is on. For an overview of IBS, see section 15.3 Instance based security (IBS).

Figure 67: User management



A *User* with user management rights can see all the other *Users*, except those with either the right *Security Management* or *System Configuration*, which includes SuperUser. Therefore, if a *User manager* does not have administrator rights, it cannot see the SuperUser in the interface. A User without user management rights can see only the details of the current *User*. The access rights of a *User* are independent of the *User manager* that created the *User*. *Groups* do not affect the right that a user manager has to edit a *User*. To manage a *User* that has administrator rights, the *User manager* must also have administrator rights.

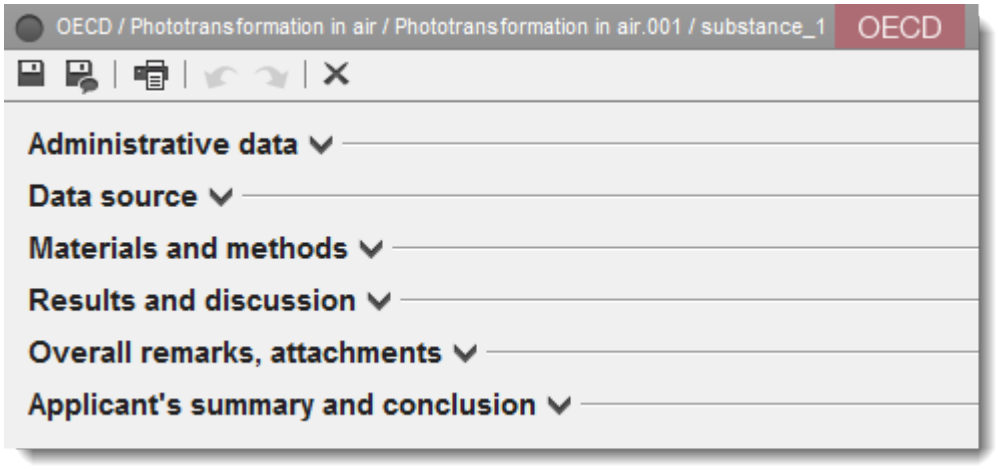
A *User manager* cannot perform user management on its self. The SuperUser does not need to do user management on itself because it has complete access to everything, which cannot be removed.

15.1.2.1. Preferences

Username identifies the *User* throughout the system, and so should be chosen with care. Persons logging in to IUCLID 6 must enter it, along with the password, to prove that they have the right to access the *User*. The values of the *last name* and *first name* are only for internal identification purposes. The email address may be used for information purposes, and if applicable, in a function that allows the reset of a password. For information purposes, an entity of type *Contact* can be attached to the *User*.

The filed *Set the default behaviour of sections in documents determines* whether by default all the sections shown in the data panel are either expanded or collapsed. An example of an endpoint study record with all sections collapsed is shown below:

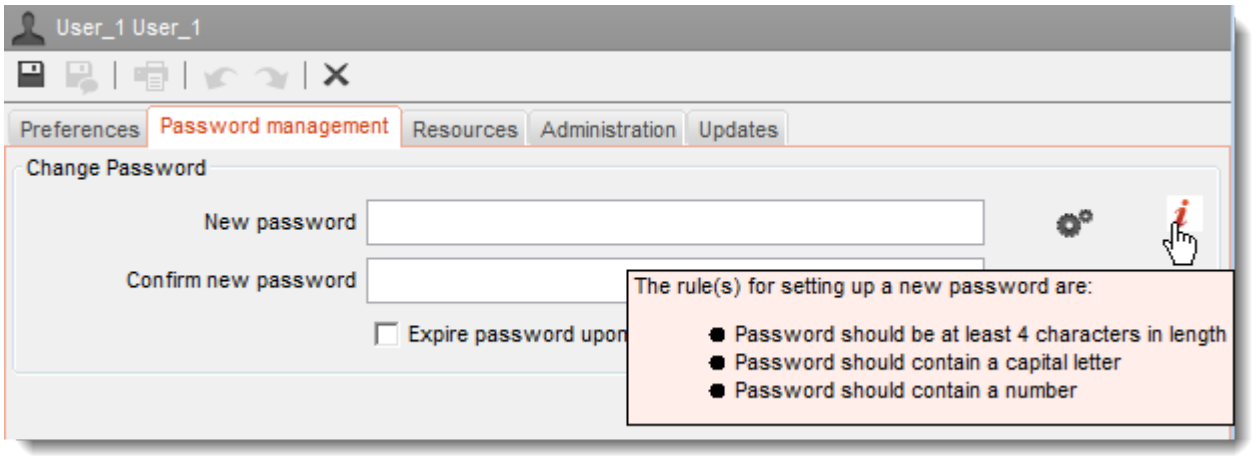
Figure 68: An example of an endpoint study record with all sections collapsed



15.1.2.2. Password management

The *password* is used in combination with the *username* to authenticate a person when logging in to a *User*. IUCLID 6 has a feature that ensures the values of passwords conform to a minimal set of security criteria. The rules are set under the menu *Admin / System administrative / Security policy*. They can be viewed by clicking on the information icon at the top right of the pane for *password management*, as shown in the example below.

Figure 69: Password management



Key for Figure 69:

1. Generate a password automatically
2. View the security rules for passwords

If the password you enter is too weak according to the security rules, on attempting to save it, an error message is displayed that explains what a password must contain. For example, the default settings require the password to be at least 5 characters in length, and to contain at least one uppercase letter, and one digit. The security policy can also be used to force users to change their

passwords periodically. The length of the period is set in the following field accessible from the main menu:

Admin / System administration / Security policy / Force users to change their password after X days.

The policy for the SuperUser is the same as that for all other *Users*.

Generate , automatically creates a password that conforms to the security policy. The value of the password is copied into the fields in to the interface, and the clipboard of the operating system upon which IUCLID 6 is running. In addition, the value is displayed in a pop-up information message.

If the password is a temporary one, the user manager will most likely want to force the user to change the password on next logging in. This is done by ticking the box labelled *Expire password upon next log in*.

15.1.2.3. Resources

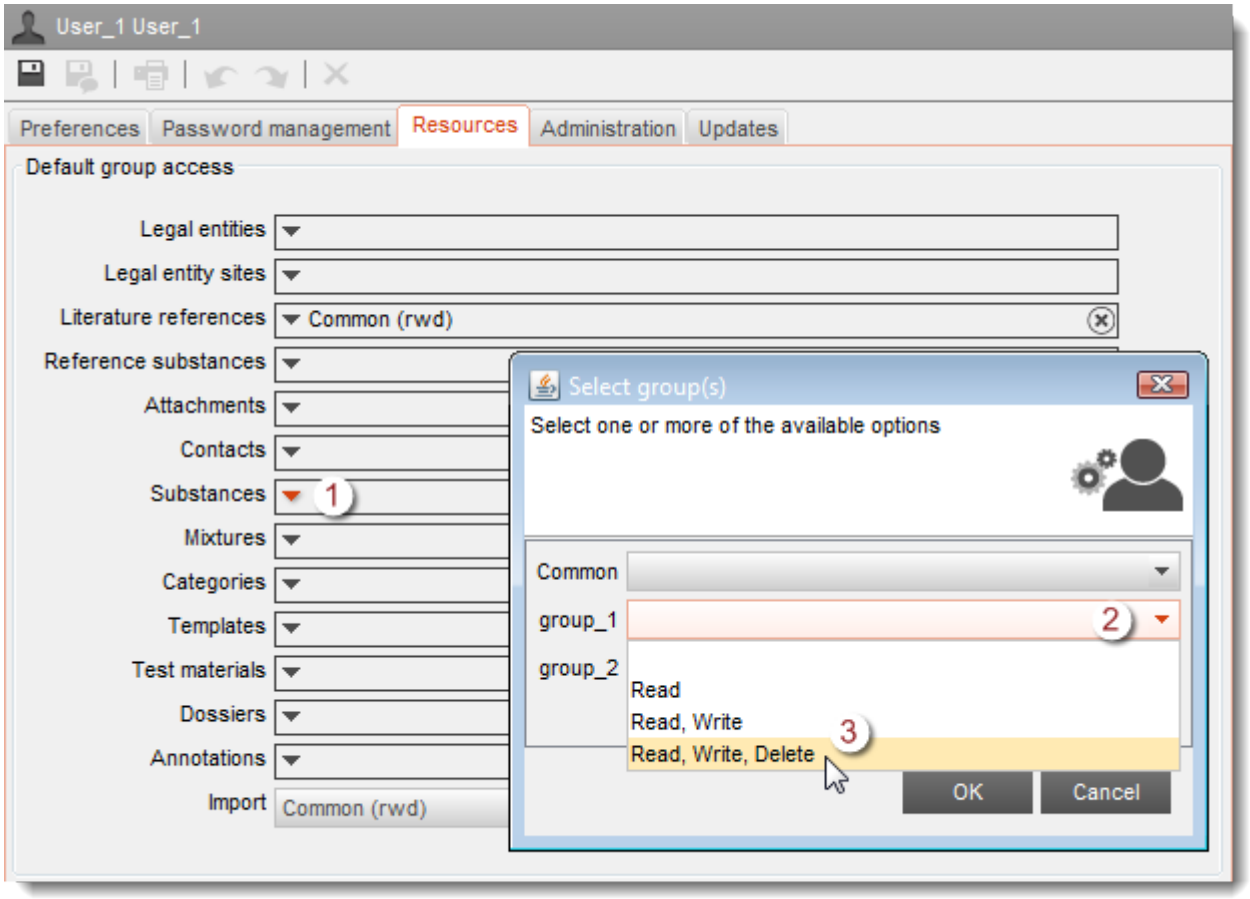
This tab is shown only when instance based security (IBS) is on. For a description of IBS, see section 15.3 Instance based security (IBS).

The options shown under this tab define the default levels of access and sharing per type of entity, per *Group*, per document created or imported by the *User*. These values may be over-ridden manually per document, or during importation.

Clicking on the downward pointing arrow opens a list of all the *Groups* to which the *User* belongs, including *Common*. To set the access for a *Group*, click on the name of the *Group*, and then select one of the following options from the drop-down menu: **no value**, **read**, **read/write**, **read/write/delete**.

For example, if the value for *Substances* is **read/write/delete** for a *Group* named `group_1`, by default, *Users* in `group_1` can read, write and delete all *Substances* created by the *User*. Such a selection is shown in the figure below.

Figure 70: Resources for a User



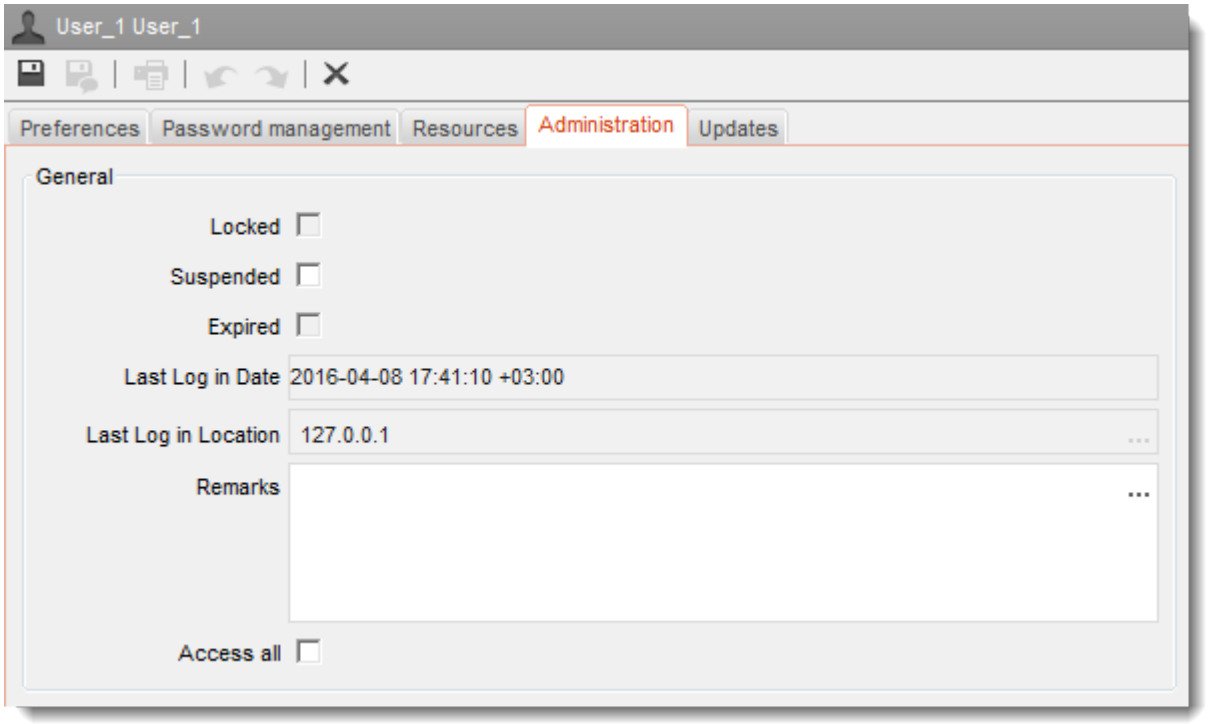
15.1.2.4. Administration

Various properties of the *User* are defined that affect access to data, and to the *User* itself. The first set of fields are shown below.

15.1.2.4.1. General

The first fields relate to access to the *User*.

Figure 71: User management / Administration / General



Locked means that the maximum number of attempts to log in to the *User* has been exceeded. The value of the limit is set under the menu *Admin / System Administration / Security policy*. The default value is three. To unlock the *User*, untick the box. The change takes effect as soon as the change is saved. A user manager cannot lock a *User*. The *User* SuperUser cannot be *Locked*.

Suspended may be used as a manual method of preventing access to the *User*, for whatever reason. If the box is ticked, no one can log in to the *User*. To cancel the suspension, untick the box. The change takes effect as soon as the change is saved. The *User* SuperUser cannot be *Suspended*.

Expired means that no one has logged in to the *User* for the number of days set in the field *Admin / System administration / Security policy / Automatic expiry of unused accounts after x days*. The default value is sixty. To cancel the expiration, untick the box. The change takes effect as soon as the change is saved.

The *last log in date* states when the most recent previous log in occurred for the *User.*

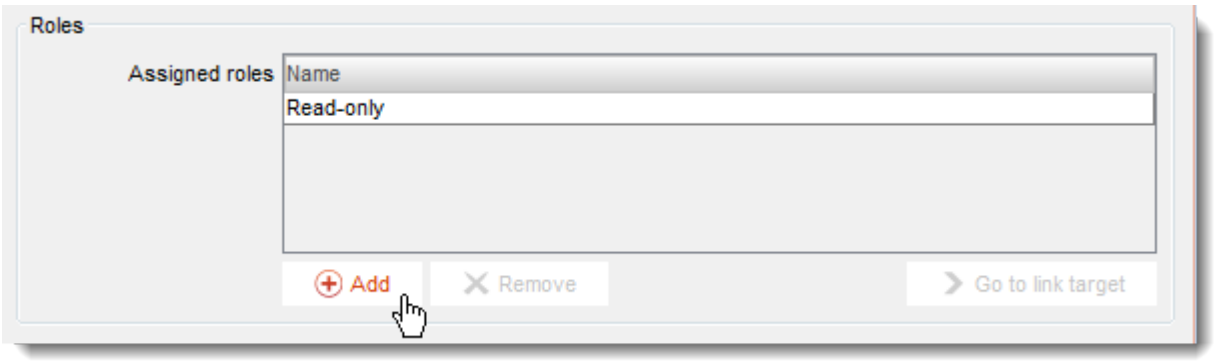
The *last log in location* states the IP address of the computer from which the most recent previous log in occurred for the *User*. For the desktop type of installation, this value will be that for localhost (127.0.0.1).

Remarks is a free text field provided to allow the user manager to make notes about the *User*. It can contain up to 32,768 characters.

The option *Access All* is shown only when instance based security (IBS) is on. For a description of IBS, see section 15.3 Instance based security (IBS). This option turns the *User* into an equivalent of SuperUser in terms of access to data. All possible restrictions that may apply via *Groups* or ownership are lifted. This option cannot be turned off for the *User*, SuperUser.

15.1.2.4.2. Role

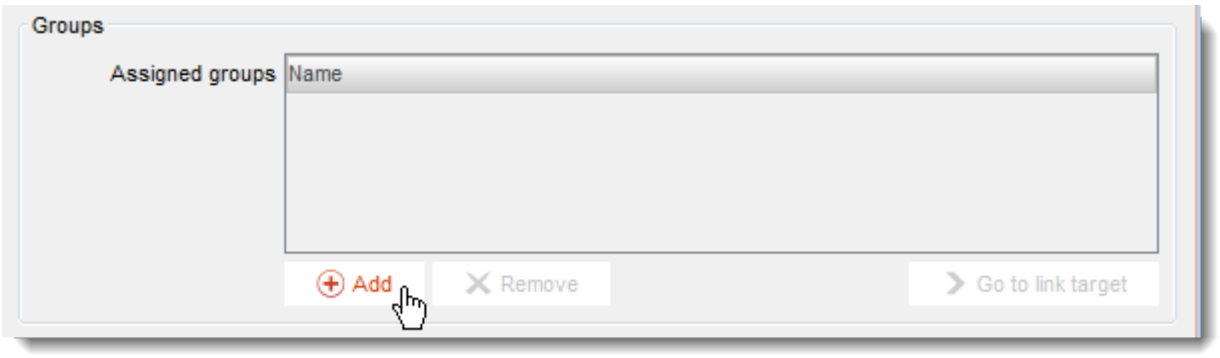
Figure 72: Adding a Role to a User under User management / Administration / Role



This field is used to define the *Roles* of the *User*. Roles are described in section *15.2* Role. A *User* must have at least one *Role*. By default, a new user is given the built-in *Role* of *Read-only*. The built-in roles are described in section 15.2.4 Built-in roles. If a *User* has more than one *Role*, the rights given are additive. For example if a *User* has a *Role* that allows only reading for a particular entity, and another *Role* that allows deletion for the same entity, the *User* can delete that type of entity.

15.1.2.4.3. Group

Figure 73: Adding a User to a Group under User management / Administration / Group

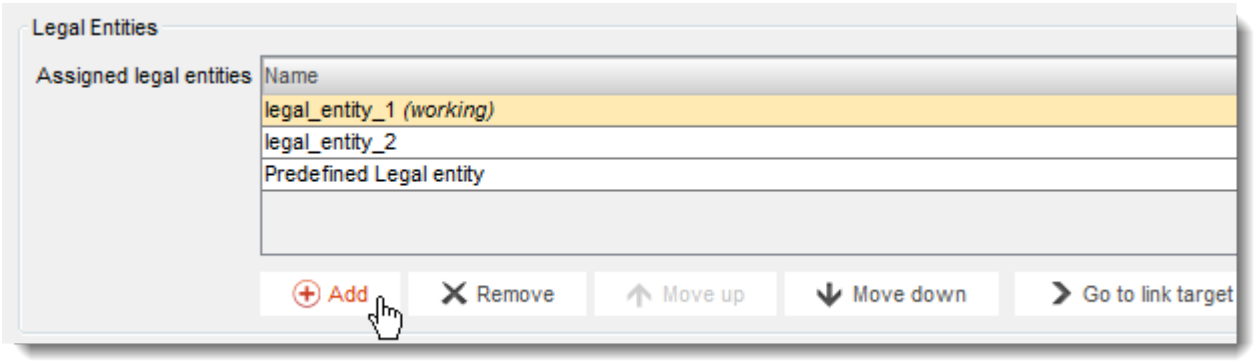


This field is shown only when instance based security (IBS) is on. For a description of IBS, see section 15.3 Instance based security (IBS).

This field is used to add and remove the *User* from *Groups*. This can also be done by a *Group manager* via the *Group* tab. A *User* can be in no *Groups*. See the section on Instance Based Security for more information on *Group*.

15.1.2.4.4. Legal entity

Figure 74: Adding a Legal entity to a User under User management / Administration / Legal Entity



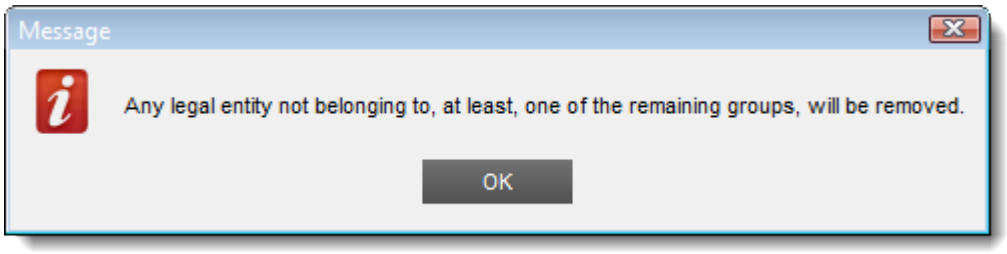
A *User* must have at least one *Legal entity* assigned to it. A *Legal entity* can either be created in IUCLID 6 or imported. IUCLID 6 comes with a built-in *Legal entity* named *Predefined Legal entity*. This is supplied as a means of getting users started, but for regulatory purposes it is recommended to use one specific to your own needs.

To set a *Legal entity* as the working one, move it to the top of the list using the buttons labelled *Move*.

When the assignment is made, it does not matter which of the *Legal entities* is the working one for the user manager's *User*.

Under *Instance based security (IBS)*, a user manager can assign to *Users* only *Legal entities* that are assigned to the user manager. A user manager can assign to *Users* only *Legal entities* that have been shared to a *Group* to which the *User* belongs. If an attempt is made to assign a *Legal entity* to a *User* to whom it has not been shared, the following message is given.

Figure 75: Message shown when a User does not have access to the Legal entity(-ies) affected by an action



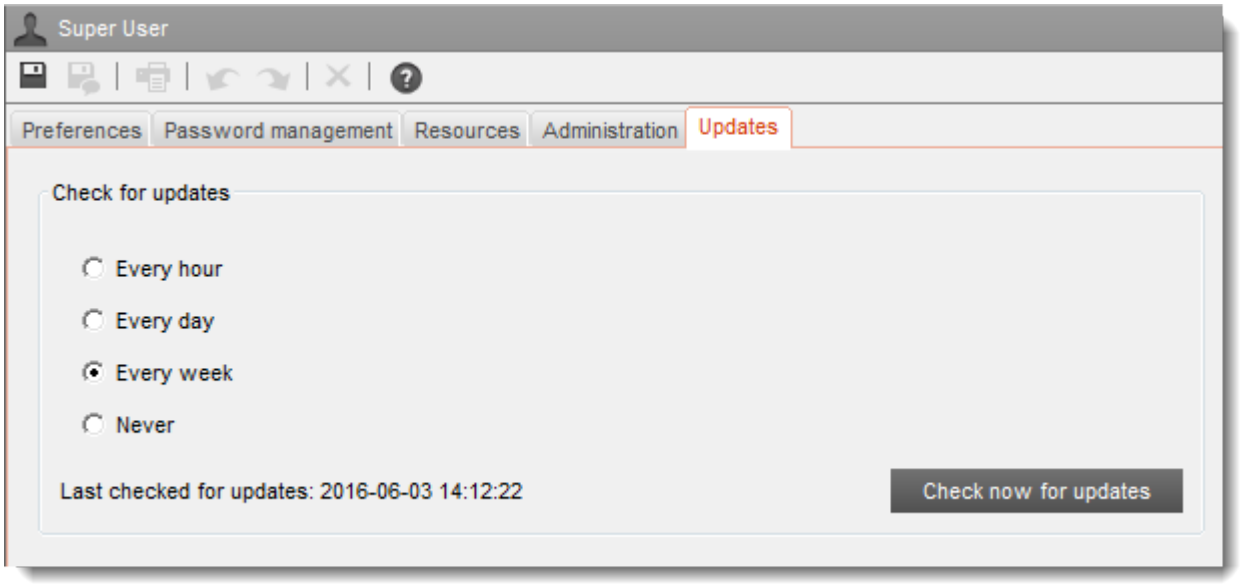
The same message is shown when removing a *User* from a *Group*, where the action also removes access to one or more *Legal entities*. In that case, the affected *Legal entities* are removed from the *User*. If this leaves the *User* with no *Legal entity*, the action is allowed, but the *User* cannot be saved until at least one *Legal entity* has been assigned to it.

15.1.2.5. Updates

The feature *Check for updates* may be used to instruct IUCLID 6 to send periodic automated requests to the IUCLID 6 web site to check whether a newer version of IUCLID 6 or its plugins is available. When IUCLID 6 detects that a newer version is available, it will notify the *User* in the

message window. If an attempt to make a check gives an error message, check the internet connection and proxy settings on the host computer.

To check immediately whether the installation of IUCLID 6 or its plugins contain the most recent version, click on the button *Check now for updates*, shown in the figure below.



If an update is available, go to the downloads section of the IUCLID 6 web site, select the option for the appropriate *Updater tool* for the system, and then follow the instructions.

Note that update process updates both the application and its plugins. There are no separate updates to be done for plugins.

15.1.2.6. Export users

The details for all the *Users* are saved to a single text file. An exported file can be imported into any IUCLID 6 system, as long as associated entities such as *Legal entities*, *Roles*, and *Groups*, are present in the destination system. This allows *Users* to be moved between two different instances of IUCLID 6. This function is accessible from the main menu item *Users*. A pop-up window opens that indicates the number of *Users* to be exported, as shown below:

Figure 76: Export users pop-up window

Click finish to start the export. The export is carried out as a background job, as described in section *1.7.3 Background jobs*.

The exported file is a plain text file. The file extension is csv for greater ease of use with spreadsheet applications, such as Microsoft Excel. There is one User per line. The fields are separated by the semicolon character ";", and the values are surrounded by double quotes. The first row contains the headers. The fields are described in the following table. Fields marked with an asterisk * must contain a value. The SuperUser is not exported.

Table 4: The fields in the text file for the function *Import users*

Header	Description
Username*	The value is used to identify the User to which data is imported. A value is mandatory per row. The value must be unique in the database.
Last Name*	Free text with a maximum of 255 characters.
First Name*	Free text with a maximum of 255 characters.
Suspended	The value of the field *Suspended*. This can be used to suspend and to unsuspend existing *Users*. [yes | 1 | true | no | 0 | false]
Remarks	Free text with a maximum of 32,768 characters.
Roles*	Name(s) of user *Role(s)* assigned to the account. Values must pre-exist in the database before import. Multiple values are allowed delimited by the semicolon character, ;, with the whole field in double quotes.
LEOs*	UUID(s) of the LEO(s) assigned to the *User*. Values must pre-exist in the database before import. Multiple values are allowed delimited by the semicolon character, ;, with the whole field in double quotes.

Groups*	Name(s) of user *Group(s)* assigned to the account. Values must pre-exist in the database before import. Multiple values are allowed delimited by the semicolon character, ;, with the whole field in double quotes.
Delete	Delete a pre-existing *User* on import. [yes | 1 | true | no | 0 | false]
E-mail	The email address associated with the *User*.
Contact	UUID of the *Contact* assigned to the *User*. Values must pre-exist in the database before import.

Below there is an example of a file containing data for three *Users*.

```
Username;Last name;First name;Suspended;Remarks;Roles;LEOs;Groups;Delete;E-mail;Contact
"admin";"Admin";"Anne";"No";"";"Read-only";"a4569f8e-a856-4520-82cc-9e76e6a46347";"Common";"No";"";"";
"reader";"Reader";"Lotta";"No";"A remark about Lotta";"Read-only";"a4569f8e-a856-4520-82cc-9e76e6a46347";"Common";"No";"";"804c707f-baac-4d03-bdd2-8a28c32ca9c8";
"user_manager";"User";"John";"No";"";"System administrator;Read-only";"a4569f8e-a856-4520-82cc-9e76e6a46347";"Common";"No";"";"";
```

15.1.2.7. Download empty users csv

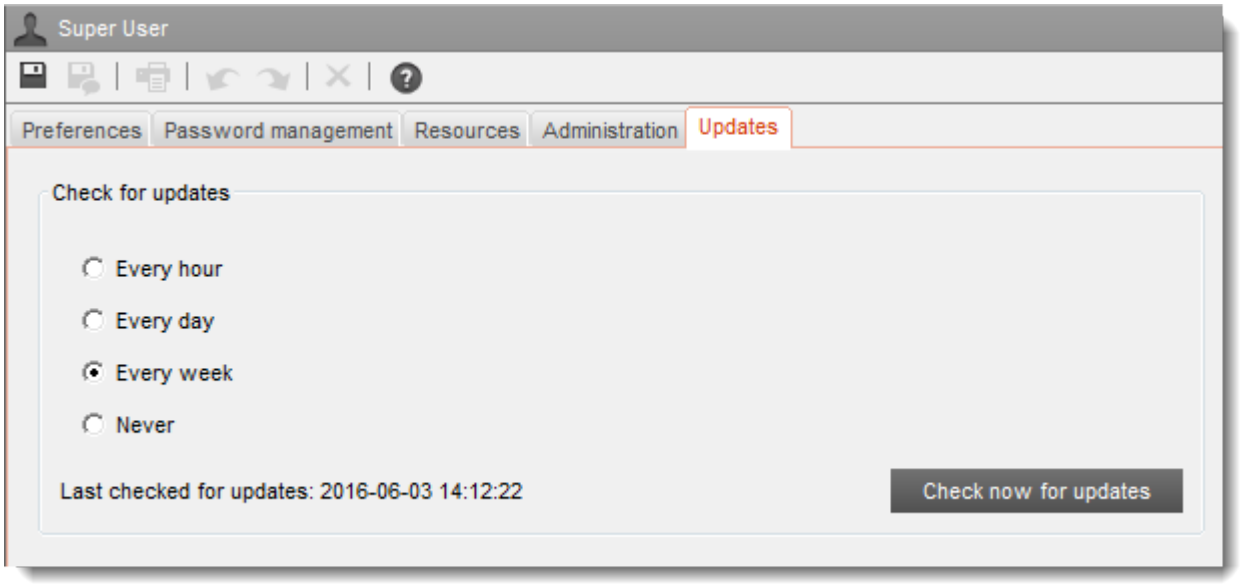
The purpose of this function is to provide a template for the creation of new *Users* in bulk. The template is a text file that is exported from IUCLID 6. The file contains only the headers described in the previous section. The details of the *Users* are entered in to the text file, which is then imported, as described in the next section.

This function is accessible from the main menu *Users*. The download of the file is done directly to a file, without any background job.

15.1.2.8. Import users

Data for *Users* can be imported into IUCLID 6 from a file that has the same format as that described in section *0 The feature Check for updates* may be used to instruct IUCLID 6 to send periodic automated requests to the IUCLID 6 web site to check whether a newer version of IUCLID 6 or its plugins is available. When IUCLID 6 detects that a newer version is available, it will notify the *User* in the message window. If an attempt to make a check gives an error message, check the internet connection and proxy settings on the host computer.

To check immediately whether the installation of IUCLID 6 or its plugins contain the most recent version, click on the button *Check now for updates*, shown in the figure below.



If an update is available, go to the downloads section of the IUCLID 6 web site, select the option for the appropriate *Updater tool* for the system, and then follow the instructions.

Note that update process updates both the application and its plugins. There are no separate updates to be done for plugins.

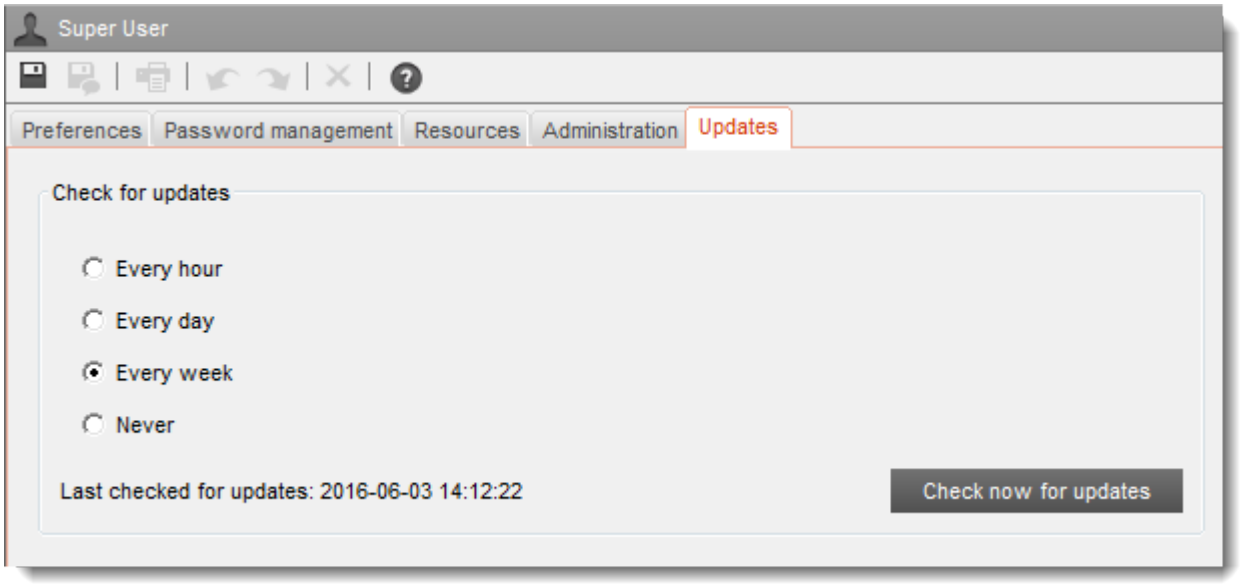
Export users. If a *User* already exists, as identified by the value of the field *username*, the data in IUCLID 6 is over-written by the data from the imported file. If a *User* does not already exist, it is created using the data from the file. This feature can be used to create many *Users* in a single action. *Users* created in this manner have an initial password of “Chang3m3”, without the quotes. Importing *User* data cannot be used to edit the current *User*.

Note that *Users* imported by the installer for IUCLID 6 Desktop are given the password “changeme”, without the quotes, which must be changed on first logging in.

This function is accessible from the main menu *Users*. Select a file and then click *Finish*. The import is carried out as a background job, as described in section *1.7.3 Background jobs*.

If there is an error message about file formatting, check the file against the format described in section *0 The feature Check for updates* may be used to instruct IUCLID 6 to send periodic automated requests to the IUCLID 6 web site to check whether a newer version of IUCLID 6 or its plugins is available. When IUCLID 6 detects that a newer version is available, it will notify the *User* in the message window. If an attempt to make a check gives an error message, check the internet connection and proxy settings on the host computer.

To check immediately whether the installation of IUCLID 6 or its plugins contain the most recent version, click on the button *Check now for updates*, shown in the figure below.



If an update is available, go to the downloads section of the IUCLID 6 web site, select the option for the appropriate *Updater tool* for the system, and then follow the instructions.

Note that update process updates both the application and its plugins. There are no separate updates to be done for plugins.

Export users. If there are any errors at all, the import process is completely abandoned, so that there is never any partial import of *User* data. This is deliberate, to avoid the corruption of personal data.

If the import is reported as a success, go to the *User management* window to confirm that.

Technical tip: The character encoding must be *UTF-8 without BOM*. A control character such as double quote (") or back slash (\), can be escaped with a back slash, therefore (\\) is imported as (\). A new line in the remark field can be entered using \n.

15.2. Role

A *Role* is a data object that defines a set of permissions that control the access a *User* has to functions and data within IUCLID 6. A *User* can have more than one *Role* at the same time, in which case, permissions are additive. For example, if a *User* has two *Roles*, one of which permits printing, whereas the other does not, the *User* can access the print function.

15.2.1. General

Role is the name of the *Role* used to identify it throughout the system. It can contain up to 255 characters.

Role description is a free text field provided to allow the purpose of the *Role* to be documented. It can contain up to 2,000 characters.

The field *assigned users*, lists the *Users* that have the selected *Role*, and provides a means of adding the *Role* to *Users*, via the buttons *Add* and *Remove*. The assignment of *Roles* to *Users* can

also be done per *User* under the *Administration* tab of *User*. A *User* can assign only *Roles* that are assigned to it.

15.2.2. Permissions

Here, the level of access to functions that directly affect entities is defined.

15.2.2.1. Access to operations

Control of access to the functions *Print*, *Export* and *Import* is set globally for all entities by ticking the relevant box.

15.2.2.2. Access to entities and inventories

Here, access can be defined per type of entity, for example for all *Mixtures*. Clicking on a field opens a drop-down menu of the types of access available: **no access**, **read**, **read/write**, **read/write/delete**.

If instance based security (IBS) is in use, the access must also be allowed through either ownership, or sharing within a *Group*.

15.2.2.3. System administration and configuration

15.2.2.3.1. Manage roles

Here, access can be defined to the entity *Role*. Clicking on the field opens a drop-down menu of the types of access available: **no access**, **read**, **read/write**, **read/write/delete**.

15.2.2.4. User management

Here, the level of access to functions that directly affect *Users* is defined.

15.2.2.4.1. Manage users

Here, access can be defined to the entity *User*. Clicking on the field opens a drop-down menu of the types of access available: **no access**, **read**, **read/write**, **read/write/delete**.

15.2.2.4.2. Assign Legal entities to users

This right permits a *User* to assign a *Legal entity* to a *User*. A *User* can assign only *Legal entities* that have first been assigned to it. Note that to assign a *Legal entity*; a *User* must have write access to that *User*.

15.2.2.4.3. Assign Roles to users

This right permits *Roles* to be added to *Users*.

15.2.2.4.4. Remove Roles from users

This right permits *Roles* to be removed from *Users*.

15.2.2.5. IBS management

These fields are shown only if instance based security (IBS) is on.

15.2.2.5.1. Manage Groups

Here, access can be defined to the entity *Group*. Clicking on the field opens a drop-down menu of the types of access available: **no access**, **read**, **read/write**, **read/write/delete**.

15.2.2.5.2. Assign users to groups

This right permits change of *Group* membership.

15.2.2.5.3. Manage private groups

This right permits change of ownership of a document.

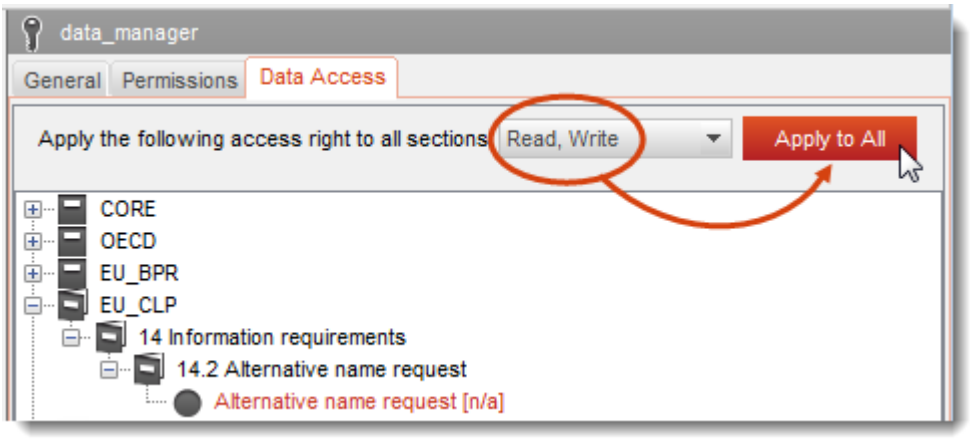
15.2.2.6. Plugin configuration

These fields control access to each individual plugin. If access is denied, the plugin icon on the home page is not clickable, and the option is not shown in the right-click menu.

15.2.3. Data access

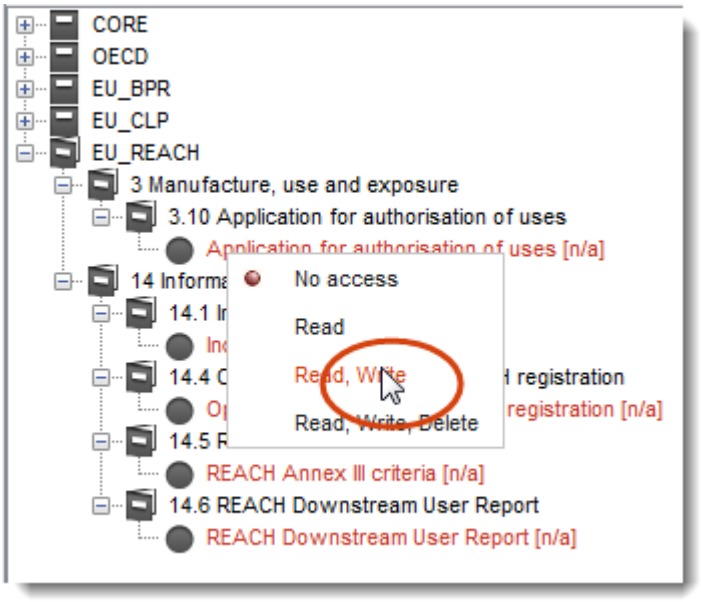
Here, access to data in *Substances* can be controlled at the level of section. The sections are shown in the default tree structure. Access rights can be set to one of the following values: *no access*, *read*, *read/write*, or *read/write/delete*. For a newly created Role, by default, the access is set to *no access* for all sections. Rights can be set either to all sections in one action, or per section. To set all sections to the same level of access, select a value from the drop-down menu, and then click *Apply to All*, as shown below:

Figure 77: Change access rights for all sections for a Role



To set access for an individual section, right-click in the section tree on the section's endpoint study or endpoint study summary, and then select a value from the drop-down menu. An example is shown below for *Application for authorisation of uses*:

Figure 78: Change access rights to an individual section for a Role



The level of access per section is indicated in the tree by appending a code after the section name and colouring the name as indicated in the table below:

Table 5: Indication of access rights for documents

Access	Colour	Code
no access		[n/a]
read		[r/]
read/write		[r/w]

Access	Colour	Code
read/write/delete	■	[r/w/d]

The rights defined here apply across all documents of type *Substance*. If instance based security (IBS) is in use, the access to a particular document must also be allowed through either ownership, or sharing within a *Group*.

15.2.4. Built-in roles

IUCLID 6 is supplied with various *Roles* built in for the convenience of users. Built-in *Roles* can neither be edited nor deleted. IUCLID 6 Desktop is delivered with the roles *System administrator*, *Full access* and *Read-only*. The possible built-in *Roles* are described below.

15.2.4.1. System administrator

Grants all possible permissions. Applying this *Role* gives the *User* the same permissions as the built-in *User*, SuperUser.

15.2.4.2. Full access

Grants read, write and delete access to all data such as *Substances* and *Dossiers*, but not administrative data

15.2.4.3. Read-only

Grants read access to all data such as *Substances* and *Dossiers*, but not administrative data.

15.2.4.4. User manager

This Role is available only when IUCLID 6 is used in a multi-*User* environment, hosted on a server. It grants only the permission to manage *Users*. There is no read-access to other types of data such as *Substances* and *Dossiers*.

If instance based security (IBS) is on it allows the *User* to determine the group membership of other *Users*. It does not permit the creation of *Groups*. For a description of IBS, see section 15.3 Instance based security (IBS).

15.2.4.5. Group manager

This *Role* is available only when instance based security (IBS) is on. For a description of IBS, see section 15.3 Instance based security (IBS).

It grants the permission to create, modify and delete *Groups*, and to be made a *Group manager* by an existing manager of a *Group*. The role *Group manager* does not give a *User* the automatic right to manage all *Groups*.

15.3. Instance based security (IBS)

IBS is intended for use with only *IUCLID 6 Sever*, not with *IUCLID 6 Desktop*. If IBS is not available and you think it should be, contact the system administrator of the instance of *IUCLID 6 Server*.

Instance based security allows access within IUCLID 6 to be controlled per document per *User*. Access can be controlled on a personal level by providing each person who uses an instance of IUCLID 6 with a unique *User*. In a large organisation with a centralised IUCLID 6 database that contains data held for a range of different purposes, it is often required to divide access to the data amongst different groups of people. IBS provides the entity *Group*, which is simply a collection of *Users*. A *User* can be in more than one group at the same time. *Groups* are used to organise access to data. They are also a convenient way to give access to more than one *User* in a single action.

For example, if all members of a particular team in an organisation need the same access to a subset of a centralised database, they may all be given their own personal *User*. The *Users* are then placed in a *Group*, and then the data is shared across the *Group*.

The levels of access that can be applied to a document under IBS are:

No access, Read, Read/Write, or Read/Write/Delete

Access to a document can be determined in four ways:

1. on creation of the document according to the settings in *Resources* under *User*;
2. on importation into IUCLID 6;
3. manually via the function *share*;
4. by a change of ownership.

The four methods listed above are controlled from different points within the IUCLID 6 interface, but they all have the same effect. The access for a particular document may be determined by any combination of these types of action. The functions and concepts supplied by IBS are described in the subsections that follow this introduction.

The entities and functions associated with IBS such as *Group* and *share* are available only whilst IBS is turned on.

IBS offers such a wide range of possibilities that in many installations of IUCLID 6 only a subset will be required. To obtain the expected results, it is recommended to create a documented policy of how IBS is used.

15.3.1. Group

A *Group* is a data object in IUCLID 6 that is a collection of *Users*. A *User* can be in more than one *Group* at once. If a particular type of access to a document has been shared to a *Group*, all members of the *Group* have that access. A *Group* can have one or more *Group managers*. The group management window under the tab *Groups*, shows a list of *Users* and indicates whether they are a *Group manager*. *Users* can be added and removed from the *Group* using the relevant buttons. A *User* is made a manager of a *Group* by being a member of the *Group*, having group management rights, and by having the checkbox ticked in the column *Manager*.

15.3.1.1. Common

Common can be considered to be a *Group* to which all *Users* belong. In that sense, *common* has the same meaning as *public*. In contrast, a *Group* created within IUCLID 6 is inherently *private*, because only members of the *Group* have access to the data shared within the *Group*.

15.3.2. Ownership

When a document is created or imported, its ownership is set to that of the current *User*. Ownership is transferable, but a document can have only one owner at a time; see the section below *Change ownership*. Ownership is accessible via the interface of IUCLID 6 only if IBS is on.

The search function in the navigation panel allows the search results to be filtered by owner. All the search results owned by the current *User* can be viewed by selecting the search criterion **Owned by me**. To view other documents, select **Owned by others**. Note that all the search criteria defined in the search function are applied at once.

15.3.2.1. Change ownership

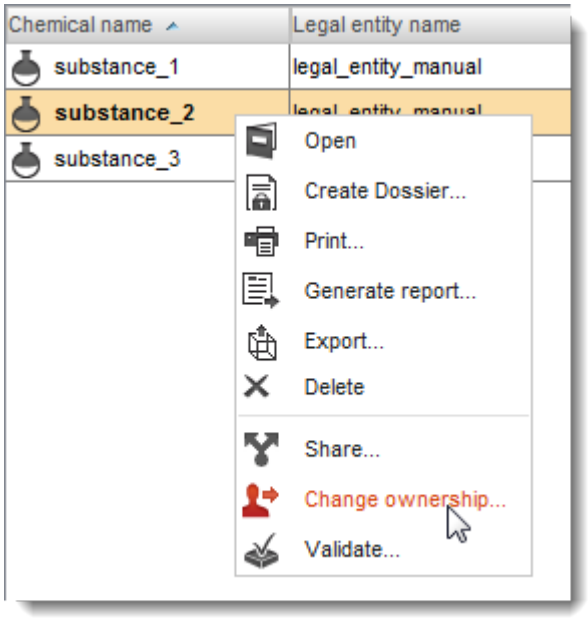
Ownership can be transferred only within the group of the owner, and only by a manager of the group. To change ownership, a *User* must have either the built-in role, *Group manager* or a custom role with at least the following rights.

Table 6: Rights of a group manager

Field	Value
Access to entities and inventories	Read all
Manage users	Read
Manage groups	Read
Manage private groups	yes

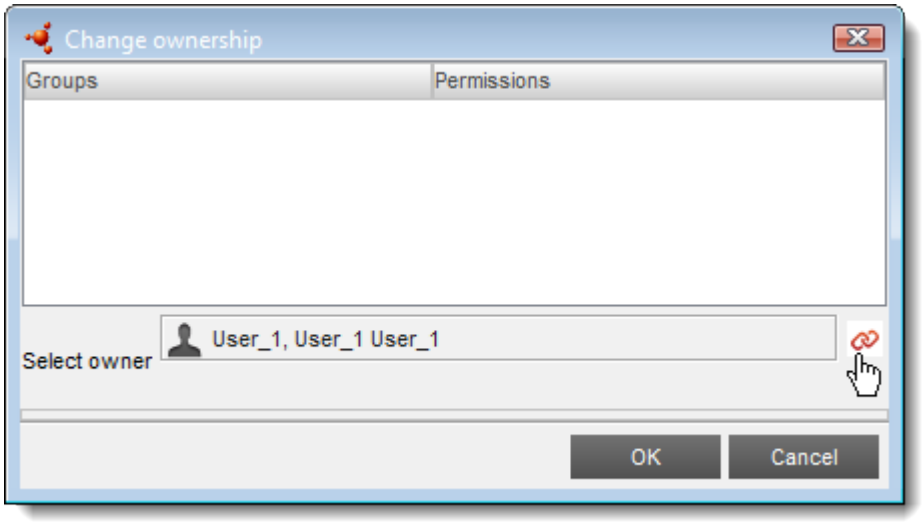
Change of ownership of a document is accessed by right-clicking on the record of the document in the search results, as shown below.

Figure 79: Open the function for changing ownership



This opens a window that states the sharing of the document per group, and the name of the *User* that owns the document. To change the ownership, click on the chain-link icon, search for the new *User*, select it, and then click the assign button, as shown below.

Figure 80: Select a different User as the owner of a document



The ownership of more than one entity can be changed in a single action by first making a multiple selection of entity records. That can be done using either of the standard methods of: shift-click and/or control-click.

15.3.3. Share

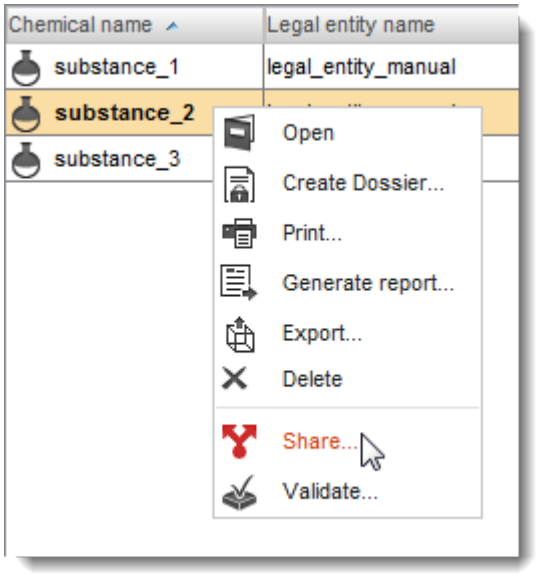
Share is an action in which access is granted manually to a document for the *Users* in a *Group* or *Groups*. This over-rides any access defined at the time of creation or importation of the document. The function share allows one of the following four states to be applied to a document per *Group*:

Not Shared, **Read**, **Read/Write**, or **Read/Write/Delete**

A share can be applied by the owner of a document, and any *Group manager* of any *Group* to which the owner belongs. Thus, a share can be applied to the *common* group to which all *Users* belong.

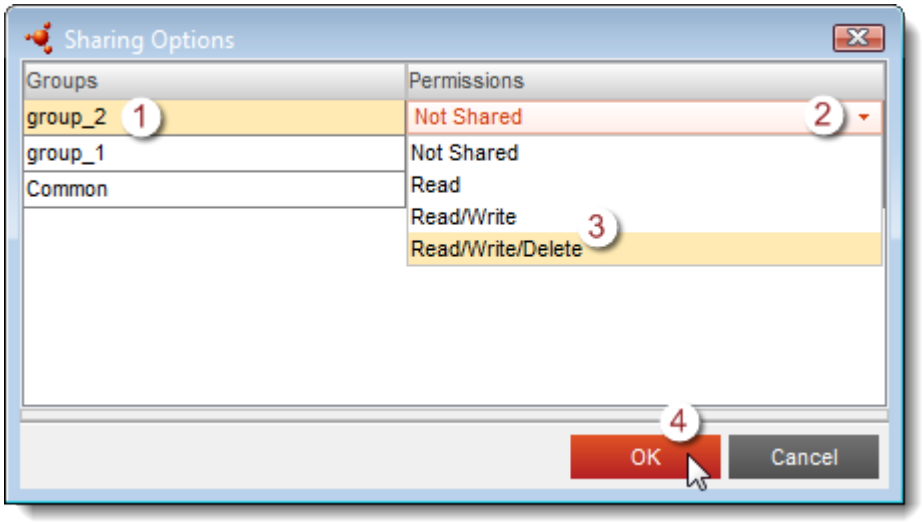
The option to share a document is accessed by right-clicking on the record of the document in the search results, as shown in the figure below. Sharing via the right-click method can be done for a multiple selection of documents.

Figure 81: Opening the sharing function



The sharing options window presents a table with two columns, *Group* and *Permissions*. The column *Group* contains a list of the *Groups* to which the *User* applying the share has access. The column *Permissions* states the access per *Group*. To change an access per group, click in the column *Permissions* next to the required *Group*. Select from one of the four possible levels of access, as shown below.

Figure 82: Setting the sharing of one or more documents



When a *User* creates a document, it inherits the sharing defined per *User* under the IUCLID 6 section User / Resources. When a *User* imports a document, the *User* can choose to over-ride the default settings during the import process. For example, if the default resource settings do not provide the required access to a document for a particular *Group*, the access can be changed manually using the *share* function.

If a *User* has access to a document only because it has been *shared*, it cannot pass that access on via sharing.

15.3.4. Exercise on IBS

The following exercise provides a brief introduction to IBS by actually using it. If the concepts and terminology of IBS are not clear to you, try doing the exercise.

Prerequisites:

Ensure that IBS is active. Log in as SuperUser. Create two *Groups* named: group1 and group2. Create four new *Users* named: userA, userB, userC, and userD. Set the properties of the *Users* as shown in the table below. Ensure that all four *Users* have the same *Legal entity*. Under the tab *Resources*, ignore the default values for *Literature references* and *Import*. For *Substances*, add the values shown below.

Table 7: IBS exercise - properties of Users

User	Role	Group	Legal Entity	Resources \ Substances
userA	Full Access	group1	<same as other *Users*>	group1(rwd)
userB	Full Access	group1	<same as other *Users*>	Common(rwd), group1(rwd)
userC	Full Access	group2	<same as other *Users*>	group2(rwd)
userD	Full Access		<same as other *Users*>	

In the following exercises, find out the access rights of the *Users* by logging in as the relevant user, and then trying in the interface to read, write and delete the documents, for example, *Substance* and *Dossiers*.

action 1: userA creates Substance1, and then Dossier1 from Substance1.

result 1: The following access has been granted.

Table 8: IBS exercise - result 1

User	Substance1	Dossier1	Comment
userA	(rwd)	(rwd)	userA created both documents and therefore owns them. Ownership gives full access.
userB	(rwd)		userB is in group1. The settings under *Resources* \ *Substance* for userA mean that when userA creates a *Substance*, all members of group1 are automatically given rwd rights to it. No rights are given for *Dossiers*.
userC			There are no settings under *Resources* for userA that automatically confer access rights to userC for *Substances* or *Dossiers*.
userD			There are no settings under *Resources* for userA that automatically confer access rights to userD for *Substances* or *Dossiers*.

action 2: userB creates Substance2, and then Dossier2 from Substance2.

result 2: The following access has been granted.

Table 9: IBS exercise - result 2

User	Substance2	Dossier2	Comment
userA	(rwd)		userA is in group1. The settings under *Resources* \ *Substance* for userB mean that when the *User* creates a *Substance*, all members of group1 are automatically given rwd rights to it. No rights are given for *Dossiers*.
userB	(rwd)	(rwd)	userB created both documents and therefore owns them. Ownership gives full access.
userC	(rwd)		The setting *Common(rwd)* under *Resources* \ *Substance* for userB mean that when the userB creates a *Substance*, all *Users* are automatically given rwd rights to it. No rights are given for *Dossiers*.
userD	(rwd)		The setting *Common(rwd)* under *Resources* \ *Substance* for userB mean that when the userB creates a *Substance*, all *Users* are automatically given rwd

			rights to it. No rights are given for *Dossiers*.

action 3: userA checks what *Substances* can be shared by right-clicking on the records in the search results list in the *Navigation panel*.

result 3: The sharing allowed is shown below.

Table 10: IBS exercise - result 3

Substance	Groups under sharing	Permissions under sharing	Comment
Substance1	group1	(rwd)	userA owns Substance1. userA is in group1. Therefore, userA can edit the permissions for group1. Being able to change these permissions confers the ability to *share* the document. The permissions are rwd because the settings under *Resources* \ *Substance* for userA mean that when userA creates a *Substance*, all members of group1 are automatically given rwd rights to it.
	Common		userA owns Substance1. All users are in group Common. Therefore, userA can edit the permissions for group Common. Being able to change these permissions confers the ability to *share* the document. There are no permissions because the settings under *Resources* \ *Substance* for userA mean that when userA creates a *Substance*, not all *Users* are automatically given rwd rights to it.
Substance2			No sharing is allowed because userA does not own Substance2.

action 4: userB checks what *Substances* can be shared by right-clicking on them.

result 4: The sharing allowed is shown below.

Table 11: IBS exercise - result 4

Substance	Groups under sharing	Permissions under sharing	Comment
Substance1			No sharing is allowed because userB does not own Substance1.
Substance2	group1	(rwd)	userB owns Substance2. userB is in group1. Therefore, userB can edit the permissions for group1.

Substance	Groups under sharing	Permissions under sharing	Comment
			Being able to change these permissions confers the ability to *share* the document. The permissions are rwd because the settings under *Resources* \ *Substance* for userA mean that when userB creates a *Substance*, all members of group1 are automatically given rwd rights to it.
	Common	(rwd)	userB owns Substance2. All users are in group Common. Therefore, userB can edit the permissions for group Common. Being able to change these permissions confers the ability to *share* the document. The permissions are rwd because the settings under *Resources* \ *Substance* for userB mean that when userB creates a *Substance*, all *Users* are automatically given rwd rights to it.

action 5: Log out. Log in as SuperUser. Change the ownership of Substance1 from userA to userB. The ownership of a document is changed by right-clicking on the entry for the document in the search window, and then selecting *Change ownership*. Log out. Log in as userA. Check what can be shared.

result 5: Neither Substance1 nor Substance2 can be shared. This is because userA owns neither of the *Substances*. Dossier1 can be shared because userA still owns it.

action 6: Log out. Log in as userB. Check what *Substances* can be shared.

result 6: Substance1, Substance2 and Dossier2 can be shared because userB own them.

action 7: userB shares Substance1 with Common(r). To do that, first right-click on the entry for the document in the search window, and select *Share*. Then, in the table that appears, on the row that has a value of Groups equal to Common, click in the cell for the field Permissions, and then select the value Read.

result 7: What are the access rights of *Users* to Substance1?

Table 12: IBS exercise - result 7

User	Access	Comment
userA	(rwd)	userA does not own Substance1 so it cannot share it, but it has rwd access because the User is in group1.
userB	(rwd), share	userB owns Substance1. Ownership gives full access,

		including sharing.
userC	(r)	Previously userC had no access rights, but now the userC can at least read the document because all *Users* have been granted that right as part of this exercise.
userD	(r)	Previously userD had no access rights, but now userD can at least read the document because all *Users* have been granted that right as part of this exercise.

action 8: Log out. Log in as SuperUser. Add userD to group1.

result 8: userD gains rwd access to Substance1 because all members of group1 have it. There are no other changes.

action 9: Log out and then log in as userB. Remove all sharing for Substance2.

result 9: UserA, userC and userD cannot see Substance2 in the user interface, but userB can. UserB retains full access and can still share the document.

16. Import

IUCLID 6 allows you to import one or more of the following files into your IUCLID system; *Dossiers*, *Substances*, *Mixtures*, *Templates*, *Categories*, *Legal entities*, *Legal entity sites*, *Reference substances*, *Annotations*, *Contacts*, *Literature references*, *Attachments* and *Test materials*. You can import these files for the purpose of exchanging data between different IUCLID installations and importing previously exported data back into IUCLID.

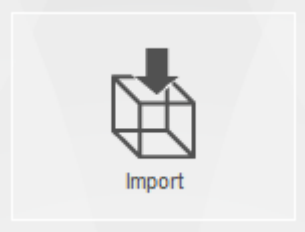
16.1. Important information on importing

As a starting point for importing files into IUCLID 6, please take note of the following:

1. You can only import files with the file name extensions **.i6z** or **.i5z** which have been exported from IUCLID 6 and the latest version of IUCLID 5 (version 5.6), as well as inventories with the file extension **.i6l**.
2. When you want to import two or more files, you can only import files with the same file extension (either i6z, i5z, or i6l). If you have files with different extensions, you will need to import these together in a separate import. Additionally, when you import an i5z file it will be automatically converted into a IUCLID 6 file with the i6z extension.
3. When importing i5z files, you will only be able to import the unzipped i5z file, which is an archive of all your stored records. For i6z files, as well as having the option to import the entire unzipped file, you can also select specific records within the i6z file which you would like to import.

16.2. How to Import

To import one or more files into IUCLID 6, click on **Import** in the **Administration** task panel found on the IUCLID 6 home page.



This will launch the **Import assistant** that will take you through to the end of the import process. Read the instructions below for a brief guide for using the Import assistant.

16.3. Step 1 of Import

When opening the Import assistant, first add the file or files you wish to import. Do this by clicking on *Add files…* and selecting from the popup browser the file(s) in your local IT environment you wish to import. When you have selected the file(s) you will see that the first field in the Import assistant will be populated with information about the file(s) you have selected using the following headings:

1. *Pathname* (the pathway to the location of your file on your local IT environment)
2. *Filename* (the full name of your file)
3. *Size* (byte size of the file)
4. *Modified* (date the file was last modified).

You can find further information about your selected file(s) by looking in the *Content* and *Remarks* tabs below the *Add files…* button.

You can remove any file during the Import assistant process by highlighting the file(s) you wish to remove so that they are coloured orange and clicking on the *Remove* button next to *Add files….* Note that any files you untick, using the checkbox in the *Import* column, will not be imported.

You can then select specific criteria which tell IUCLID how to treat the file(s) you wish to import if the same Universal Unique Identifier (UUID) for the file already exists in your IUCLID system. There are three criteria to select from;

5. *Always* (by selecting this criterion, the file(s) you have selected to import will replace any duplicated file which exists in your IUCLID system, i.e. any file with the same UUID as an existing document or dataset).
6. *Never* (by selecting this criterion, no existing dataset or document in your IUCLID system with the same UUID as the imported file will be imported).
7. *If newer than existing* (by selecting this criterion, the file to be imported will only be imported if it was modified more recently than the existing dataset or document in your IUCLID system).

If Instance Based Security (IBS) is enabled in IUCLID 6, a field is shown called *Default import pool*. For more information about IBS, see section 15.3 Instance based security (IBS). Default import

pool can be used to over-ride the default *Group* access settings for the current *User*. The field contains a drop-down menu that presents options for read, write and delete **<Group name> (R/W/D)** for each of the *Groups* of which the current *User* is a member. This includes the *Group* named *Common*. For example, if the default access for the *User* to the *Group* named *Common* is read-only, access to imported data can be set to read, write and delete by choosing the setting **Common** (R/W/D).

If you are importing an i6z file, you will have the option to untick the field named *Skip content verification (document selection screen).* By unticking this field, you will be able to define specific records within the file you would like to import (in the second step of the Import assistant). Note that this option is not available when importing two or more files.

16.4. Step 2 of Import

In S*tep 2* of the Import assistant (only available when importing a single i6z file), there are four panels of information. The first two panels are editable and are used to specify what you want to retain or omit in your imported file. The third and fourth panels are read-only information. These panels are described below.

8. The first panel called *Entities list* displays all the high-level entities (such as Legal entities, Contacts, Substances, Dossiers etc.) which are contained in the file. Each entity is by default ticked and selected to be imported. If you wish to omit any of these entities from your import, deselect them by unchecking the tick box in the column named **In**.
9. The second panel named *References to* displays the records which the high-level entity contains. Click on any high-level entity to view the records it contains. For instance, in this panel a dossier or a substance dataset will contain the entire section tree of records. Again, by default every record will be ticked and selected to be imported. If you wish to omit any specific record from your import, deselect them by unchecking the tick box. Note that in entities with section tree records you can uncheck the tick boxes for entire sections as well as individual sections.
10. The third panel named *Referenced from* displays the entities or records that are linked to the entity which you selected in the *first panel.* For instance, a contact in the first panel will be linked to a legal entity also displayed in the first panel, and you can view the legal entity affected in this third panel. This will give you a view of what entities are affected by deselecting any of the entities or records in the first and second panels.
11. The fourth panel named Final outcome displays what entities and records will be imported when you press Finish in the Import assistant.

From this point you can either click the Back button to change any fields in step 1 or you can click the Finish button to complete the import. Note that if you press Back, any changes you made in step 2 of the Import assistant will not be retained and you will need to make those changes again.

When the import is complete (whether successful or not) a popup notification appears on the bottom right-hand corner of the IUCLID 6 screen. You can click on this or the flashing red circle to show the *Background job console*. Here you can see if the import succeeded or failed. If you want to know more detailed information about the import, double click on the red bar to bring up the *Import Log*.

17. Export

IUCLID 6 allows users to export the following entities, as well as the datasets or documents contained within them; *Legal entity, Legal entity site, Substance, Mixture, Template, Category, Dossier, Reference Substance, Contact, Annotation.* The function *Export* contains a wizard that provides context sensitive options in selecting what will be exported. Exporting can be done either in bulk or at a lower level, such as down to a single endpoint study record.

To launch the function *Export* for a single document that has a record in the search results, click on the export icon,  , located either just above the *Filter* function, or in the menu opened by right-clicking on the record. To export a single document that can be viewed from a table of contents (TOC), right-click on its entry in the TOC, and then select the export icon.

Bulk export can be launched from the main menu *File*, from the home page, or by making a multiple selection from the search results, and then launching *Export* in the same way as for a singular selection.

The advantage of *Bulk export*, is that you can export in bulk either *all dossiers, all substances, all mixtures, all categories, all templates,* or *all reference substances*. You can also export different dataset types in the one and same export, for instance a combination of substance datasets, mixture datasets and reference substances. Note that if you wish, you can also select single datasets or documents through the *Bulk export* (see manual selection below).

The advantage of *Export* of a single document is that you can quickly export a single specific dataset or document directly from where you are in the entity, for instance a single mixture dataset or a single endpoint study record. If the *Export* icon is clicked whilst more than one search record is selected in the *Navigation pane*, the wizard for *Bulk export* is opened.

17.1. Important rules when exporting

When you export from IUCLID 6 please note some important rules below that govern what is, and can be, exported:

1. To be able to export information and data from IUCLID you will need to be a user who has been assigned a role with access rights to export (set in the Permissions tab of Roles in User management). If you do not have these access rights, contact the user with system administrator rights to IUCLID who is responsible for assigning access rights to other users.
2. Only those entities, datasets and/or documents which directly reference (links to) other entities, such as when a substance references a contact, will these referenced entities also be exported.
3. As an addition to (a), the exported entity, dataset or document will not export an entity, document or dataset which it is referenced in or only indirectly linked to. For example, when a mixture is exported, a substance which is directly linked to that mixture will also be exported but not the category which is linked to the linked substance.
4. When exporting a document (flexible record or summary) that is part of a dataset, its parent entity (substance, mixture/product or template) is also exported. However, when you do export a document, no other document or template in that entity is exported.

5. Linked entities might be filtered out because of security or confidentiality claims (which is set in **User management** by a user with sufficient access rights), regardless whether the entity is a mandatory field or not.
6. An Inventory entry cannot be exported on its own and can only be exported with an entity that makes a reference to it.

17.2. How to use the Export assistant

The **Export assistant** can be generated by either clicking on **Bulk export** in the **Tools and administration** task panel on the IUCLID 6 front page or, by directly right-clicking on the specific dataset(s) or document(s) contained within these entities which you want exporting and then selecting *Export* from the menu. Below you can find guidelines on:

1. How to use the first step of a Bulk export using the Export assistant.
2. How to complete all other steps of the Export assistant process. This is divided between different entities.

Note that to define what is exported in the export assistant, in many steps of the export assistant process you will need to actively deselect what information and data you do not want to export.

17.3. Bulk export

The first step of the Export assistant process when launched from the Bulk export icon on the IUCLID 6 front page or when you directly *Export* two or more datasets or documents from an entity, is called *Step 1 – Document selection*. In this first step you can either:

1. Choose to export at the entity level all dossiers, all substances, all mixtures, all categories, all templates, or all reference substances, or;
2. Manually choose a specific dataset/document or multiple datasets/documents within an entity. With this option, you have the added flexibility of selecting different datasets from different entities, for example a dataset from both the substance and the mixture entities'.

For a) select the appropriate radial button next to the entity you wish to export. To opt for (b), select the radial button next to **manual selection** and then, below the **Document/Entity** results box, click the *Add…* button. This will generate a *Query* box where you can specify the dataset(s) and document(s) you wish to export. This Query box has four search fields to help you filter your selection as outlined and described below:

3. *Result type* – choose from the dropdown list of entities you wish to export.
4. *Query type* – choose from the search criteria you wish to search by and from the resulting choice, fill in some or all of the corresponding search fields to find the dataset you are looking for.
5. *UUID* (search only appears when *Document* is selected in *Result type*) – enter here the *Universal Unique Identifier* number of the dataset or document you are searching for. *Ownership* (this option only appears when *Instance Based Security* is switched on) – choose from two options:

6. *Owned by me* – this option only searches for the entities that are in your *private security pool*.
7. *Owned by others* – this option only searches for the groups you belong to or are a manager of and which are not in your *private security pool.*
8. *Group* (this option only appears when *Instance Based Security* is switched on) – choose from the groups listed in the dropdown box. When selecting a group, only the entries that are assigned to the selected group are displayed.

Note that when you intend to export an Endpoint Study Record, an Endpoint Summary, or a dataset using the bulk export assistant, you can only search for these documents using the query box and entering the Universal Unique Identifier number of the document in the UUID search field.

When you have filled in the search information in the Query box click *Search* to display the results or *Clear* to start the same search again. After pressing *Search* a list of results will be displayed in a results box with the information for each result divided into four columns; *Chemical Name, Legal entity name, Reference substance, Last modification date.* To quicken up your search you can also do a quick search using the information you would expect to appear in these four columns. To do this, type in the *Filter by representation* text box (found just above the search results), the first letters, numbers or words of the *Chemical Name, Legal entity name, Reference substance, Last modification date*. This will automatically generate and filter a list of results for you to choose from.

When you have finished your search using the Query box, click on the *Assign* button to populate the Document/Entity results list in the first step of the Export assistant. These will be the datasets and/or documents which will be exported. You can *Add* or *Remove* your selected datasets and/or documents at any time. If you directly export from an entity two or more datasets or documents the first step of the Export assistant will automatically populate the *Document/Entity* results list with your chosen datasets or documents. These results can be edited at any time of the Export assistant process through the *Add* and *Remove* buttons.

17.4. Export of Substances

When choosing *all substances* in the Bulk export option or when exporting a substance or substance(s) directly from the substance entity, the steps to follow in the Export assistant are the same except for the step called *Verify selected documents: Verify the selected documents or select/deselect as appropriate.* This step only appears when exporting a single dataset or document and allows you to deselect entities and documents which are referenced by your substance, for example a *Legal entity* or an endpoint study record.

17.4.1. Select submission type

This step of the Export assistant (the first step for single exports, the second step for bulk exports) has two options as distinguished by the two tabs at the top-left hand corner of the screen; *Substance* and *Use related categories*.

The Substance tab allows you to define by submission type what substance will be exported. For instance, if the substance(s) you are exporting have been assigned to a particular substance type such as *BPR Active substance application*, only the substance(s) with this submission type will be selected in the Export assistant. Select your submission type by clicking on the radio button next to

the submission type you wish to export. Your selection will be displayed in the information area of every step that follows in the Export assistant process.

The Use related categories tab allows you to specify whether category-related information should be used in your export. This option only involves substances that are related to a category and only when you have at least Read access to Categories.

There are three options to choose from:

1. *Yes* (selected by default) – click this option to export all the data related to all categories the substance is linked to.
2. *No* - click this option to not include in your export any categories and their related information.
3. *Select category(ies)* - when this option is checked, a panel containing all related categories is displayed. From this list of related categories you can select one or more categories by clicking on them. Only the categories selected are included in the export.

17.4.2. Data protection flags

This step helps you to define what confidential information you wish to include in your export.

1. The first option named *Detail level of document fields* provides you with three preferences to choose from:
   a. *All fields, including confidential test material information* - Choose this option if you want all fields and all test material information to be exported.
   b. *All fields, excluding confidential test material information* - Choose this option if you want all fields to be exported but to exclude all test material information.
   c. *Basic level* - Choose this option if you want only 'basic' fields to be included in your export. Basic fields include every field *except* for the endpoint study records in the following IUCLID sections under the OECD legislation; *Physico-chemical properties, Analytical methods, Degradation and accumulation, Effects on biotic systems, Efficacy, Health effects, Pesticide residue chemistry*.
2. The second option named *Confidentiality* is where you choose what information will be exported.
   All confidential information is automatically selected to be exported. To pick and choose what confidential information you want exporting click on the dropdown box and deselect from the list of options what flagged fields you do not want to export:
   CBI – confidential business information
   IP – intellectual property
   No PA – not publicly available
   You can also choose to only export confidential information by deselecting the *Not confidential* box.
3. The third option named *Use restricted to selected regulatory programmes* allows you to define what regulatory purposes, if any, have been assigned to the substance(s) you are exporting and you wish to export.
   From the drop down box you will open a list of regulatory programmes. All regulatory

programmes are automatically selected to be exported. Deselect the regulatory programmes that you do not want to be included in your export.
You can also deselect *No regulatory purposes* from the drop down list which will export any field in your substance entity that was not flagged with a regulatory programme.

17.4.3. Administrative data properties

This step allows you to define in more detail your export through various elements of your substance data as outlined below:

1. Robust study summary
   The dropdown box automatically selects to export all fields where details of a *Robust study summary* were entered in the entities, datasets or documents you are exporting. You can deselect *Yes* to exclude any field where robust study summary information was entered. You can deselect *No* to include only fields where robust study information was given. You can deselect *Where Robust study summary is not applicable (e.g. endpoint summaries)* to exclude any field where robust study summary is not applicable.
2. Used for classification
   The dropdown box automatically selects to export all fields where details of *Used for classification* were entered. You can deselect *Yes* to exclude any field where robust study summary information was entered. You can deselect *No* to include only fields where robust study information was given. You can deselect *Where Used for classification is not applicable (e.g. endpoint summaries)* to exclude any field where robust study summary is not applicable.
3. Used for MSDS
   The dropdown box automatically selects to export all fields where details of *Used for MSDS* were entered. You can deselect *Yes* to exclude any field where robust study summary information was entered. You can deselect *No* to include only fields where robust study information was given. You can deselect *Where Used for MSDS is not applicable (e.g. endpoint summaries)* to exclude any field where robust study summary is not applicable.
4. Purpose flag
   The dropdown box automatically selects to export every field where the following Purpose flags were entered; key study, supporting study, weight of evidence, disregarded study, where purpose flag is empty, where purpose flag is no applicable. Deselect any of these options to not export the corresponding purpose flag.
5. Data waiving
   The dropdown box automatically selects to export every field where *Data waiving* data was entered such as *Study not technically feasible* or *Exposure considerations.* To not export this information, deselect the corresponding box.
6. Study result type
   The dropdown box automatically selects to export every field where a *Study result type* was entered such as *Experimental result* or *Read-across based on grouping of substances (category approach).* To not export this information, deselect the corresponding box.
7. Reliability
   The dropdown box automatically selects to export every field where *Reliability* data was

entered such as *reliable without restrictions* or *not assignable.* To not export this information, deselect the corresponding box.

17.4.4. Settings

This step allows you to select whether you wish to include or exclude *Attachments* and *Annotations* which are linked to the substance(s) you are exporting. You can only select one preference from the options in *Annotations* and *Attachments.* Note that the default selection includes all related annotations and to not export your attachments.

17.4.5. Verify selected documents (only for single exports)

This step only appears when exporting a single dataset or single document.

You will see that there are four panels of information. The first two panels are editable and are used to specify what you want to retain or omit in your exported file. The third and fourth panels are read-only information. All these panels are described below.

1. The first panel called *Entities list* displays all the high-level entities (such as Legal entities, Contacts etc.) which are contained in the file. Each entity is by default ticked and selected to be exported. If you wish to omit any of these entities from your export, deselect them by unchecking the tick box in the column named *In*.
2. The second panel named *References to* displays the records which the high-level entity contains. Click on any high-level entity to view the records it contains. For instance, in this panel a dossier or a substance dataset will contain the entire section tree of records. Again, by default every record will be ticked and selected to be exported. If you wish to omit any specific record from your export, deselect them by unchecking the tick box. Note that in entities with section tree records you can uncheck the tick boxes for entire sections as well as individual sections.
3. The third panel named *Referenced from* displays the entities or records that are linked to the entity which you selected in the first panel. For instance, a contact in the first panel will be linked to a legal entity also displayed in the first panel, and you can view the legal entity affected in this third panel. This will give you a view of what entities are affected by deselecting any of the entities or records in the first and second panels.
4. The fourth panel named Final outcome displays what entities and records will be exported when you have finished and pressed *Finish* in the Export assistant.

17.4.6. Enter additional administrative information

Enter here in the *Remarks* box (maximum 32,365 characters) any comments you wish to adjoin to your export.

17.4.7. Select the folder of the exported files

In this final step you can specify the location on your local IT environment where your export will be saved. Click on *Browse* to select the destination of your export.

To help you manage the file structure of the export, you can also use the option to *create new subfolder after* [X number of] *files.* This option is used for older file systems that cannot support a large amount files per folder. The default number for this option is 1000 but this value can be changed to any number between 500 and 10000.

17.5. Export of Mixture/Products

The export of mixtures has many similar steps to the export of substances. Where there is overlap between the two types of export, the guidance text below will provide a link to the section where it is fully described as well as pointing out any differences, should they exist, between the two types of export.

17.5.1. Select submission type

The Select submission type step is similar to the equivalent step when exporting substances but with two differences:

1. There is a reduced list of submission types to select from in accordance with what submission types are available for mixture/product datasets.
2. There is an added option called *use mixture components*. Here you can select *Yes* to include all endpoint data from the entities which are linked to the mixture/product will be exported. If you select *No*, this same endpoint data will not be exported.

17.5.2. Data protection flags

See the section Data protection flags

17.5.3. Administrative data properties

See the section Administrative data properties

17.5.4. Settings

See the section Settings

17.5.5. Verify selected documents (only for single exports)

See the section Verify selected documents

17.5.6. Enter additional administrative information

See the section Enter additional administrative information

17.5.7. Select the folder of the exported files

See the section Select the folder of the exported files

17.6. Export of Categories

The export of categories has many similar steps to the export of substances. Where there is overlap between the two types of export, the guidance text below will provide a link to the section where it is fully described as well as pointing out any differences, should they exist, between the two types of export.

17.6.1. Select submission type

The Select submission type step is similar to the equivalent step when exporting substances but with one difference. There is a reduced list of submission types to select from in accordance with what submission types are available for categories.

17.6.2. Data protection flags

This step is the same as when exporting substances but with one difference. There is no option to define what test material, if any, is also exported. See the section Data protection flags for a description of this step.

17.6.3. Administrative data properties

See the section Administrative data properties

17.6.4. Settings

See the section Settings

17.6.5. Verify selected documents (only for single exports)

See the section Verify selected documents

17.6.6. Enter additional administrative information

See the section Enter additional administrative information

17.6.7. Select the folder of the exported files

See the section Select the folder of the exported files

17.7. Export of Templates

The export of templates has many similar steps to the export of substances. Where there is overlap between the two types of export, the guidance text below will provide a link to the section where it is fully described as well as pointing out any differences, should they exist, between the two types of export.

17.7.1. Select submission type

See the section Select submission type

17.7.2. Data protection flags

See the section Data protection flags

17.7.3. Administrative data properties

See the section Administrative data properties

17.7.4. Settings

See the section Settings

17.7.5. Verify selected documents (only for single exports)

See the section Verify selected documents

17.7.6. Enter additional administrative information

See the section Enter additional administrative information

17.7.7. Select the folder of the exported files

See the section Select the folder of the exported files

17.8. Export of Reference substances

The export of reference substances has many similar steps to the export of substances. Where there is overlap between the two types of export, the guidance text below will provide a link to the section where it is fully described as well as pointing out any differences, should they exist, between the two types of export.

17.8.1. Data protection flags

This step is the same as when exporting substances but with one difference. There is no option to define what test material, if any, is also exported. See the section Data protection flags for a description of this step.

17.8.2. Settings

See the section Settings

17.8.3. Enter additional administrative information

See the section Enter additional administrative information

17.8.4. Select the folder of the exported files

See the section Select the folder of the exported files

17.9. Export of Dossiers

The export of dossiers has many similar steps to the export of substances. Where there is overlap between the two types of export, the guidance text below will provide a link to the section where it is fully described as well as pointing out any differences, should they exist, between the two types of export.

17.9.1. Settings

This step is the same as for substances, see the Settings section above, but does not provide the option for exporting attachments.

17.9.2. Enter additional administrative information

See the section Enter additional administrative information

17.9.3. Select the folder of the exported files

See the section Select the folder of the exported files

17.10. Export of all other entities, datasets and documents

There are other entities, datasets and documents which you can export in addition to the principle entities above. These other entities, datasets and documents are only available to select and export through the manual selection option as described above or directly, by right-clicking on the documents or datasets themselves in the entity.

The Export assistant process is set out below for the remaining entities, datasets and documents and divided between the steps in the Export assistant process. The steps start from the second step of the Bulk export process and from the second step when exporting a single dataset or document directly from an entity. The process for exporting these is similar to the steps described above and where there is overlap, a link is given to the fuller description of what you can do in that step.

17.11. Export of Legal entities and Legal entity sites

The guidance text below will provide a link to the section where the step is more fully described as well as pointing out any differences, should they exist, in the particular step.

17.11.1. Data protection flags

This step is the same as described in the section Data protection flags but with one difference. No option exists to define what test material, if any, is also exported.

17.11.2. Settings

See the section Settings

17.11.3. Verify selected documents (only for single exports)

See the section Verify selected documents

17.11.4. Enter additional administrative information

See the section Enter additional administrative information

17.11.5. Select the folder of the exported files

This step is the same as described in the section Select the folder of the exported files, but does not give the option to create a subfolder after 500 or more files.

17.12. Export of Contacts

The guidance text below will provide a link to the section where the step is more fully described as well as pointing out any differences, should they exist, in the particular step.

17.12.1. Enter additional administrative information

See the section Enter additional administrative information

17.12.2. Select the folder of the exported files

See the section Select the folder of the exported files

17.13. Annotations

The guidance text below will provide a link to the section where the step is more fully described as well as pointing out any differences, should they exist, in the particular step.

17.13.1. Data protection flags

This step is currently empty, please press *Next*

17.13.2. Settings

This step is the same as described in the section Settings above, but with one difference. It only has the option for exporting or not exporting attachments with no option for exporting or not exporting annotations.

17.13.3. Verify selected documents (only for single exports)

See the section Verify selected documents

17.13.4. Enter additional administrative information

See the section Enter additional administrative information

17.13.5. Select the folder of the exported files

See the section Select the folder of the exported files

17.14. Endpoint records

The guidance text below will provide a link to the section where the step is more fully described as well as pointing out any differences, should they exist, in the particular step.

17.14.1. Data protection flags

See the section Data protection flags

17.14.2. Administrative data properties

See the section Administrative data properties

17.14.3. Settings

See the section Settings

17.14.4. Verify selected documents (only for single exports)

See the section Verify selected documents

17.14.5. Enter additional administrative information

See the section Enter additional administrative information

17.14.6. Select the folder of the exported files

See the section Select the folder of the exported files

18. Print

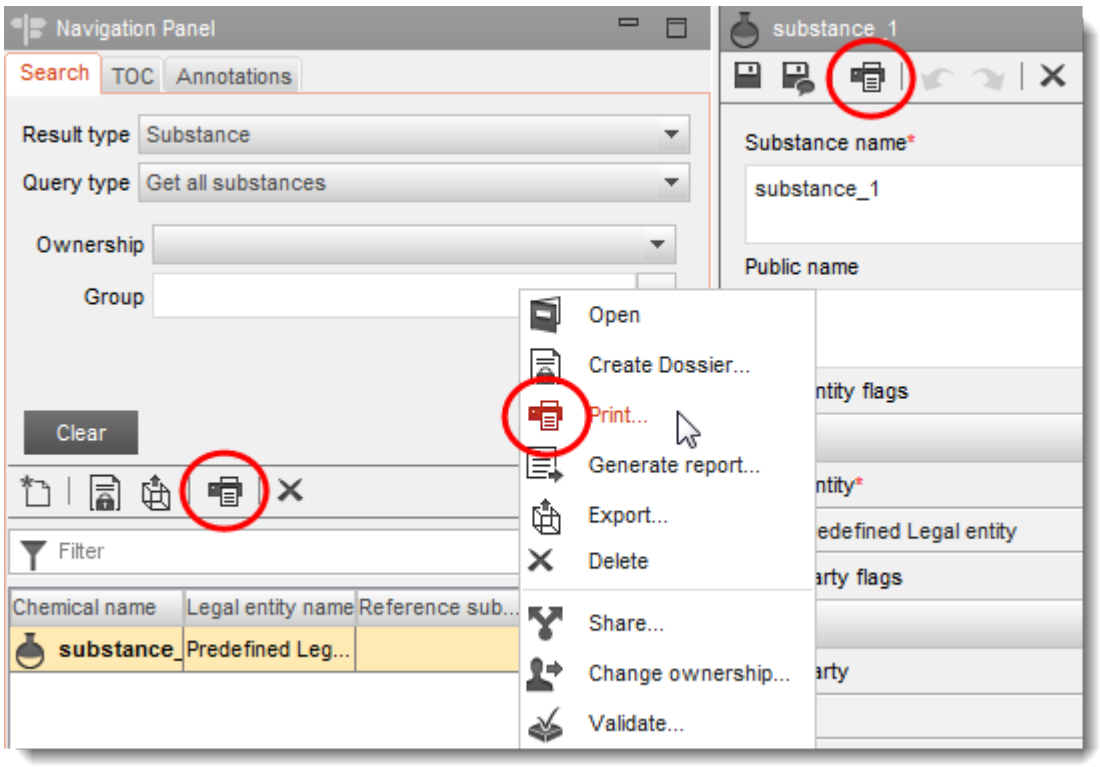
IUCLID 6 allows you to generate PDF documents and print the following files; *Substance datasets, Mixture/Product datasets, Templates, Categories, Dossiers, Endpoint study records, Endpoint summary records, Reference substances, Literature references, Legal entity sites, Legal entities, Contacts, Annotations, Test Materials.*

There are some important points to note before generating a PDF and printing;

1. You can only generate a PDF and subsequently print if your IUCLID user account is assigned to a role which has been given permission to print. This is set in the Permissions tab of Roles in **User management.**
2. You cannot print more than one of the above files at any one time. If you wish to print two separate endpoint summaries for example, you will need to generate two individual PDFs.
3. Any information which is flagged as confidential will be included in the PDF.
4. Any entities which are referenced by the dataset or document you print will also be included in the PDF. For instance, if you print a Category which is linked to a Legal entity, the Legal entity information will also be included in the PDF.
5. Inherited Endpoint study and summary records from a template cannot be printed individually, but are included in the PDF when printing an entire dataset.

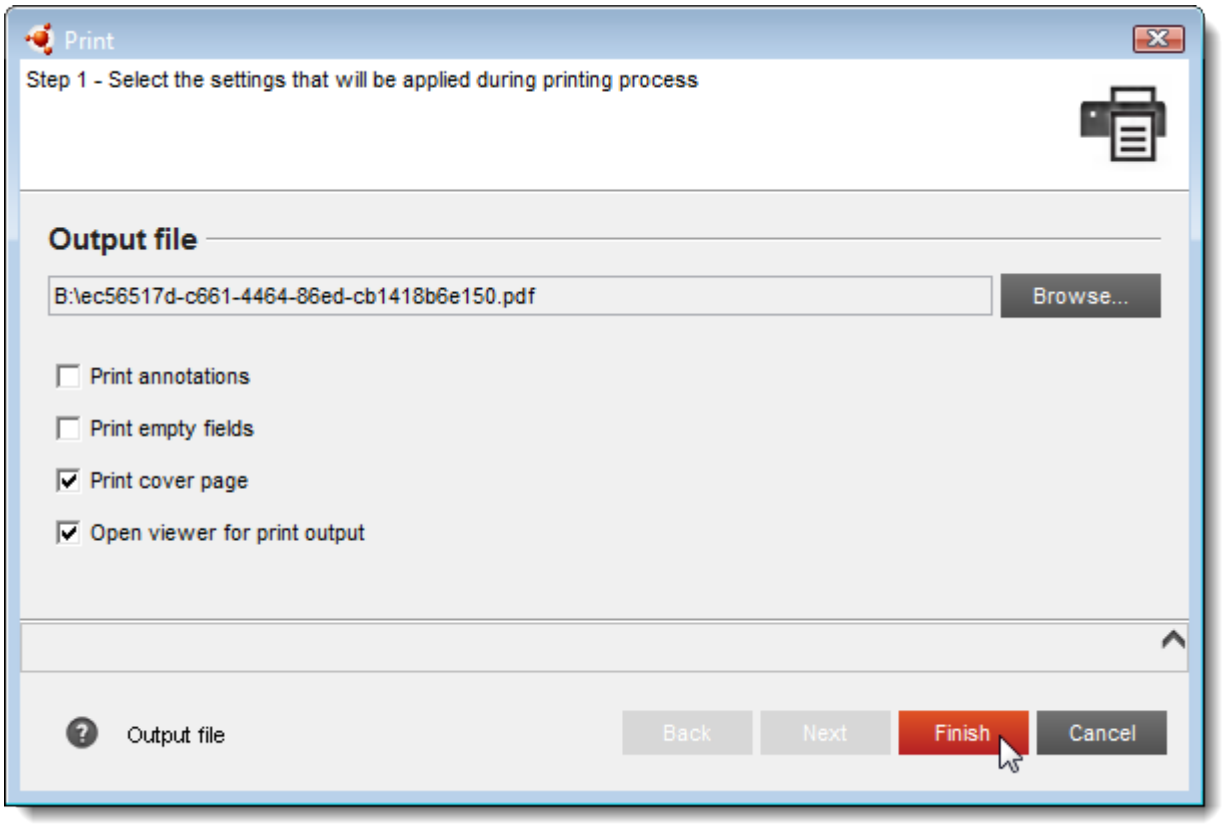
18.1. Print assistant

To launch the printing function, click on the print icon, , located as shown in the figure below. The menu is opened from within the *Navigation pane* by right-clicking on the search record of what is to be printed.



The Print assistant generates a PDF file in a single step, as shown in the figure below.

Figure 83: The options for printing to a PDF file



Under the heading *Output file* enter the path of the folder where the output will be saved. Click the *Browse* button to change the path.

There are four options:

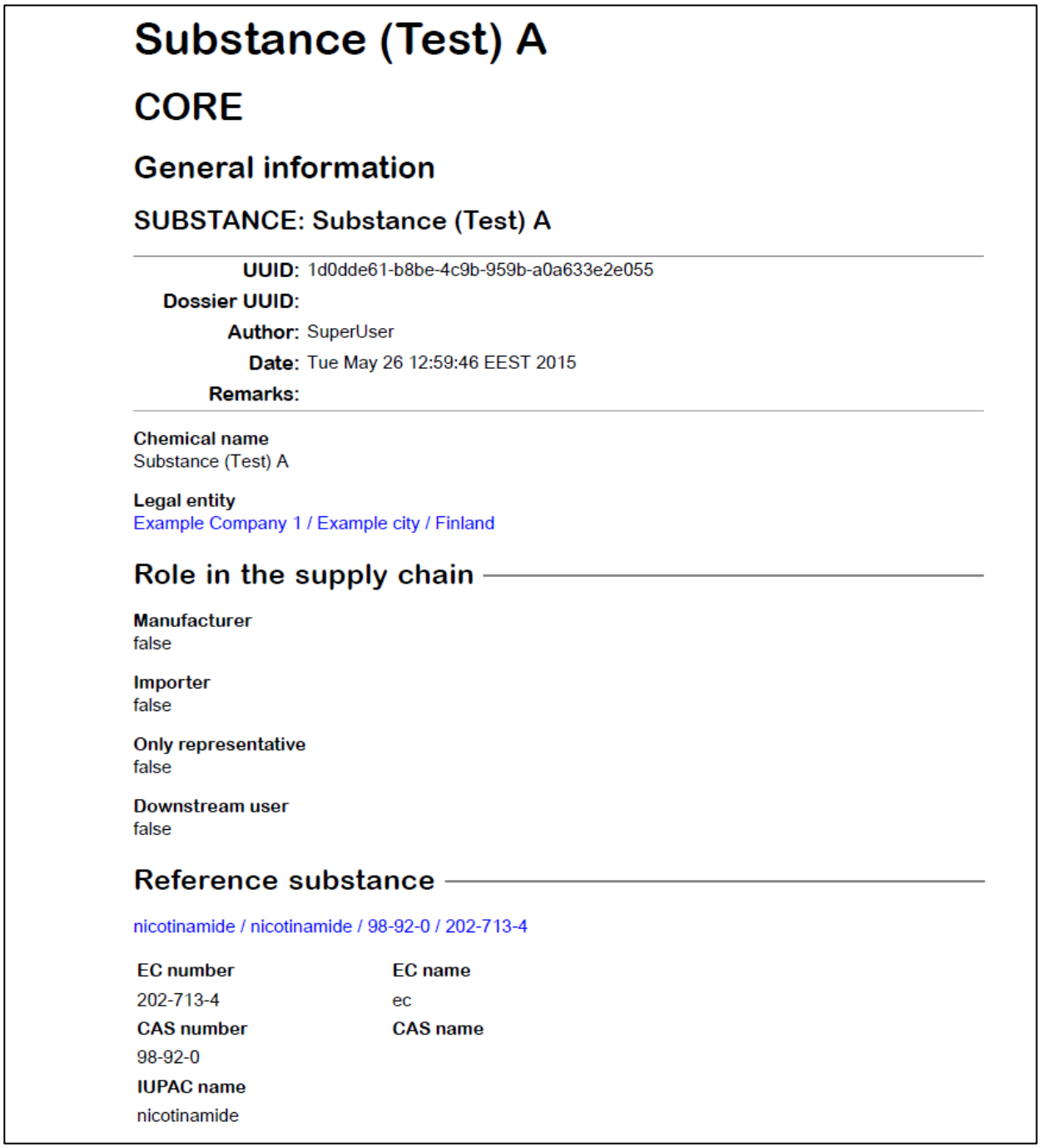
1. *Print annotations* (by default unchecked)
   If you check this option, all the annotations of your dataset, document or entity will be included in the generated PDF.
2. *Print empty fields* (by default unchecked)
   If you check this option, all the empty fields of your dataset, document or entity will be included in the generated PDF.
3. *Print cover page* (by default checked)
   If you leave this box checked, the generated PDF will have a cover page which includes the following information;
   a. Substance name
   b. Legal Entity owner
   c. Printing date
4. *Open viewer for print output* (by default checked) -
   If you leave this box checked, the PDF will be opened automatically in the default PDF viewer for the host computer.

The print process is handled as a background job, as described in section *1.7.3 Background jobs*.

18.2. Table of contents and structure of PDF

In the generated PDF you will see underneath the cover page a table of contents. This will help you locate the information you wish to view. For large files such as datasets, the PDF will be structured according to the sections which contain information, see the examples below.

Table of Contents



Substance (Test) A

CORE

General information

SUBSTANCE: Substance (Test) A

UUID: 1d0dde61-b8be-4c9b-959b-a0a633e2e055
Dossier UUID:
Author: SuperUser
Date: Tue May 26 12:59:46 EEST 2015
Remarks:

Chemical name
Substance (Test) A

Legal entity
Example Company 1 / Example city / Finland

Role in the supply chain

Manufacturer
false

Importer
false

Only representative
false

Downstream user
false

Reference substance

nicotinamide / nicotinamide / 98-92-0 / 202-713-4

EC number
202-713-4
EC name
ec
CAS number
98-92-0
CAS name
IUPAC name
nicotinamide

19. Validation assistant

19.1. Introduction

The aim of the Validation assistant is to assist users in the preparation of IUCLID dossiers so that they can be successfully submitted to and processed by the relevant authority. To this end, the Validation assistant carries out validations on the data provided in a IUCLID dataset or dossier

according to a set of pre-defined rules to verify that the information was provided as expected. The outcome of the validation is a report, which lists all the rules for which the validation failed.

The Validation assistant currently supports the validation of all dossier types that industry can submit to the European Chemicals Agency (ECHA) under the REACH and CLP regulations. It can be customised to validate other types of dossiers, as needed.

The following chapters describe the principles of the Validation assistant, its current coverage of dossier types, and how it is used.

19.2. Structure

The Validation assistant is based on the following components:

- *Scenarios*. A scenario refers to a specific submission type. For simple submission types, a scenario equals a dossier template, but for more complex types, additional parameters are calculated.
- *Rules*. A rule carries out a specific validation on certain content in the dataset or dossier. Each rule is identified by a unique rule ID.
- *Rule sets*. The rule sets are used to configure which rules should be run for each scenario.
- *Messages*. The messages are displayed to the user when a rule is not fulfilled. They inform the user of what caused the failure.

For the end user, it is not necessary to understand this structure; however, it may be useful if in doubt about the outcome of the validation to verify that the validation scenario was the intended one.

19.3. Supported validations

The current version of the Validation assistant allows the users to perform the following checks on their dossiers or substance datasets:

- The *completeness check* on the technical dossier (TCC), for REACH registrations and PPORD notifications
- The verification of those *business rules* that do not rely on information from the ECHA database (e.g. submission history), for all supported dossier types
- In addition, the future versions of the Validation assistant will include *quality checks* to support users in improving consistent reporting of information.

19.3.1. Completeness check

According to Articles 9(3) and 20(2) of the REACH regulation, registration dossiers and PPORD notifications are subject to a completeness check. This completeness check consists of two parts: the financial completeness check (FCC) and the completeness check on the technical dossier (TCC). The Validation assistant enables registrants and PPORD notifiers to check within their IUCLID installation the completeness of their substance datasets and dossiers prior to submission to ECHA via REACH-IT.

While the Validation assistant largely simulates the completeness check carried out by ECHA, it does not capture exhaustively all possible situations in which a dossier may be found incomplete. This includes situations where the registrant deviates from the standard information and needs to provide a justification for the deviation, or when a joint submission member registers a higher tonnage band than the tonnage band of the joint submission and needs to provide the additional study information in his dossier. In such cases, completeness of the dossier will be ensured by manual verification of the information at ECHA. The responsibility remains with the company ensure that their submission fulfils all the relevant legal requirements.

Please refer to the manual *How to prepare Registration and PPORD Dossiers* for detailed information on how to fill in the information for these dossier types in IUCLID format. The manual is available at: http://echa.europa.eu/manuals

19.3.2. Business rules

The Validation assistant also incorporates several of the business rules (BR) checked at ECHA. The following dossier types are supported for business rules check:

- REACH Application for authorisation
- REACH Downstream user report
- REACH Inquiry notification
- REACH Notification of substance in article
- REACH PPORD notification
- REACH Registration
- REACH Substance evaluation dossier
- CLP alternative name request
- CLP notification
- CLP Annex VI – CLH dossier

As some of the business rules depend on contextual information that is stored within the REACH-IT database (e.g. submission history), the Validation assistant cannot simulate all the business rules checked at ECHA.

Please refer to the dossier preparation manuals for detailed information on how to fill in the information for these dossier types in IUCLID format. The manuals are available at: http://echa.europa.eu/manuals

19.3.3. Quality checks

The Quality checks feature will be developed in a future version of the Validation assistant.

19.4. Using the Validation assistant

The Validation assistant is by default installed with IUCLID 6. This chapter describes how you can launch the Validation assistant, and how to understand its output.

19.4.1. Launching the Validation assistant

You can launch the Validation assistant from a variety of locations, according to preference and way of working.

19.4.1.1. Checking existing dossiers / substance datasets

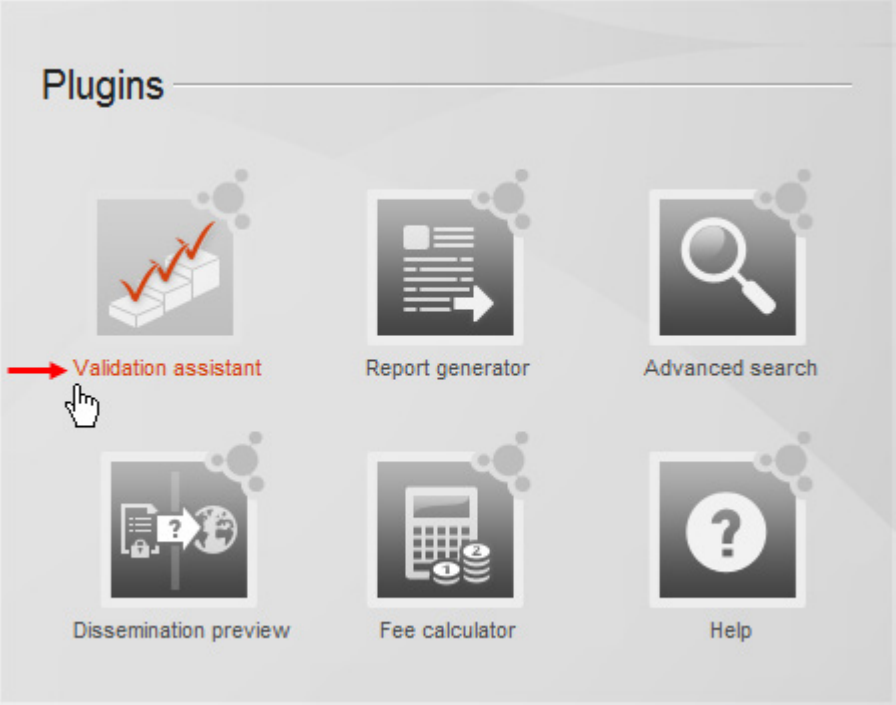
If the purpose is to run the Validation assistant on an existing dossier or substance dataset in the IUCLID application, the following approach may be adopted.

Step 1. Launch the Validation assistant by clicking on the icon in the Plugins section of the home view, as shown in the figure below.

Step 2. Click on the icon to select the dossier or substance dataset to be validated. A query window is opened where you can perform a search using standard criteria.

Step 3. If you selected a dossier, click *Next* to see the validation report. If you selected a substance dataset, first provide the requested information on the type of dossier and submission context, and then click *Next* to see the validation report. See section 19.4.2.2 for further information.

Figure 84: Launching the Validation assistant from the IUCLID home page



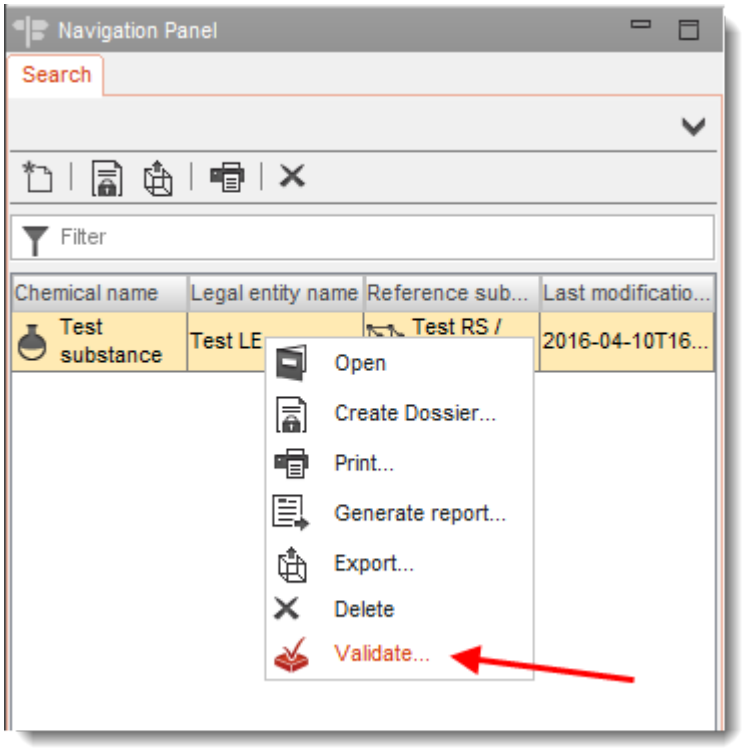
19.4.1.2. Checking a dossier / substance dataset you are working on

The following approach is most suitable in the case that you working inside the Substance or Dossier menus of IUCLID, i.e. (i) you are working on a substance dataset and want to interactively check its validation status while entering the data; or (ii) you just finalised the preparation of a dossier and want to run a validation on it.

Step 1. While in the Substance/Dossier menu, right-click on the name of the relevant substance dataset/dossier in the Search list of the Navigation Panel on the left, and select Validate, as shown in the figure below.

Step 2. If you selected a dossier, click Next to see the validation report. If you selected a substance dataset, first provide the requested information on the type of dossier and submission context, and then click Next to see the validation report. See section 19.4.2.2 for further information.

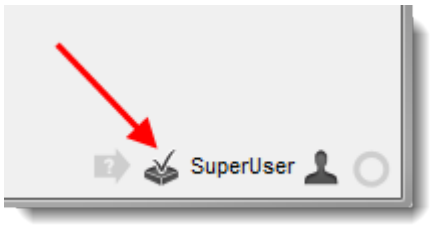
Figure 85: Launch the Validation assistant from the Search list of the Navigation Panel by right-clicking on the name of the relevant dossier or substance dataset.



19.4.1.3. Hide/display the Validation assistant window

The Validation assistant window can be minimised by clicking on an icon located at the top right corner of the window ( ). This action will hide the Validation assistant window, but retain all the information about the ongoing validation. To display the Validation assistant window again, click on the Validation assistant icon in the bottom right corner of the IUCLID window, as shown in the figure below.

Figure 86: A dark grey Validation assistant icon in the bottom right corner of the IUCLID window indicates that a Validation assistant instance is active. If you minimised the Validation assistant window, clicking on this icon will restore it maintaining the same.



You cannot launch multiple instances of the Validation assistant at the same time. You therefore need to close a running instance of the Validation assistant, before launching a new validation.

19.4.2. Checking dossiers and substance datasets

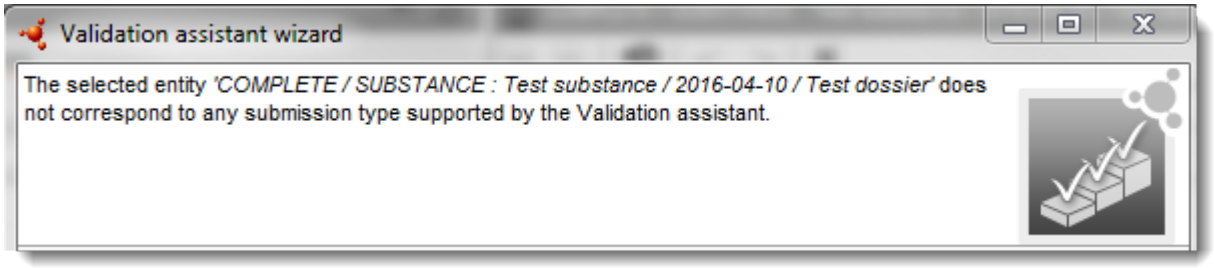
This section explains how to use the Validation assistant to check a dossier or a substance dataset.

19.4.2.1. Checking dossiers

When you launch the Validation assistant on a dossier, it will calculate the submission type (scenario) and by default execute the relevant rules for that scenario.

- For dossiers created with any of the REACH registration templates (and the template REACH PPORD), the Validation assistant performs a completeness check according to the tonnage band information and joint submission status from the dossier template and header. In the same report, the outcome of the business rules check is included.
- For the remaining templates supported by the Validation assistant (see Chapter 19.3), a business rules check is performed.
- If you attempt to run the Validation assistant on a dossier type that it does not support, a message is displayed at the top of the Validation assistant results window, as shown in the figure below.

Figure 87: Running the validation on a dossier template not supported by the Validation assistant gives the above message.



19.4.2.2. Checking substance datasets

Unlike dossiers, substance datasets do not correspond to a specific type of submission and therefore the user needs to provide the Validation assistant with sufficient information to be able to determine the submission type (scenario) against which the dataset should be checked. This information is similar to what is provided in the dossier header during dossier creation.

Step 1. Launch the Validation Assistant plug-in as described in section 19.4.1.

Step 2. Select the type of dossier for which you want to validate the dataset. If you wish to filter the information included in the validation based on confidentiality and regulatory programme flags, check the box *Use advanced settings* and select the appropriate flags to be included/excluded. Otherwise, directly click *Next*.

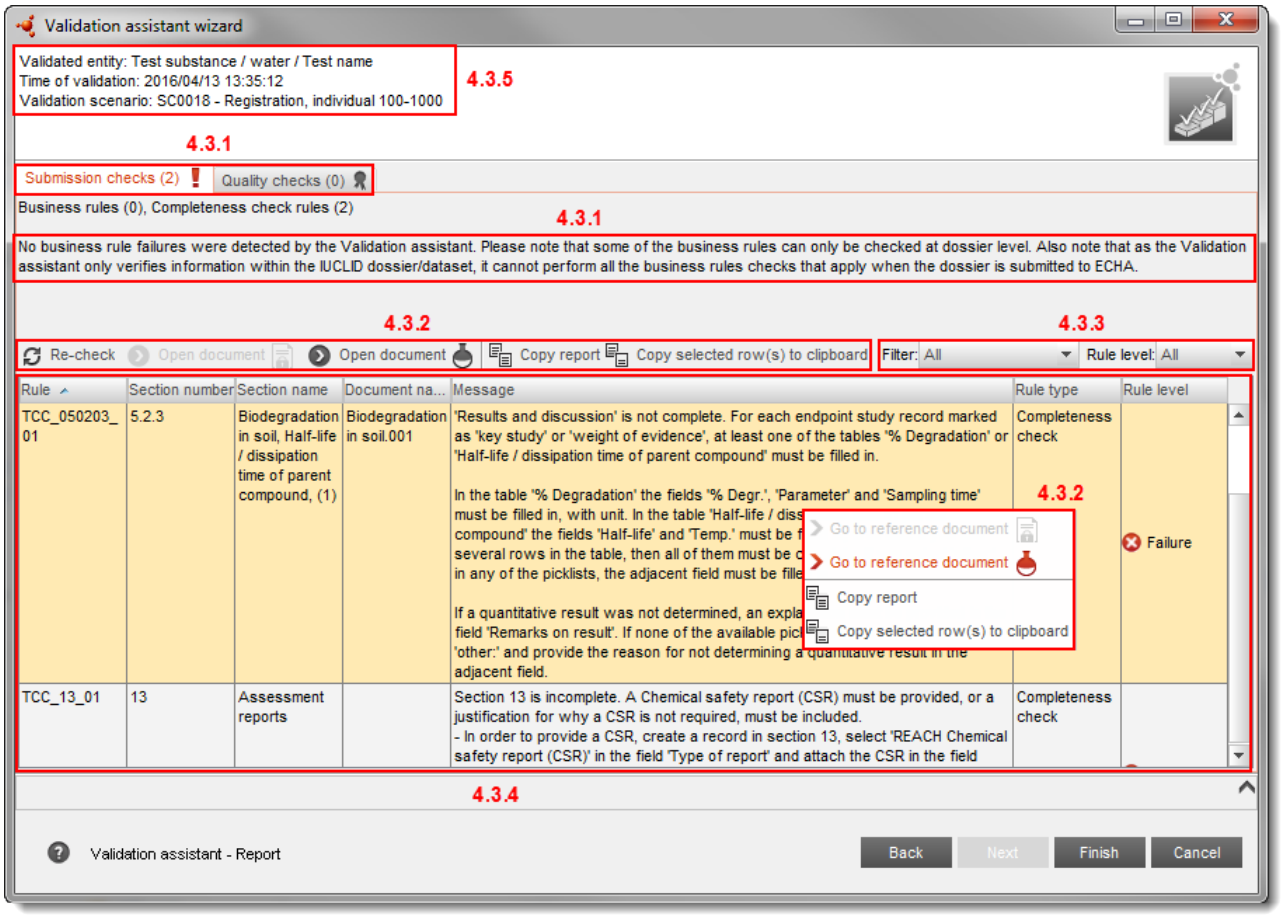
Step 3. Provide information on the type of submission for which you want to validate the dataset. The available fields depend on the type of dossier selected in step 2. For example, when validating the dataset for a REACH inquiry dossier, no further information needs to be provided in this step. However, when validating the dataset for a REACH registration, information on the tonnage band and the joint submission status must be entered for a correct result. Follow the instructions for the specific submission type, available in the dossier preparation manuals.

Note that a IUCLID dossier consists of two parts: a substance dataset, and the so-called dossier header. The dossier header is generated during the dossier creation process. The dossier header contains important parameters to determine the validation scenario. Therefore, even if validating your substance dataset does not trigger any failures by the Validation assistant, it is very important that you validate also the dossier you have generated from the substance dataset. This will ensure that the data is validated against the correct submission type (scenario) and that all the information provided in the dossier header has been considered.

19.4.3. Validation assistant results window

The last step of the Validation assistant wizard displays the outcome of the performed checks. The different parts of the results display are further described in the following subchapters.

Figure 88: Validation assistant results display. The numbers shown for the different interface elements corresponds with the numbering of the following subsections.



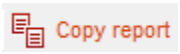
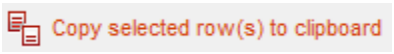
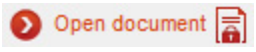
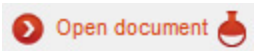
19.4.3.1. Submission checks tab and Quality checks tab

As shown in the figure above, the Validation assistant results window is split into two separate parts (tabs). When entering the results window, the tab that is opened by default is the one containing the results of the checks that are relevant for a successful submission, i.e. the business rules and completeness check. The Quality checks feature is not yet developed in this version of the Validation assistant.

In the tab headers, numbers are displayed in brackets. They indicate the number of messages (validation errors) displayed for each tab. When no validation errors occur for a certain type of rule, an information message is displayed in the upper part of the active tab, explaining the implication to the user.

19.4.3.2. Validation assistant report toolbar

The Validation assistant report toolbar contains the following elements:

	Refresh the report. When working in a substance dataset, you can edit the data and refresh the Validation assistant result to see the impact of the modification. Remember to save the changes made in the dataset, for the refresh to be effective.
	Copy the entire report table to the clipboard (for pasting to e.g. Excel, Word). Also achieved by right-clicking in the report table and selecting *Copy report*, or by using the keyboard shortcuts CTRL+A and CTRL+C.
	Copy the selected row(s) from the report table to the clipboard (for pasting to e.g. Excel, Word). Also achieved by right-clicking in the report table and selecting *Copy selected row(s) to clipboard*, or by using the keyboard shortcut CTRL+C.
	Navigate to the document in the dossier (only for dossiers). If you select any row and press this button, it will open the document that contains the validation error in the dossier that was checked. The same action can be achieved by right-clicking on a row in the report, and selecting *go to reference document*. Navigation to a document is not possible when the validation error is caused by a *missing* document.
	Navigate to the document in the substance dataset. If you select any row in the report table and press this button, it will open the document that contains the validation error in the substance dataset that was validated or the substance dataset that was used to create the dossier (if a dossier was validated). The same action can be achieved by right-clicking on a row in the report, and selecting *go to reference document*. Navigation to a document is not possible when the validation error is caused by a missing document. This option is not available if you were validating a dossier but the substance dataset that was used to generate the dossier is not available in your IUCLID database.

19.4.3.3. Rule types and filtering of the report table

The Validation assistant verifies rules of different types. You can use the field *Filter* to display the outcomes of a certain type of rule in the report table. Rule outcomes may also be of different level. In the Validation assistant, the rule levels *failure*, *warning* and *reminder* exist, implying different consequences if present in the submitted dossier. The field *Rule level* can be used to display the outcomes with a certain level in the report table. All messages reported in the *Submission checks* tab are of the level failure; if not corrected; the dossier will not be successfully submitted.

19.4.3.4. Validation assistant report table

The Validation assistant report table contains the following elements:

Rule	The name of the validation rule that was not fulfilled. This is mainly relevant if you need to exchange information with colleagues or helpdesks about the validation report; in this case it is useful to identify particular rules with their name.
Section number	Displays the IUCLID section number in which the validation error occurred.
Section name	Displays the IUCLID section name in which the validation error occurred. For rules that check information in repeatable structures, such as tables or blocks, the section name is displayed together with the number of the incomplete row/block in parenthesis (see the figure above). For rules that check information in multiple tables, the section name is followed by both the indication of the incomplete table name and row number. For example, the section name "Biodegradation in soil, Half-life / dissipation time of parent compound, (1)" means that the failure is located in the first row of the table *Half-life / dissipation time of parent compound* of section 5.2.3 - Biodegradation in soil. When rules that check repeatable structures fail due to that no information at all was provided, then no indication of the table or row number is shown.
Document name	If the validation error was triggered by incomplete information in an existing document, the document name is displayed. If the error is triggered by the absence of a document, this column will be empty. When choosing to navigate to a document in the substance dataset or dossier (see Chapter 19.4.3.2), this is the location that will be opened.
Message	Provides the description of what caused the validation error.
Rule type	Displays the type of the rule. The messages reported in the *Submission checks* tab are of the type business rule or completeness check rule. Both of these rule types are crucial for submitting the dossier; any failure reported by the Validation assistant on business rules or completeness check rules must be corrected to achieve a successful submission.
Rule level	Displays the level of the rule, i.e. failure, warning or reminder. All messages reported in the *Submission checks* tab are of the level failure.

By default, the validation report displays the outcome sorted by the first column *Rule*, in ascending alphabetical order. By clicking on a column header of the validation report, you can sort the report by that column in ascending or descending order. This may be helpful if you wish to correct all failures reported for a certain section.

When updating a registration that was previously a notification under Directive 67/548/EEC for another reason than a tonnage band update, or to become the lead of a joint submission, less

information is required than for a standard registration dossier. The minimum information to be provided in this case is described in Annex 4 (Minimum information required for updating a registration under previous Directive) of the manual How to prepare Registration and PPORD Dossiers available at http://echa.europa.eu/manuals.

The Validation assistant does not offer the possibility to verify the completeness of only these reduced information requirements (especially, since all new and updated information needs to be checked for completeness), but will check the full requirements for the selected submission type. Consequently, the Validation assistant can be used to check the completeness of these datasets and dossiers but only the TCC failures related to the information requirements indicated in the manual should be considered in the result.

19.5. Version update

It is important to use the latest version of the Validation assistant. New versions are made available either as part of a new release of the IUCLID application, or through an update of an individual component. The user can choose to be notified of when new versions of the IUCLID application or its components are available, as described in section *15.1.2.5 Updates*.

19.6. Disclaimer

The checks performed by the IUCLID Validation assistant do not cover all of the verifications carried out on a dossier submitted to ECHA. It is the responsibility of the submitter to ensure that the dossier fulfils the appropriate data requirements and to monitor the outcome of the submission process in REACH-IT.

20. The Report generator

The Report Generator extracts data from a IUCLID dataset or dossier in a different format, usually generating a printable output.

The Report Generator is using a set of predefined templates such as the Chemical Safety Report (CSR) under the REACH Regulation but can also accept customised report templates in order to generate user-tailored reports.

The Report Generator plugin is launched from the IUCLID main menus, in the Plugins section. Clicking on the corresponding icon, the Report Generator dialogue appears. The access to the same function is also provided as right-click on a selected substance or dossier.

From the Report Generator dialogue the user can select the type of Report he wants to generate.

The plugin generates documents in RTF, PDF or XML format.

The capture of IUCLID data is controlled by a number of rules used to extract and transfer the relevant information. Example of these rules, used to generate specific document, can be found in the following sections.

20.1. Preparing the Chemical Safety Report (CSR) with the Report Generator

The Report Generator plugin generates the complete structure of the Chemical Safety assessment (CSR) including all main sections and subsections according to the to section 7, Annex I of REACH and a more detailed breakdown as laid down in the CSR template version of July 2008 made available by the ECHA. In details, the Report Generator pre-fills Part A and the sections 1 to 8 of Part B with the information captured from IUCLID.

As outlined in the ECHA Guidance on information requirements and chemical safety assessment, Part F: Chemical Safety Report (ECHA 2008), the main goal of the chemical safety report (CSR) is to document the chemical safety assessment (CSA), including its conclusions and results, with regard to the standard elements of the CSA. The report should be readily understandable as a stand-alone document. The principles applied, the assumptions made and the conclusions drawn should be transparent. The key data should be easily identifiable without the need to revert to the underlying data sets. In order to keep the CSR as concise as possible, only the most relevant information reported in the technical dossier (in IUCLID) is extracted.

20.1.1. General principles

The capture of IUCLID data is controlled by a number of rules used to extract and transfer the most relevant information, filtering out less relevant information.

The Report Generator can be used in an iterative process: entries in the IUCLID source fields can be optimised as appropriate. In this respect, the cyclic improvement of the source data and re-run of the plugin can be useful in verifying that the appropriate information has been entered in IUCLID.

Knowing beforehand what kind of IUCLID information is used or not used by the plugin may prompt the IUCLID user for a more anticipating, i.e. CSR-oriented, completion of the relevant fields.

Although possible, editing of the generated CSR using any text processing program, should be limited to (rare) cases where data cannot be edited upfront in the data source(s). Be aware of the risk that any manual changes made to IUCLID-borne information in the CSR may result in inconsistencies, if the IUCLID records are not updated accordingly.

Note: it cannot be guaranteed that all relevant information is captured and/or copied into the appropriate CSR section. The user is responsible to verify that the relevant CSR information is included, and if not, to update the CSR by updating the source records and/or by modifying, supplementing or deleting any information in the CSR manually as appropriate.

20.1.2. CSR part A

Part A of the CSR consists on the following three subsections:

1. 1. Summary of risk management measures
2. 2. Declaration that risk management measures are implemented
3. 3. Declaration that risk management measures are communicated

All parts can be easily completed by the user in section 13.1 of IUCLID. For each of the three subsections a rich text area is provided which can accommodate plain text, but also tables and specific formatting of text entered.

The Part A is specific to the type of CSR generated in terms of "Own CSR", "Joint CSR" or "All uses CSR". In this way, for a single substance, up to three different sets of part A can be entered which are linked to the respective selection made by the user.

20.1.3. Generation of own / joint CSR

The Report Generator allows the generation of different types of Chemical Safety Report (CSR). This has an impact on the selection of uses that are described in section 2 of the CSR and the part A. It has no impact on the information reported in any other sections related to the hazard assessment.

The Report Generator creates different CSRs according to the selection made in the first record of IUCLID section 13.1 "Chemical Safety Report (Part A)".

If the user decides to prepare its "Own" CSR, all uses in IUCLID section 3.5 flagged as "Use covered by an own CSR" (as well as "Use not assessed") will be reported in section 2 of the CSR.

In case the user instead decides to prepare a "Joint" CSR, only the uses flagged in IUCLID section 3.5 as "Use covered by a Joint CSR" (including those flagged as "Use covered by a Joint CSR but not a lead own use" and the "Use not assessed) will be reported in section 2 of the CSR.

The option "all uses" can be chosen to populate CSR section 2 with all uses reported in IUCLID section 3.5, regardless of whether and how they have been flagged. However users should be very careful when using this option, especially if some uses have been already identified as own or joint.

20.1.4. General rules underlying the CSR generation

In this section the general rules underlying the CSR generation are explained and exemplified. It is demonstrated how the Report Generator works and what kind of IUCLID information is generally captured.

20.1.4.1. Text labels (prompts) preceding transferred IUCLID values

In the IUCLID data entry forms, the data entry fields are specified by prompts, which are text labels describing the kind of information expected to be entered (e.g. "Type of information"). In the overview tables generated by the Report Generator, the following approach is used:

- No text labels are printed if the kind of information transferred is self-explanatory in order to keep the tables as concise as possible. Typical examples where the placeholders are replaced by the field value without any further preceding label include: Guideline, Principles of method if other than guideline, Reliability, Adequacy of study, Type of information, Author, Year, …
- Text labels are printed if they help understand the meaning of the information or to avoid misinterpretation.

20.1.4.2. Handling information captured from repeatable blocks of fields

In IUCLID, most results data are included in repeatable blocks of fields, which are grouped in a dialog box and usually displayed in tabular form on the data entry screen. The Report Generator concatenates all or selected subfields according to specific rules.

Note: For technical reasons, several pieces of information (e.g. Remarks) are set in parentheses, as it would otherwise be difficult to set them apart by punctuation marks.

20.1.4.3. Discarding picklist phrase "no data", "other:", "other .....:"

In many IUCLID picklist (drop-down list) fields, the phrase "no data" can be chosen. By convention, this phrase is not transferred to the CSR as this would cause confusion or give false meanings. For instance, if no text label is provided, the plain text "no data" would not be understood.

The picklist phrases "other:" or "other guideline:" are also ignored. However, the free text entered next to the list field is indeed transferred.

20.1.4.4. Handling information captured from text fields and rich text areas

In IUCLID, different text field types are provided. Information captured from these fields is handled as follows:

- Single-line text field: The content of these fields is transferred without any changes.
- Multi-line text field: The content of these fields is transferred as is including line breaks. Only in some cases the latter may be removed.
- Rich text (html) area: allows to specify fonts, colours, bullets, and other text attributes and to insert tables. The Report Generator keeps most of the formatting including tables.

20.1.4.5. Assessment entities

Currently the Report Generator does not convey the information on assessment entities available in a specific substance dataset/dossier

20.1.5. Guidance on specific CSR sections B.1 to B.3

Part B of the CSR template mainly refers to the sections and subsections comprising the hazard assessment, basic information on manufacture and uses, classification and labelling, and PBT and vPvB assessment.

20.1.5.1. CSR section B.1 IDENTITY OF THE SUBSTANCE AND PHYSICOCHEMICAL PROPERTIES

Specific guidance notes:

- Table "Physicochemical properties": Information is captured from the relevant endpoint summaries, but not from endpoint study records.
- Data waiving: see section 2.7 Data waiving information.

- Testing proposal: see section 2.8 Information on testing proposals.

20.1.5.2. CSR section B.2 MANUFACTURE AND USES

Reports the tables in the IUCLID sections "3.2 Estimated quantities", "3.5 Life Cycle description" and "3.6 Uses advised against"

20.1.5.3. CSR section B.3. CLASSIFICATION AND LABELLING

The Report Generator only extracts data from "3.1 Classification and labelling according to CLP / GHS".

To distinguish the C&L information transferred from multiple records the heading "Substance: <Name>" is inserted. Make sure that this field is completed appropriately. As a fall-back, the heading "Substance: <Reference substance name>" is inserted.

Subsection "3.2 Classification and labelling according to DSD / DPD" is not captured by the Report Generator.

20.1.6. Guidance on CSR sections B.4 to B.7 (HAZARD ASSESSMENT)

The following approach is applied for generating the hazard assessment sections:

- Overview tables are generated for summarising all relevant and possibly relevant studies as requested in the ECHA guidance documents:
  - Present the key information provided in the IUCLID dataset in a brief table format and reference, rather than repeat the details (cf. ECHA 2008).
  - In addition to the key studies, information available in other studies could also be used by the registrant as supporting information or as part of a weight of evidence approach (cf. ECHA 2012a).

Note: The IUCLID fields "Conclusions" and "Executive summary" are not addressed by the Report Generator: this is in line with the ECHA guidance that the description of key information should preferably be done in tabular form.

- Data waiving and testing proposal ("Type of information = experimental study planned") records from each endpoint section are transferred.
- The conclusions from the hazard assessment should be presented in the relevant endpoint summaries of IUCLID which is then transferred to the relevant CSR subsections (cf. ECHA 2008).

20.1.6.1. Overview tables for summarising the relevant studies

The following approach is applied for generating overview tables:

- An overview tables is generated if at least one endpoint study record is available in the IUCLID dataset

- Each overview table is preceded by a default statement such as "The results of studies on skin irritation are summarised in the following table.".

20.1.6.2. Sorting data from multiple endpoint study records of the same source section

When data from multiple records are inserted in a CSR table, the order is controlled by the following sort rules:

(I.) Endpoint-specific criteria (if applicable): (1) e.g. freshwater; (2) e.g. saltwater; (3) etc.

(II.) Field "Adequacy of study" = (1) "key study"; (2) "supporting study"; (3) "weight of evidence"; (4) disregarded due to major methodological deficiencies.

(III.) If multiple records fulfil the same combination of sorting criteria (e.g. several key studies of type freshwater), the order of records follow the one used in the source IUCLID.

Note: In the tables of "Human information" sections (Table # "Exposure-related observations on ... in humans"), the primary sort rule is determined by the source section. This means that any relevant records from section 7.10.1 are inserted first, followed by those from 7.10.2, etc.

20.1.6.3. Sorting data from multiple fields within the same endpoint study record

Data from multiple fields or blocks of fields are normally ordered as entered in the IUCLID source field(s).

20.1.6.4. Elements included in overview tables

20.1.6.4.1. Information on method (Guideline, Principles of method, specific fields)

In the column "Method", the key information is inserted, which includes specific descriptors such as Test type, Species, Route of administration, Exposure duration and the following generic descriptors: guideline and principles of method if other than guideline.

Information on study results

In the column "Results", the most relevant study results and conclusions are inserted. In most cases structured fields are extracted, e.g. "Effect levels" or "Interpretation of results". In some cases multi line free text fields or text areas are addressed in addition or exclusively. In these cases, manual intervention may be necessary to ensure that the tables contain only brief descriptions of the relevant information.

Examples:

- Several CSR sections: Field "Principles of method if other than guideline"
- CSR section "5.1 Toxicokinetics": Fields "Doses / concentrations", "Details on in vitro test system (if applicable)".
- Several CSR sections: The "Results" column of Table "Exposure-related observations on ... in humans" includes information from the following free text fields: "Results", "Results of examinations", "Outcome of incidence".

20.1.6.5. Information on test material

In the column "Remarks", the identity of the test material used in the study is inserted in the result tables. However, if no information on the test material is available, then this default statement appears in the CSR >>>??? information missing in IUCLID<<<.

20.1.6.6. Administrative information (Reliability, Adequacy of study, Type of information)

In the column "Remarks", the following administrative information is given:

- Reliability: The value from the corresponding source field is inserted.
- Adequacy of study: The value from the corresponding source field is inserted, i.e., either "key study", "supporting study", "weight of evidence" or "disregarded due to major methodological deficiencies".
- Type of information: The value from the corresponding source field is inserted, i.e., either "experimental result", "estimated by calculation", "read-across based on grouping of substances (category approach)", "read-across from supporting substance (structural analogue or surrogate)", "(Q)SAR" or free text (if "other:" is selected). "robust study summary"

Note: The phrase "experimental study planned" in field "Type of information" triggers the transfer of the relevant information to the corresponding part "Testing proposal" (see section 2.8 Information on testing proposals).

20.1.7. Data waiving information

Data waiving information is captured based on the following rules:

- Data waiving records from each endpoint section are transferred to the corresponding section of the CSR. Please note: In the previous version of the Report Generator data waiving information was captured only where REACH foresees this possibility (cf. ECHA 2012b).
- If the field "Data waiving" is populated, this field and the field "Justification for data waiving" are captured and inserted under the CSR heading "Data waiving".
- If, in the same endpoint study record, "Data waiving" is indicated and "Adequacy of study" is populated, the data waiving information is ignored, while the relevant study summary information is transferred to the overview table.

Note: This approach reflects the indication that "an individual Data waiving record should stand alone and not be mixed with other data such as existing study summaries".

- Since multiple data waivers are possible for a given endpoint, each data waiving information starts with the heading "Information requirement: <Endpoint>", e.g.

20.1.8. Information on testing proposals

Information on testing proposals is captured based on the following rules:

- Testing proposal records from each endpoint section are transferred to the corresponding section of the CSR. Please note: in the previous version of the Report Generator testing

proposal information was captured only where REACH foresees this possibility (cf. ECHA 2012b).

- If the field "Type of information" contains the phrase "experimental study planned", the values of the following fields are captured and inserted under the CSR heading "Testing proposal":
  - Guideline
  - Specific fields characterising the study design, e.g. Study type, Type of method, Test organisms (species).
  - Principles of method if other than guideline
  - Study period

- Test material information

20.1.9. Information from endpoint summaries

In the hazard assessment part of the CSR, the human health hazard, physicochemical hazard and environmental hazard should be assessed and reported in the endpoint summaries in IUCLID .

In the IUCLID Endpoint sections 4 to 10, Endpoint summary records can be created, and they can be used to give an appraisal of all data compiled in a given Endpoint section. Hence, an endpoint summary addresses, in a very condensed form, the most relevant and reliable data or provides a weight of evidence evaluation based on several studies.

Endpoint summary records can also be created at a higher level, i.e., for main sections. At the highest level of the main sections "6. Ecotoxicological Information" and "7. Toxicological information", specific summary templates are provided for recording more integrated information, i.e. PNECs and DNELs, respectively, and other hazard conclusions including relevant input parameters.

The relevant endpoint summary information is printed either under the heading "Additional information" or in a subsection titled "Summary and discussion of ..."

Note: in IUCLID, several summaries can be created per endpoint. The Report Generator captures all endpoint summary records by printing them one after the other. The name of the endpoint summary record defined in the IUCLID tree view is printed in order to distinguish the different records.

The following fields are captured from endpoint summaries, if available:

"Additional information": The information from this field is inserted in the CSR normally after the heading "Additional information". As an exception, in section "B.1.3 Physico-chemical properties", it is transferred to the overview table.
In this IUCLID field, the assessment made for the given endpoint should be described, including the rationale for the choice of the key study(ies). This includes a discussion of the key information identified and in some instances of studies which are considered to be unreliable, but give critical results. A discussion as to why they were discarded in favour of other studies should then be included. Vice versa, a weight of evidence analysis based on less reliable data should be justified.

"Description of key information": The information from this field is normally inserted in the CSR after the default statement: "The following information is taken into account for any hazard / risk

assessment:".
In section "B.1.3 Physico-chemical properties", it is transferred to the overview table.
In this IUCLID field a short description of the most relevant endpoint data should be included, i.e., the most relevant details, e.g. the test guideline used, test organism and exposure duration, and the key results. Also several key studies can be referenced, particularly if several data requirements are discussed, e.g., in vitro vs. in vivo or gene mutation vs. chromosome aberration in the section "7.6 Genetic toxicity". In general, the characterisation of the endpoint data should be kept as concise as possible and not repeat verbatim the narrative in the field "Additional information".

"Key value for chemical safety assessment": The information from field(s) subsumed under this heading is inserted in the endpoint-related CSR summary subsections after the text label: "Value used for CSA:", e.g. Value used for CSA: 255 °C at 101.3 kPa

In addition, the key values from the toxicological endpoints are used to generate the table "Available dose-descriptor(s) per endpoint as a result of its hazard assessment" in the CSR section "Overview of typical dose descriptors for all endpoints".

Note: In IUCLID endpoint summaries, only a minimum number of structured and hence, searchable fields are provided as "Key value". This has been foreseen for the use of estimation tools. Key values are intended to condense the data summarised in the field "Description of key information" to one single numeric value or concluding remark (e.g. negative / positive) chosen from a drop-down list. Where a numeric field is provided, only a clear value can be entered, that is, no range and no less than or greater than qualifiers.

The information from endpoint summaries of the main ecotoxicological and toxicological sections is transferred as follows:

IUCLID section "7. Toxicological information": The relevant information is transferred to the CSR section "5.11.2. Selection of the DNEL(s) or other hazard conclusions for critical health effects":

- The DNEL(s)/DMEL(s) or qualitative hazard conclusions are transferred to the tables "Hazard conclusions for workers" and "Hazard conclusions for the general population" together with the information from the fields "Most sensitive endpoint" and "Route of original study".

IUCLID section "6. Ecotoxicological Information": The relevant information is transferred to CSR section "B.7.6. PNEC derivation and other hazard conclusions":

- All PNEC values and/or qualitative hazard conclusions are transferred to the table "Hazard assessment conclusion for the environment", together with "Assessment factor:", "Extrapolation method" and "Justification for (no) PNEC .... derivation".

- The information from the field "Environmental classification justification" is inserted under the heading "Environmental classification justification".

20.1.10. Information to be added manually

With the Report Generator all relevant CSR elements of section B are automatically completed with IUCLID data except for the following items:

Section 9: EXPOSURE ASSESSMENT

Section 10: RISK CHARACTERISATION

20.1.11. Annexes

At the end of the CSR a list of full references available in the substance/dossier is printed (Annex 1) as well as the additional information on Test material (Annex 2).

21. Dissemination preview

21.1. Introduction

The Dissemination preview plugin allows you to simulate which information from your dossier is likely to be made publicly available by ECHA in the process known as dissemination. The plugin is delivered with IUCLID 6.

In the current version of the tool only dossiers which are in a REACH registration template, and which are not mixtures, can be previewed.

The output of the Dissemination preview is a filtered version of the input dossier, called a *Filtered Dossier*, and a *Dissemination preview report*. The Filtered Dossiers crated by the tool will be filtered so as to contain only the information which would be, if submitted to ECHA, put publicly available over the internet.

The Filtering Process in the tool, that prescribes which information is or is not present in the output Filtered Dossier, uses the same Filtering Rules as used by ECHA for publication of information on the ECHA website. Information on these Filtering Rules can be found in a dedicated Manual on the ECHA webpage.

The Dissemination preview is for information purposes only, and the resulting Filtered Dossiers may not be identical to the actual dissemination that will be performed by ECHA in accordance with Article 119 of REACH.

In particular, as the Dissemination preview cannot assess confidentiality claim(s) it will remove information claimed confidential by default. Note however, that ECHA will perform an assessment of each confidentiality claim falling under REACH Article 119(2). Should ECHA reject any such confidentiality claim(s) the information claimed confidential will be disclosed at a later stage after consultation with the registrant, in accordance with REACH Article 119(2).

In addition, the information that will be disseminated for each substance on the ECHA website will be aggregated from multiple registration dossiers at different tonnage bands, and therefore may contain additional information to filtered dossiers from the Dissemination preview tool.

The following chapters describe how you can launch the tool, and how to understand its output.

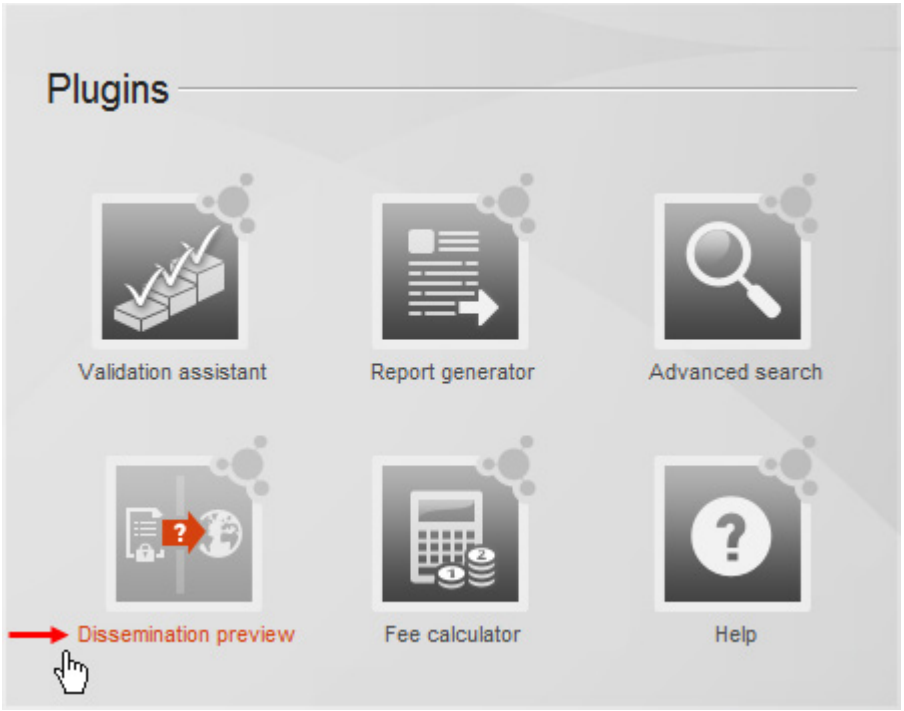
Note: It is recommended to always check that you have the latest version of the preview tool, to ensure you always have the same Filtering Rules as ECHA. Choose to be notified of when new versions of IUCLID or its components are available on the website, as described in section 15.1.2.5 Updates of the IUCLID functionalities.

21.2. Starting the Dissemination preview

21.2.1. From the IUCLID home page

From the IUCLID home page the Dissemination preview can be started by clicking on the icon in the Plugins section as shown below.

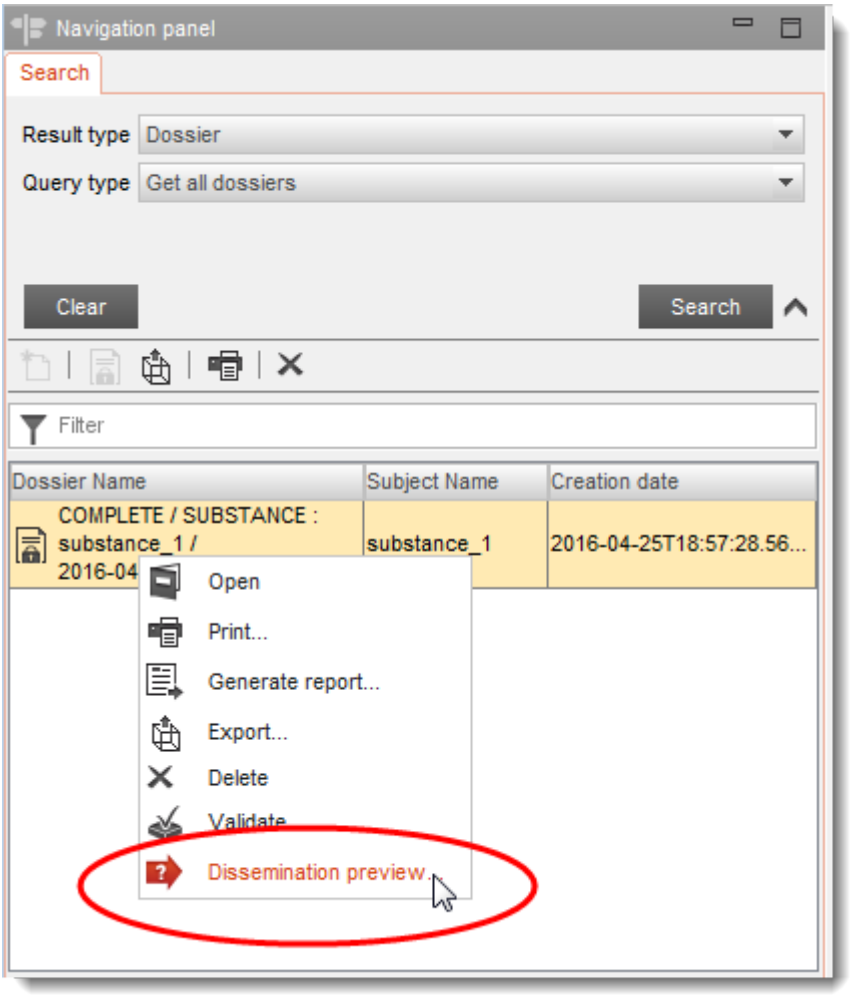
Figure 89: Starting the Dissemination preview from the IUCLID 6 home page



21.2.2. From the Dossier view

While in the Dossier menu, right-click on the name of the relevant Dossier in the Search results of the Navigation, and then select *Dissemination preview* as shown below.

Figure 90: Starting the Dissemination preview from the Dossier view



21.3. Using the Dissemination preview

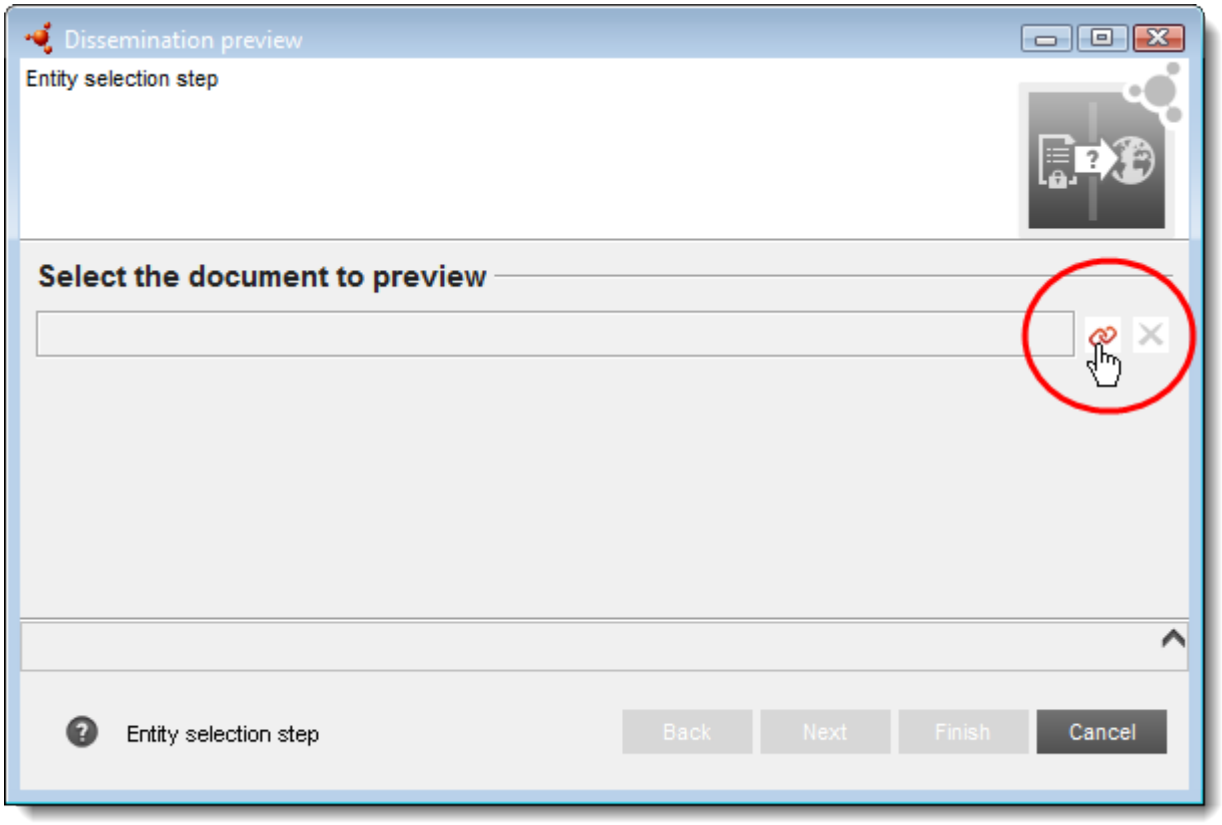
21.3.1. Step 1: Selecting a Dossier to preview

When you start the preview, a wizard will appear.

If you start the preview from the Dossier view, the dossier is pre-selected in the wizard and you will be taken directly to Step 2 *Name your Filtered Dossier.*

If you start the preview from the IUCLID Home view, you need to select the dossier to filter. Click on the icon to bring up a standard IUCLID search dialog which you can use to locate the dossier you wish to preview in a disseminated form.

Figure 91: Dossier selection from the IUCLID home page



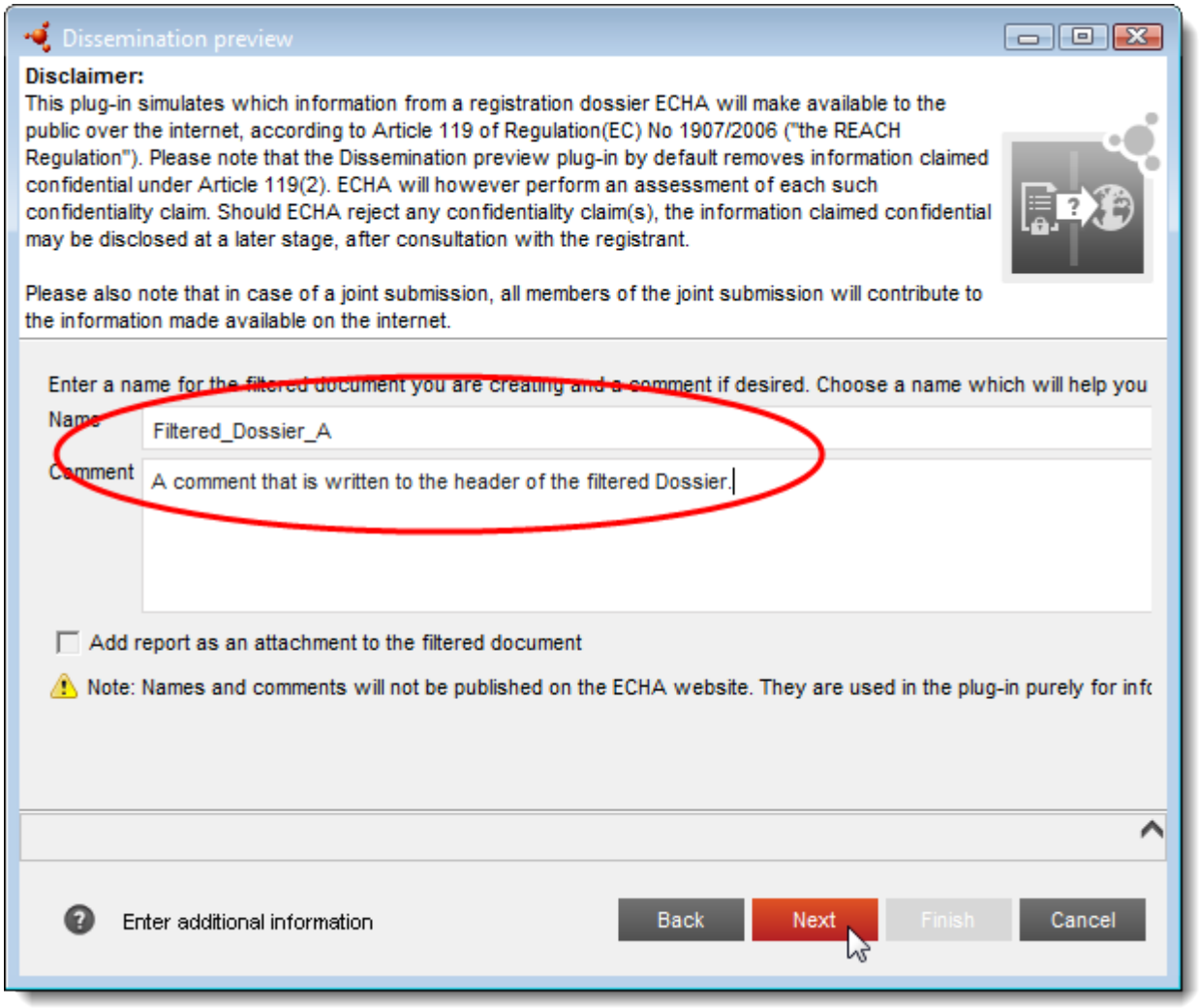
Note that only REACH Registration dossiers are accepted by the current version of the Dissemination preview tool.

21.3.2. Step 2: Name your Filtered Dossier

You will be presented with an opportunity to select a name for your Filtered Dossier. You may also add a comment.

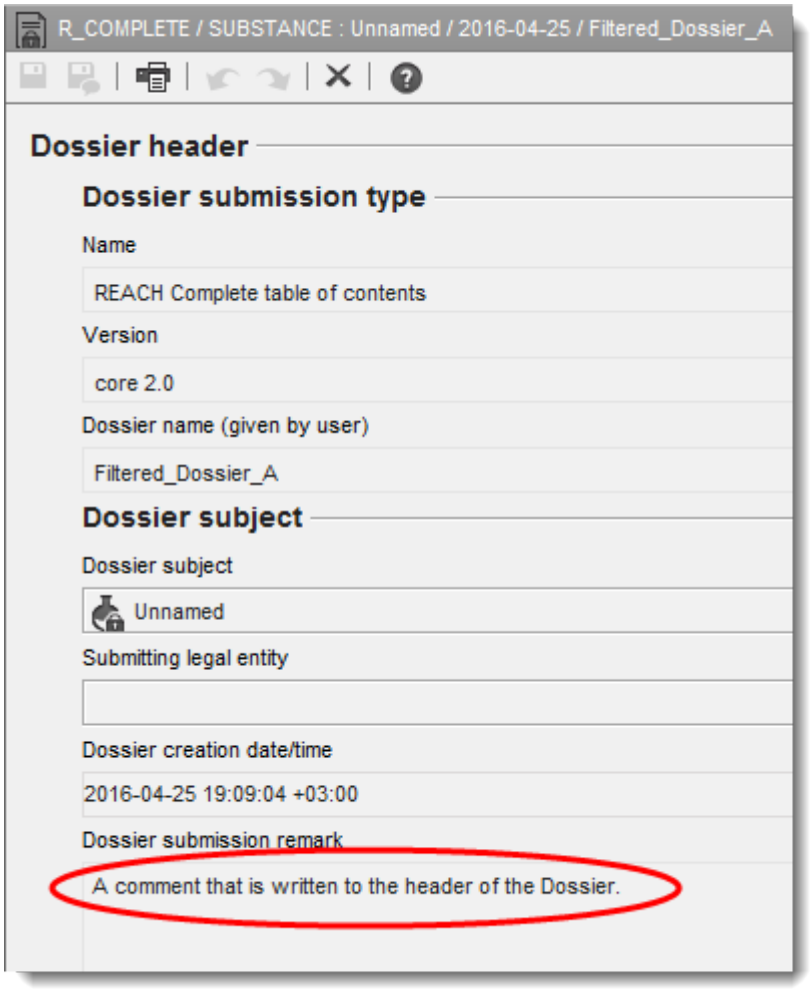
Names and comments will not be a part of actual disseminated dossiers produced by ECHA. They are created by the Dissemination preview plugin purely for informational purposes.

Figure 92: Name and Comment for Filtered Dossier



Your comment, if any, will be saved in the Dossier submission remark in the Dossier header.

Figure 93: Comment for Filtered Dossier



Click *Next*. The tool generates the Filtered Dossier.

Very Important: Do not quit IUCLID until the Dissemination preview has finished working, or there is a risk you will corrupt your IUCLID installation's database.

When the Filtered Dossier has been generated you will be presented with the Dissemination preview report as shown in the next figure.

21.4. Dissemination preview report

Once the report window appears, the Filtered Dossier is saved in your IUCLID database. The Filtered Dossiers are converted to submission type *REACH Complete*.

The Dissemination preview report indicates which information from the input dossier is and is not present in the Filtered Dossier created by the Dissemination preview tool.

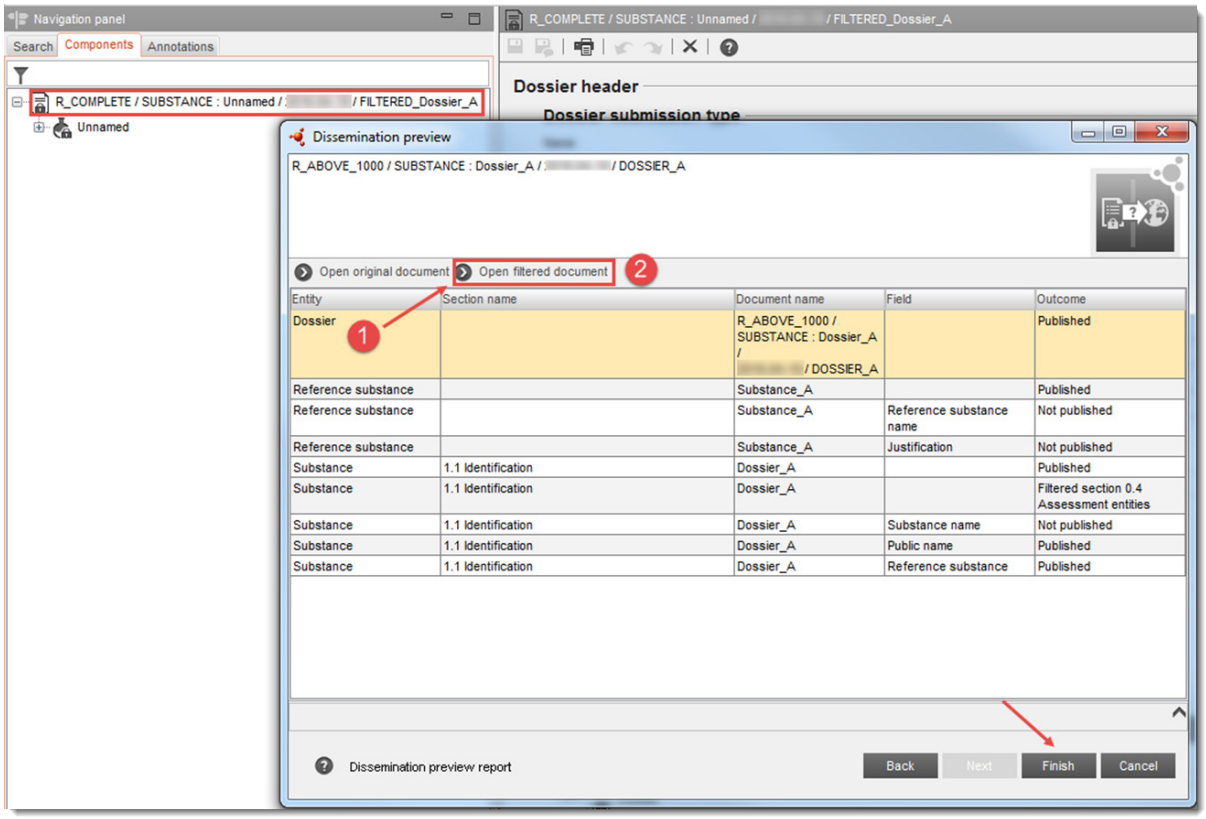
You can review more specific details on the filtering outcome from the report table.

The report table can be copied for pasting to e.g. Excel, Word. Copy report table using the keyboard shortcuts CTRL+A and CTRL+C.

Important: If you do not copy the Dissemination preview report, it will no longer be available if you close the report window.

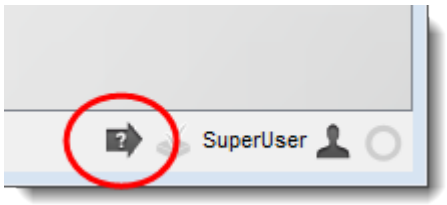
Selecting the first row of the report table *Dossier* and clicking in the report toolbar *Open filtered document*, opens the Filtered Dossier in the main IUCLID window behind the Dissemination preview report window, as shown below.

Figure 94: Dissemination preview report



The Dissemination preview window can be minimised by clicking on the icon in the top right corner, and displayed again by clicking on the Dissemination preview icon in the bottom right corner of the IUCLID window, shown below. Minimising the window hides it from view, but retains all the information about the ongoing preview.

Figure 95: Whist the Dissemination preview plugin is running, its icon in the bottom right corner of the main IUCLID 6 window is dark grey. In that state, clicking on the icon displays the plugin window uppermost.



You can sort the Dissemination preview report table by, for example,. *Section name* by clicking on the column header in the report table.

If you wish to compare specific parts of the dossier before and after filtering, select a row in the report table, and from the report toolbar *Open original document* and *Open filtered document* (can also be achieved by right-clicking on the row in the Dissemination preview report table).

Note that *Open filtered document* is inactive if the record to which the row relates is empty after filtering. Empty elements of the dossier are cleaned-up in the filtering post-processing.

Clicking on the button *Finish*, displays the Filtered Dossier. The report will not be saved unless you have copied it.

The Filtered Dossier can afterwards be located via Dossier view, or through any query searching for a dossier, by searching for the name you gave the Filtered Dossier.

Very Important: Do not submit a Filtered Dossier to ECHA as your Registration. Such Filtered Dossiers are for your own information only.

22. Getting additional help

If you need help in addition to what is presented in the IUCLID 6 help system, you can:

1. Consult the IUCLID 6 website at http://echa.europa.iuclid6 where you will find news articles, various manuals, and a collection of Frequently Asked Questions. For example, more information is available on the migration of data from IUCLID 5, and the IUCLID plugins.
2. Contact the ECHA Helpdesk free of charge through the contact form at the address http://echa.europa.eu/contact/helpdesk-contact-form. This is an online web form where you can specify the type of help you need, so that it can be forwarded to the closest matching expert. The Helpdesk team will reply to your question in English within 15 working days. You can also receive a reply in another EU language, but note that this may take longer than 15 days.

22.1. Contacting the ECHA Helpdesk for technical support

IUCLID 6 has been carefully tested. However, if you experience any problems during the installation and/or use of IUCLID 6 that appear to be caused by a technical problem with the software, you can report it via a web form provided by the ECHA Helpdesk at address:

http://echa.europa.eu/contact/helpdesk-contact-form

If you are using IUCLID 6 Server, in the first instance, report any problem to the system administrator.

The form has three steps:

1. Enter the contact details, the relationship to the EU, and select the topic *I need technical support on IUCLID 6*.
2. Enter a subject and a question and fill out the technical options as best you can. For example describe the steps you made, up until the problem occurred. If there was an error message given in the messaging area include it. If you want to send any files to ECHA, that is done on the next page.
3. You can attach file(s) here, for example screen shots and log files. Confirm all the details and then click *Send email*.

23. Backup/Restore

In the installation package of IUCLID 6 Desktop there is standalone application that can be used to both backup and restore all the data associated with an installation of IUCLID 6. The backup function writes all the data to a single file that is given the extension `i6b`. It is unlikely that the maximum permissible size of a single file will be exceeded, so long as the installation contains the amount of data for which IUCLID 6 Desktop is intended to be used, that is, up to about a hundred *Substance* datasets. The restore function reads from any file that was created by the backup function.

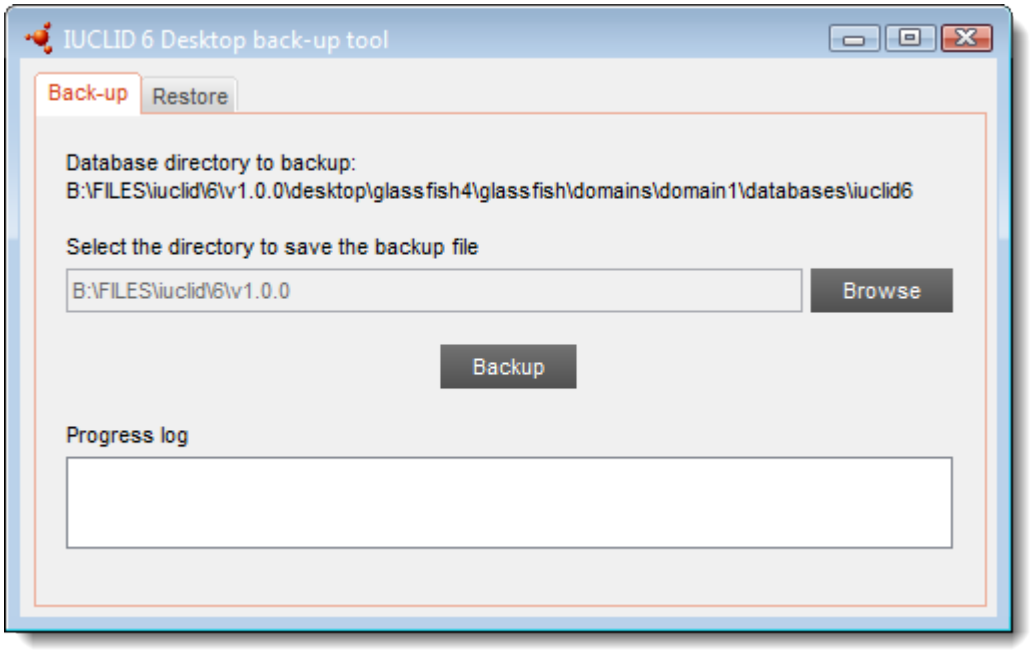
To run the backup/restore application double-click on the file `iuclid6-backup-restore.exe`. There is no need to shut IUCLID 6 down first. If IUCLID 6 Desktop is running, it is automatically shut down, and then restarted after the backup or restore process has finished.

To close the backup/restore application after use, click on the cancel icon at the top right of the window.

23.1. Backup

The backup/restore application opens with the Backup tab activated, as shown below:

Figure 96: Backing up all the data in an installation of IUCLID 6 Desktop

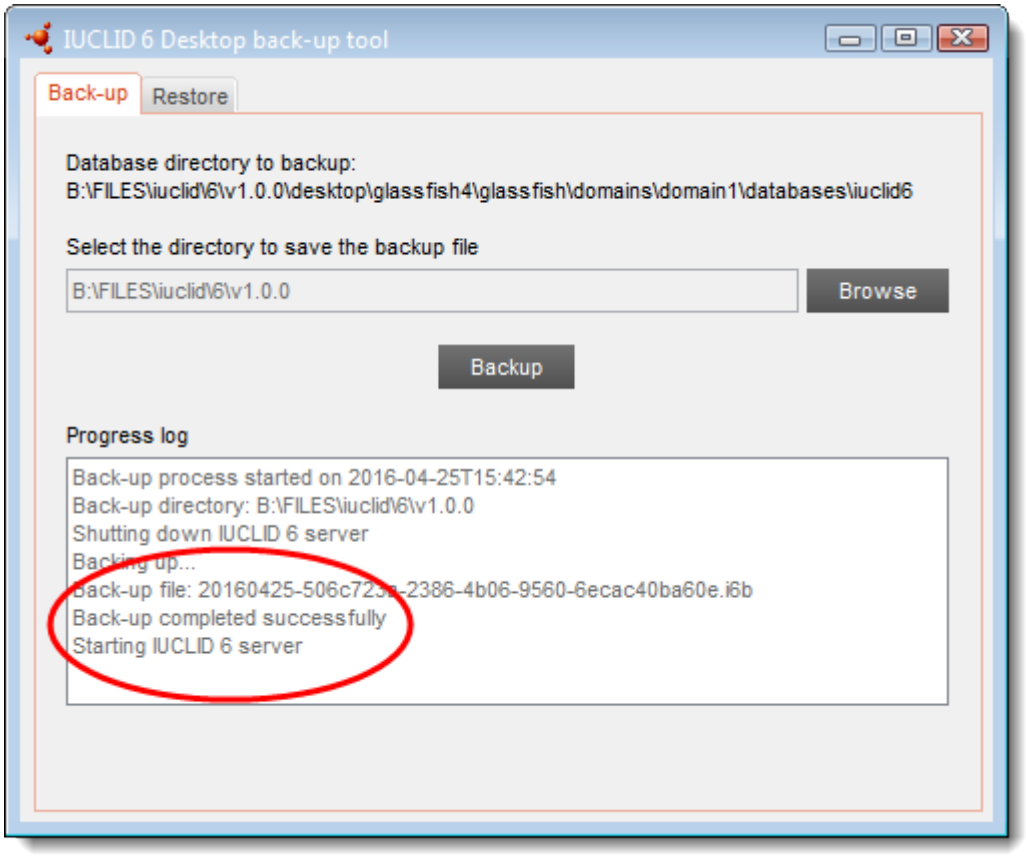


In the first field, check that the path leads to the database in the installation of IUCLID 6 that is to be backed up. The default value is:

```
<installation
folder>\glassfish4\glassfish\domains\domain1\databases\iuclid6
```

In the second field, enter the destination of the output file. The default value is the home directory of the operating system user under which the application is run. To start the backup process, click on the button *Backup*. Watch what is shown in the window labelled *Progress log*. At the end of a successfully completed backup, started whilst IUCLID 6 Desktop was running, the interface should look like the one shown below.

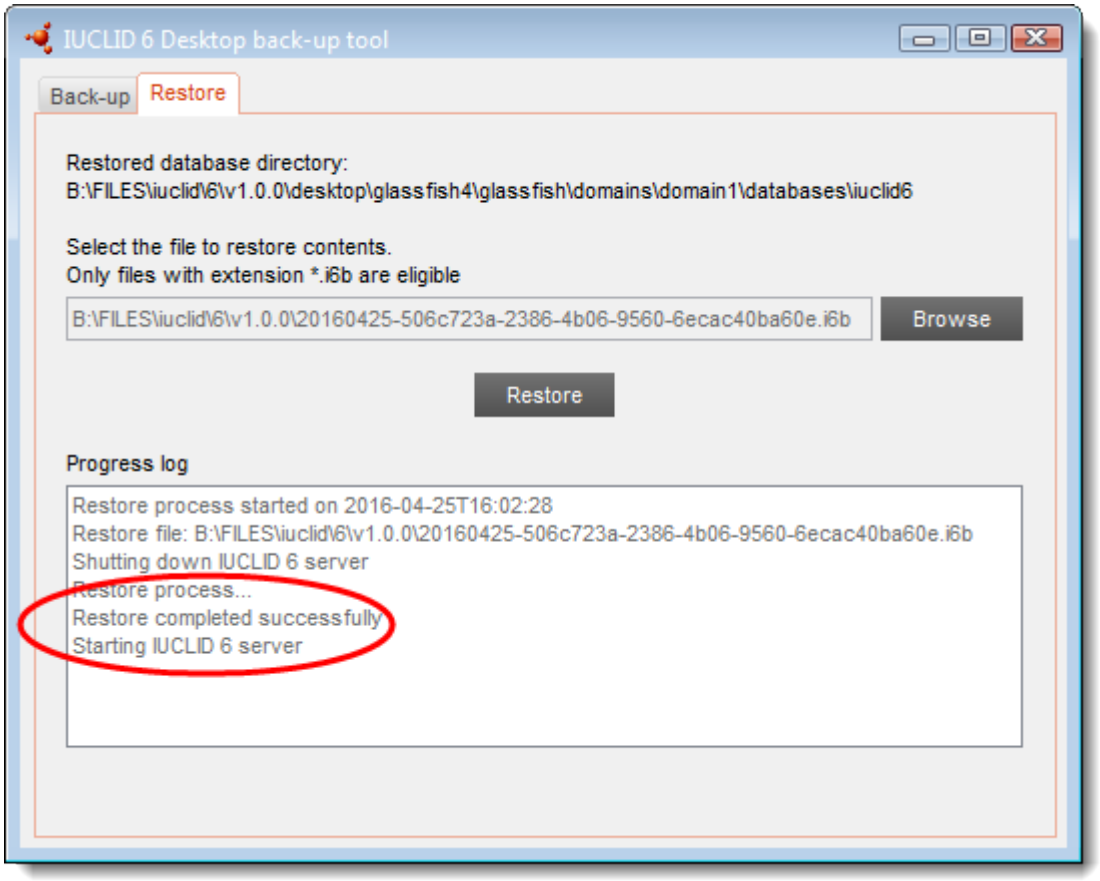
Figure 97: A successfully completed backup of the data in an installation of IUCLID 6 Desktop



23.2. Restore

Run the backup/restore application by double-clicking on the file `iuclid6-backup-restore.exe.` , and then click on the tab, *Restore*. In the first field, select the file with extension `i6b` from which the restoration is to be done. Click on the box *Restore*. At the end of a successfully completed restoration, started whilst IUCLID 6 Desktop was running, the interface should look like the one shown below.

Figure 98: A successfully completed restoration of data to an installation of IUCLID 6 Desktop



24. Updating IUCLID 6 and its plugins

IUCLID 6 is updated by running a software tool that is available on the IUCLID 6 web site. The tool updates all of the IUCLID 6 application and its plugins in one action. There is no need to update plugins separately. It is possible to set IUCLID 6 so that it automatically checks for the availability of updates, as described in section *15.1.2.5 Updates*. This section also describes how to check whether you are using the most recent version.