


Functionalities of IUCLID 6



The image displays the IUCLID 6 logo, which consists of a stylized molecular structure of three red spheres connected by lines, positioned to the left of the text 'IUCLID 6'. The text 'IUCLID' is in a grey, sans-serif font, and the number '6' is in a larger, bold, red font. The background is a faded periodic table of elements. At the bottom left, there are logos for ECHA (European Chemicals Agency) and OECD (Organisation for Economic Co-operation and Development). At the bottom right, there is a small graphic of three white spheres of varying sizes.

ECHA
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IUCLID 6 is developed by the European Chemicals Agency in association with the OECD

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Changes to this document

Date	Release	Changes
30/10/2019	4.2	Minor corrections and update of copyright date. Added warning that <i>Compare Dossiers</i> is available only in the web interface.
24/10/2018	3.1	Added a description of the field <i>Origin. Assessment entity</i> in section 0 of the substance table of contents moved to section 1.10 and renamed to <i>Assessment approach</i> . Edited definition of technical terms. For a complete list of changes, see the release notes.
13/10/2017	2.0.0	Added description of new functionality: <i>Fee Calculator</i> . Described changes to the functionalities: <i>Export, Report generator, DNEL calculator, and Flags</i> . Added a description of warnings given where dynamic fields are not filled out logically. For a complete list of changes in IUCLID 6 v2.0.0, see the release notes.
28/04/2017	1.3.0	Added description of new functionality: <i>PNEC calculator</i> . Described changes to the functionalities: <i>Create Dossier, Report generator, DNEL calculator, and Background jobs</i> . Added more detail to descriptions of <i>Legal entity</i> and <i>Import</i> .
31/01/2017	1.2.0	Added description of new functionalities: Hyperlink, DNEL calculator, ordering and bulk actions for TOC entries, Changes of visibility of plugins. Updated the specification of the file format for Import/Export Users. Report generator: custom templates and generating an XML file for use with the SPC Editor.
30/09/2016	1.1.0	Added description of new functionalities, <i>Dossier comparison</i> and <i>Inventory management</i> . Updated the description of the <i>Validation assistant</i> . Added <i>Replace</i> option for <i>Import</i> . Created links to translations of this document.
21/06/2016	1.0.2	Added a description of how to prevent the locking of the <i>User, SuperUser</i> . Stated the default passwords given to <i>Users</i> when they are imported, or created by importation of a CSV file. Updated the description of the <i>Validation assistant</i> in sections <i>19.4.3.2. Validation assistant report toolbar</i> and <i>19.4.3.4. Validation assistant report table</i> . 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.
29/04/2016	1.0.0	First version

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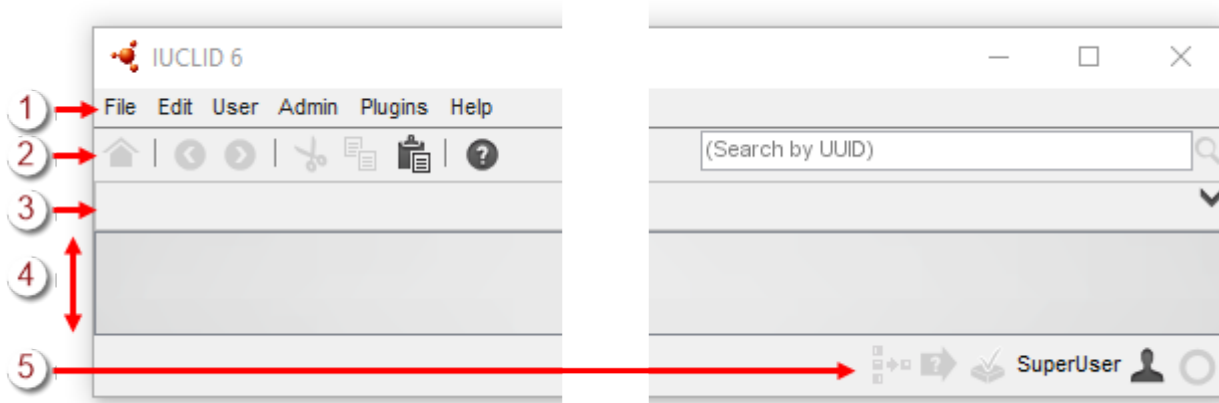
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1. Overview of the interface

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 menu 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 are defined in the context of IUCLID.

Table 1: Some technical terms in IUCLID

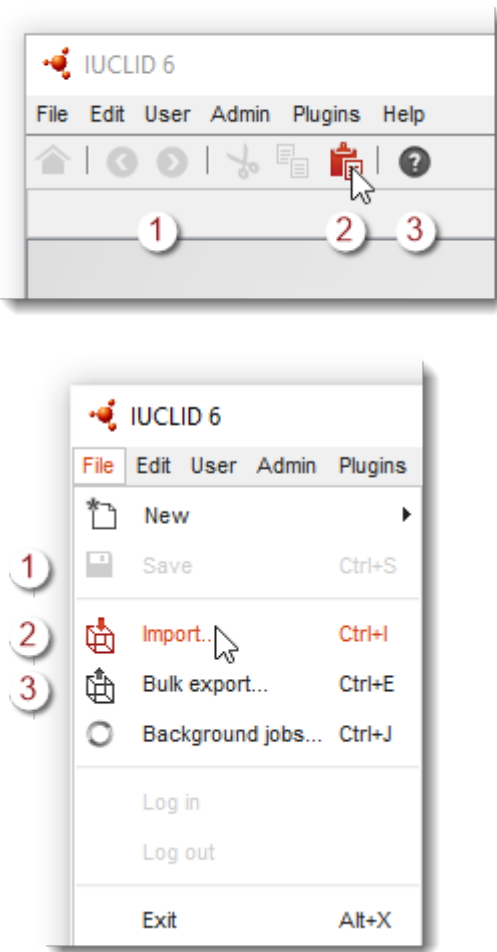
Term	Description
Entity	<p>Entities in IUCLID are software objects that are used to store data that has a particular purpose, which depends on the type of entity. The types of entity are: <i>Dossier, Substance, Mixture/Product, Category, Template, Annotation, Legal entity, Legal entity site, Reference substance, Test materials, Contact, Literature reference.</i></p> <p>Entities can be viewed, printed, and deleted individually. They can also be exported and imported as individual files. With the exception of <i>Dossier</i>, entities are designed to be referred to by other entities. This reduces duplication of data sources, and improves data consistency. On saving a change to an entity, the change is immediately seen in any other entity that refers to it. An exception to that is a <i>Dossier</i>, which is a read-only snapshot of data.</p>
Dataset	<p>A <i>dataset</i> is a collection of documents that relate to a particular chemical substance, or grouping of chemical substances. It can be of the following types: <i>Substance, Mixture/Product, Template.</i></p> <p>For clarity and where appropriate, the type of the dataset should be stated, for example <i>Substance dataset.</i></p>
Document	<p>A <i>document</i> is a page that contains functionality for creating, viewing or modifying an <i>entity</i>, a <i>record</i>, or a <i>summary</i>. The term <i>document</i> is also used to mean a standardised set of data that exists in a dataset in a particular section. For example, in the OECD harmonised templates under the section named <i>Acute toxicity: oral</i>, there can be one or more documents that all have the same structure, but do not necessarily have the same name, or contain the same values.</p> <p>For more information about types of documents, see section 1.9.2 TOC (<i>Table of Content</i>) tab in the navigation panel.</p>
Fixed	The term <i>fixed</i> means that a document is in a section that can contain only one document.
Field	A <i>field</i> is a location within an entity or document in which a specific piece of data is stored. The type of data is the same throughout an individual field, for example, the field could contain free text, a text value chosen from a drop-down menu, a number, or a date. There can be many fields in one document. An example of a field is <i>IUPAC name</i> .

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

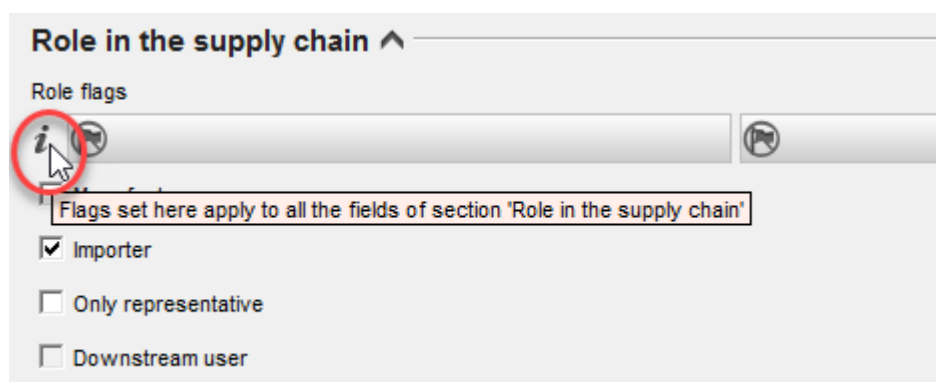
A free text template is a piece of text designed to help the user to enter all the required information into a field that can contain any text value. It provides a model text which must be edited to fit in with the particular circumstances of the user in that context.

To open a free text template, click on the icon that shows the letter A with an arrow at its lower right, **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.

1.3.2. Flag

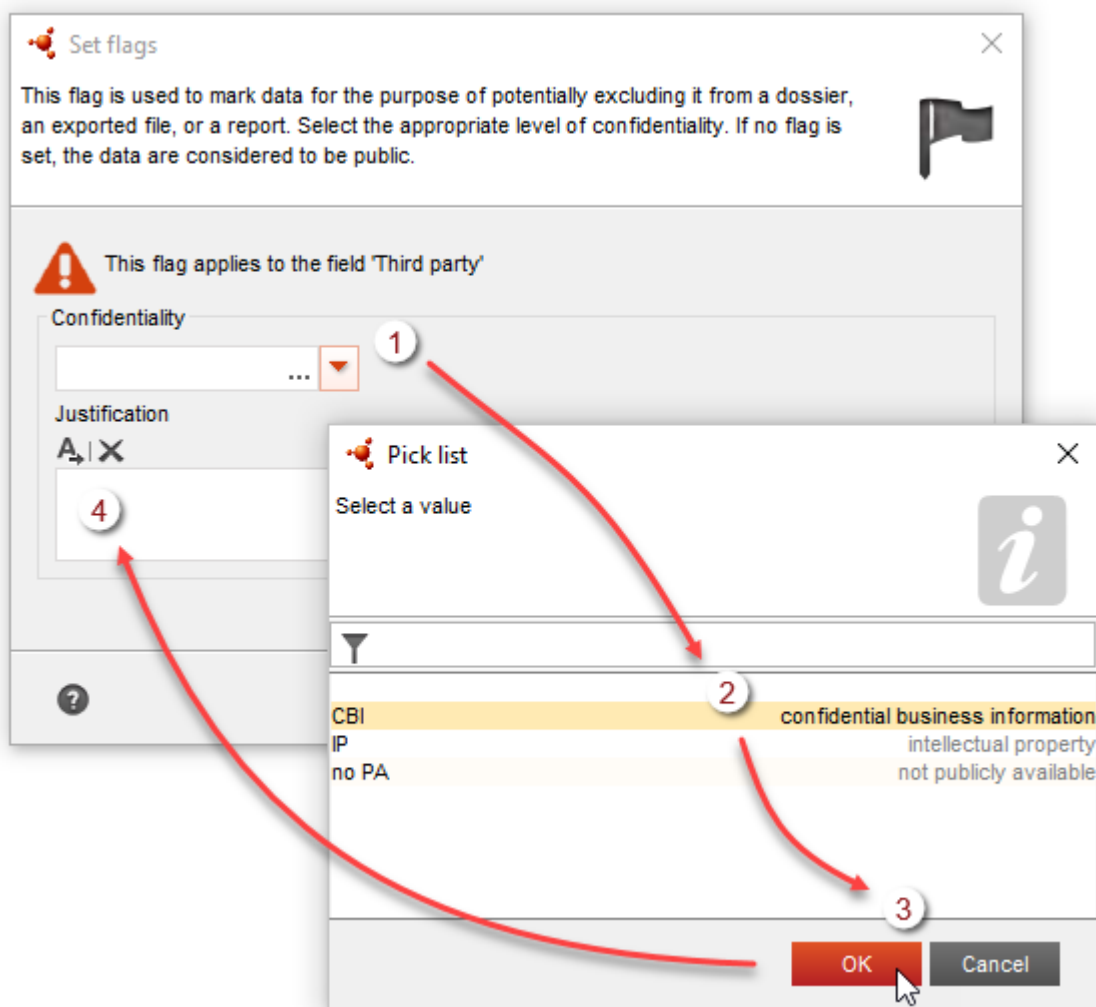
Some individual fields and groups of fields can be labelled with a flag. By default, no flags are set. In each location where flags can be set, one can be set for confidentiality, and one for regulatory programme. These are set and acted upon independently. Flags can be used to filter data when placing it in a *Dossier*, exporting or, printing. The field or fields to which a pair of flags refer is indicated by hovering over an info icon to the left of the flags, as shown in the example below:

Figure 3: Example of how to view to which data a flag applies



In the example above, the flag refers to all of the fields in the section *Role in the supply chain*.

To set a flag for confidentiality, first open the dialogue box by clicking on the left-hand flag button, as shown below.

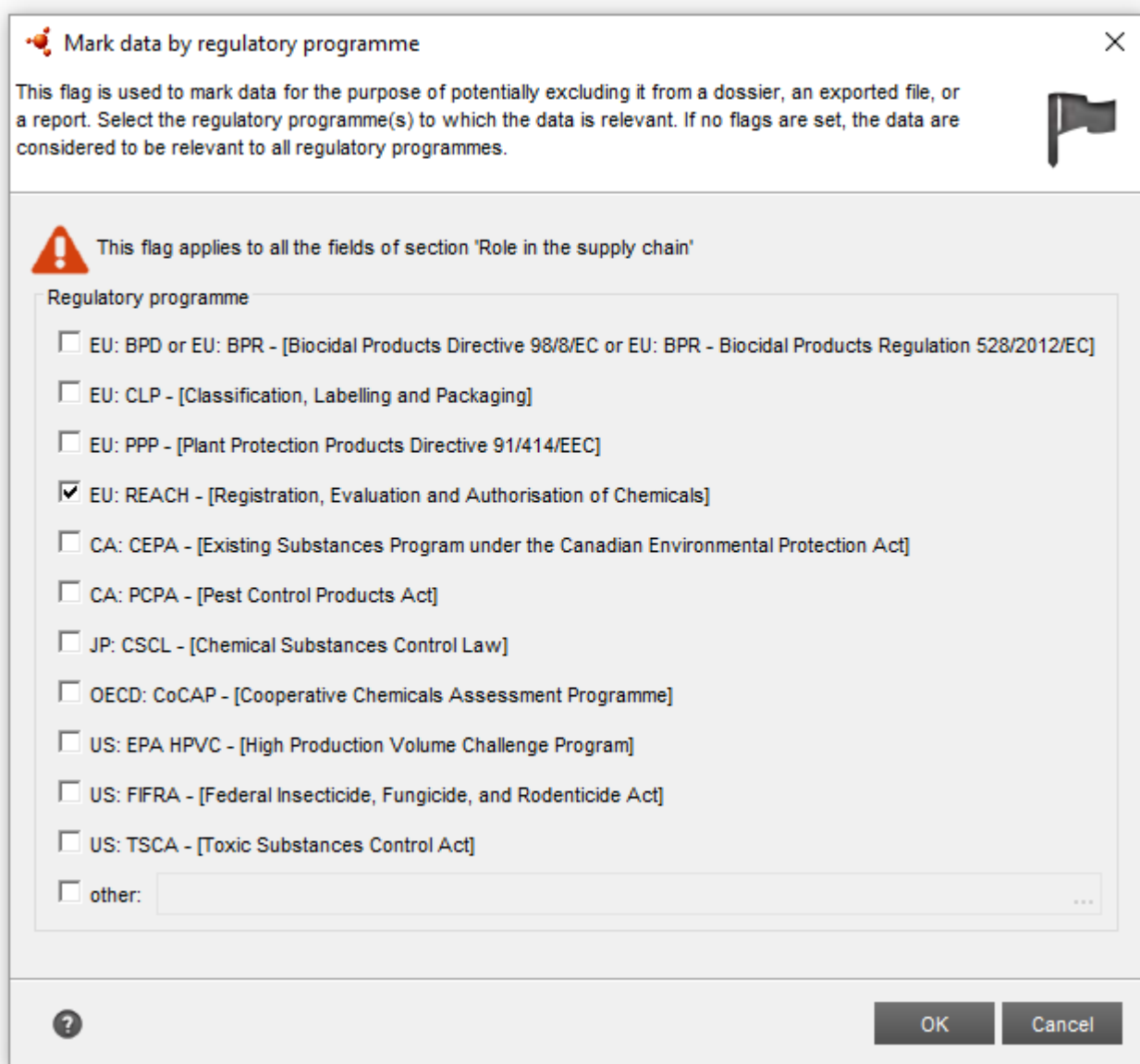
Figure 4: Set confidentiality in a flag

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

If a justification of the confidentiality is required (4), 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 a flag for an association with a regulatory programme, first open the dialogue box by clicking on the right-hand flag button. Then, tick one or more of the boxes, as shown below.

Figure 5: Set a flag for association with a regulatory programme



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

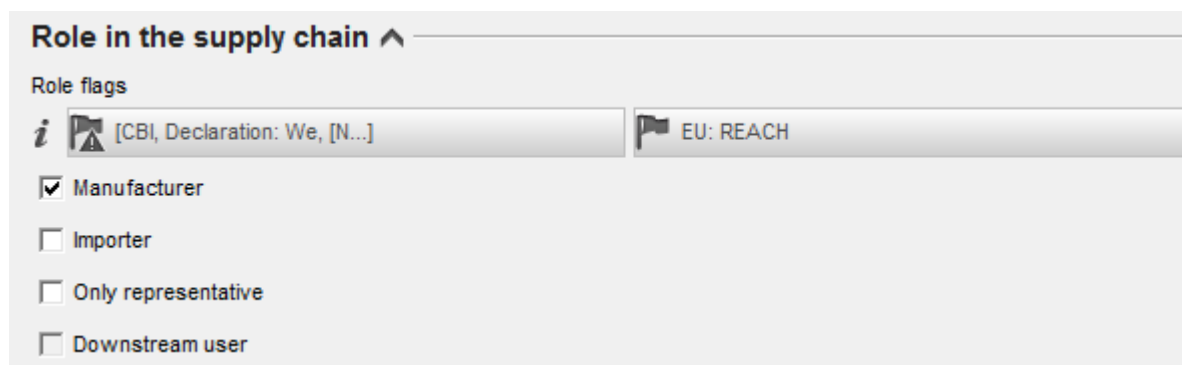
Table 2: The icons for the states of a flag

Icon	State
	No flag is set.
	A flag is set but confidentiality is not involved. The flag refers only to a regulatory programme.
	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, flags are set that indicate the field contains confidential business information, and is associated with the REACH legislation of the EU.

Figure 6: Flags applied to an example field

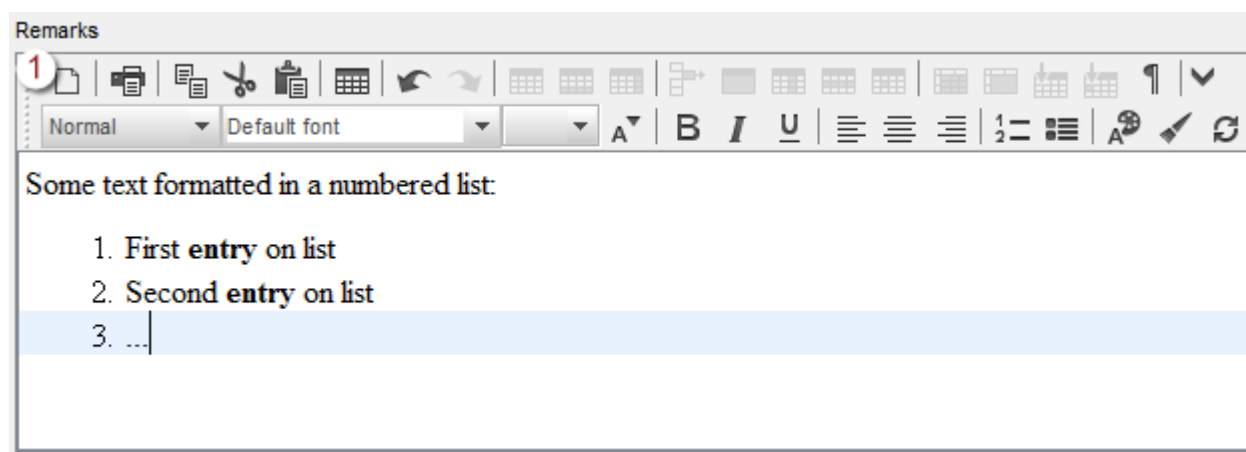


The screenshot shows a web interface for 'Role in the supply chain'. It features a section titled 'Role flags' with a dropdown menu showing '[CBI, Declaration: We, [N...]]' and a flag icon labeled 'EU: REACH'. Below this are four checkboxes: 'Manufacturer' (checked), 'Importer', 'Only representative', and 'Downstream user'.

1.3.3. Rich text input

Some fields allow text to be entered in rich text format. To see what a button does, hover the cursor over it and read the label that appears. An example of some formatted text is shown below.

Figure 7: Rich text field



The screenshot shows a rich text editor titled 'Remarks'. It has a toolbar with various icons for text formatting, including bold, italic, underline, and list creation. A red circle with the number '1' highlights the first icon in the toolbar. The text area contains a numbered list: '1. First entry on list', '2. Second entry on list', and '3. ...'.

1.3.3.1. Uploading HTML text templates in to rich text fields

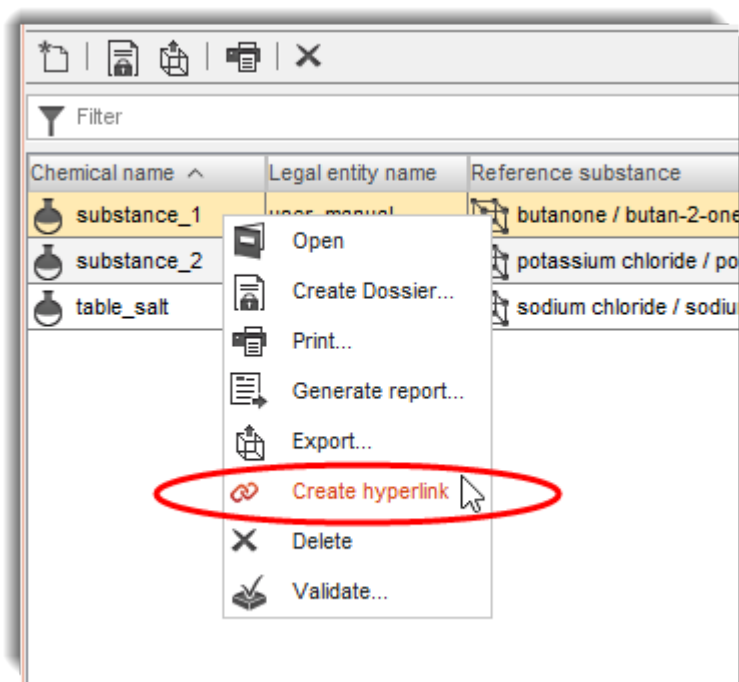
The button at the top left of the field, marked with a 1 in the screenshot above, is used to import text in HTML format. For example, if a text template has been provided for the field in HTML format, upload it using this feature.

1.3.4. Hyperlink

The feature *hyperlink* provides a way of creating a web-based hyperlink to an entity or document within IUCLID 6. After following the link, the entity or document is displayed in the data window. This feature is available only for IUCLID 6 Server.

To generate the address for the hyperlink, right-click on entity or the document, and then select *Create hyperlink* as shown below. This places the address of the hyperlink in to the clipboard of the operating system, from where it can be pasted as required. The option to create a hyperlink can be accessed from entries within the search results and the table of contents (TOC) in the *Navigation panel*.

Figure 8: Hyperlink



The hyperlink points to the UUID or UUIDs that are displayed in the *Information panel* at the time of creating the hyperlink. A hyperlink can be made to a whole Dossier, or an entity or document within a Dossier. A hyperlink to a whole Dossier points to the Dossier header.

Following the hyperlink successfully requires: access to the instance of IUCLID 6 to which the hyperlink points, User credentials to log in, and at least read-access to the entity or document itself. If the computer on which the hyperlink is followed is known to be capable of connecting to the instance of IUCLID 6, no additional configuration is required. Technical aspects of *hyperlink* are described in the subsection below.

Hyperlinks are a convenient way of providing co-workers with quick and easy access to entities and documents shared within an instance of IUCLID 6. A hyperlink can be placed on a web page, sent in an email, or included in a PDF document, just like any other hyperlink.

1.3.4.1. Technical aspects of hyperlink

The requirements for running the IUCLID 6 client are stated on the IUCLID 6 website [here](#). The hyperlink feature uses *Webservices*. When the hyperlink is followed, the IUCLID 6 client is downloaded from the server to which the hyperlink points. The specific entity or document to which the hyperlink points is identified in the hyperlink using HTTP parameters. The address of the hyperlink is an HTTP universal resource locator (URL) of the form:

```
http://<server name>:<port>/webstart/launch.jnlp?uuid=<entity or document UUID>[&snapshot=<dossier UUID>]
```

Table 3: The HTTP parameters for hyperlink

Name	Purpose
uuid	The UUID of the entity or document to be displayed in the data window.
snapshot	The UUID of the Dossier that contains the entity or document to be displayed in the data window. This parameter is required only where the hyperlink points to a Dossier, or a target within a Dossier. If the hyperlink points directly to a Dossier, the value of this parameter is the same as that for <code>uuid</code> .

Examples

A hyperlink to a Category.

```
http://<host>:8080/webstart/launch.jnlp?uuid=361577f5-df5e-4a39-a2e2-55204a9905ab
```

A hyperlink to the same Category inside a Dossier.

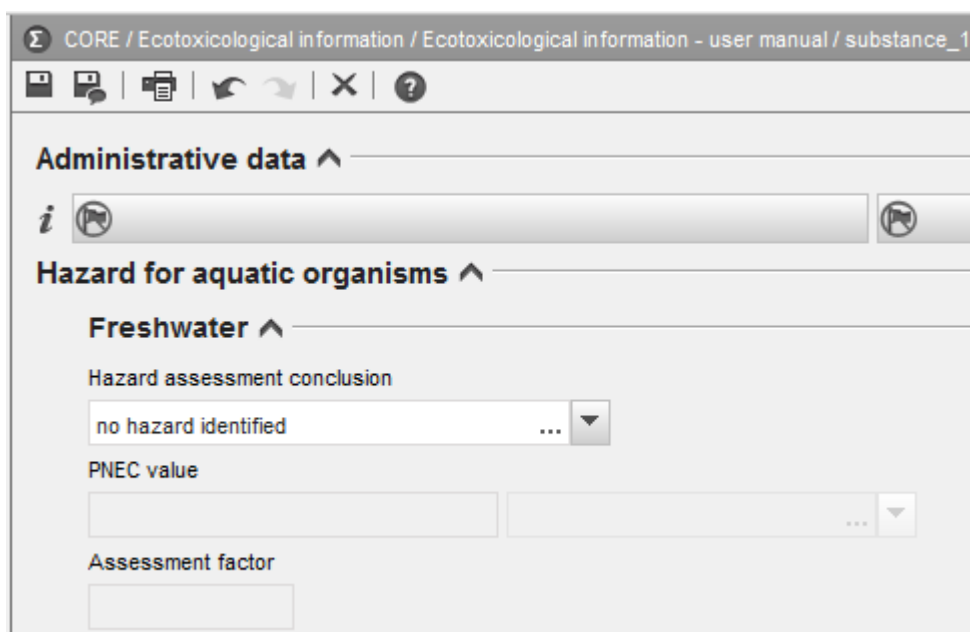
```
http://<host>:8080/webstart/launch.jnlp?uuid=361577f5-df5e-4a39-a2e2-55204a9905ab&snapshot=d0f3361e-2b24-425f-bda0-3dee0c9a8c9e
```

1.3.5. Dynamic fields

To help users to enter data in a logically consistent way, the values that can be entered into some fields are dependent on the values that are already in other fields. If a field is edited such that the rules of the dependency are broken, the affected data are shown with a yellow background. The user must then change what has been entered until it is logically consistent.

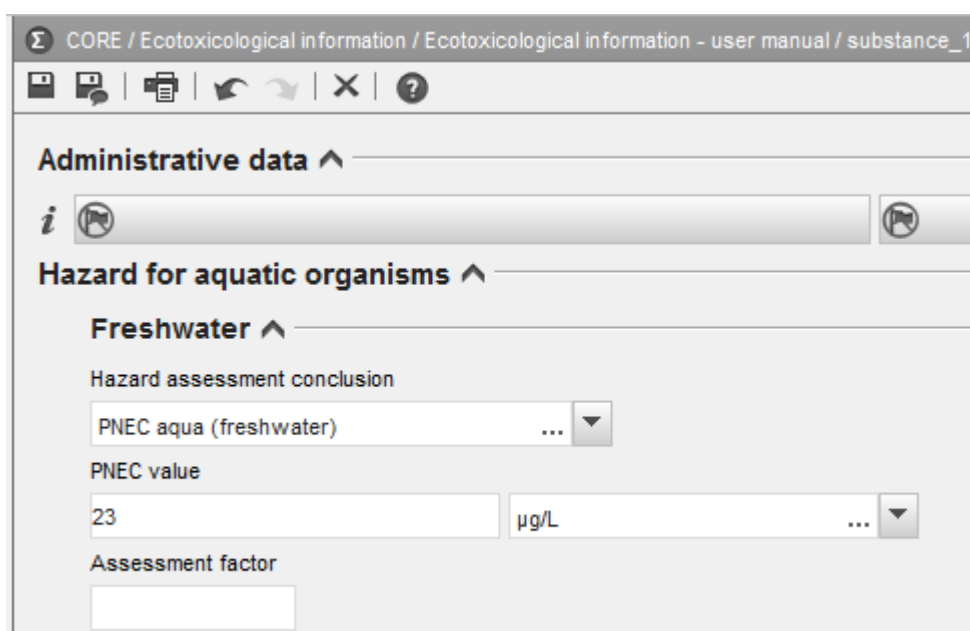
Example

In the example shown below, the field *Hazard assessment conclusion* has the value *no hazard identified*. Due to the lack of hazard, there is no meaningful value for the PNEC. Therefore, the field *PNEC value* is greyed out and no value can be entered.

Figure 9: Dynamic field dependency – example 1

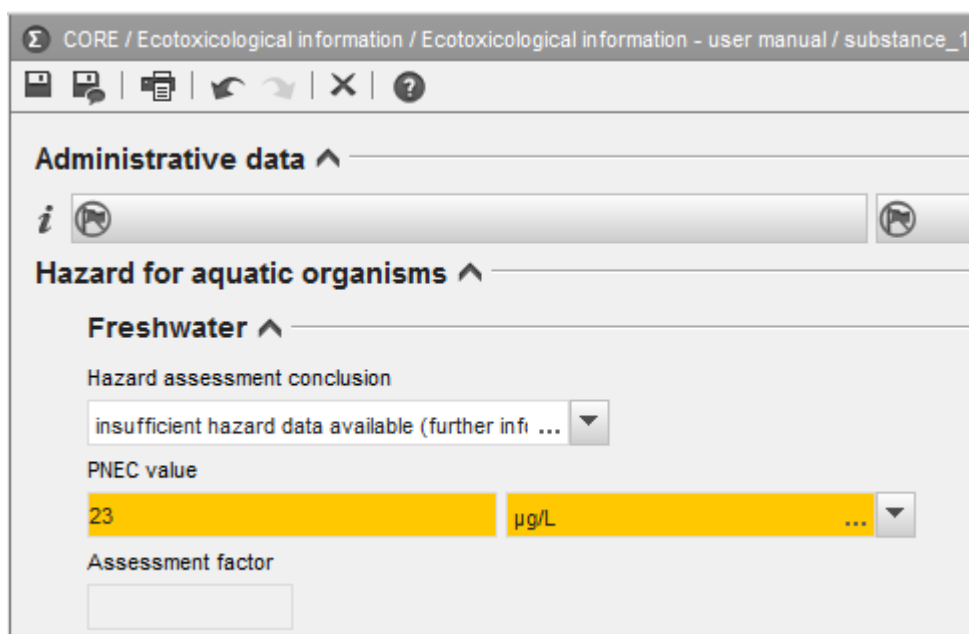
The screenshot shows a web application interface for IUCLID 6. The breadcrumb trail at the top reads: CORE / Ecotoxicological information / Ecotoxicological information - user manual / substance_1. Below the breadcrumb is a toolbar with icons for save, print, undo, redo, close, and help. The main content area is divided into sections: 'Administrative data' (expanded), a search bar, and 'Hazard for aquatic organisms' (expanded). Under 'Hazard for aquatic organisms', the 'Freshwater' section is expanded, showing three fields: 'Hazard assessment conclusion' with a dropdown menu currently displaying 'no hazard identified', 'PNEC value' with an empty input field and a unit dropdown, and 'Assessment factor' with an empty input field.

In the example shown below, the field *Hazard assessment conclusion* has the value of *PNEC aqua (freshwater)*. A value can be entered in to the field *PNEC value*. The value is *23 micrograms per litre*.

Figure 10: Dynamic field dependency – example 2

This screenshot shows the same IUCLID 6 interface as Figure 9, but with updated values. The 'Hazard assessment conclusion' dropdown now displays 'PNEC aqua (freshwater)'. The 'PNEC value' field contains the number '23' and the unit dropdown is set to 'µg/L'. The 'Assessment factor' field remains empty.

In the example shown below, the field *Hazard assessment conclusion* has been changed from *PNEC aqua (freshwater)* to *insufficient hazard data available...*, but the value of the PNEC is still in place, which is not logically consistent.

Figure 11: Dynamic field dependency – example of warning


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 *1.7.4 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 12: 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 [15.1.2.6 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. Plugins

This menu provides access to optional plugins that provide extra functionality to IUCLID 6. The plugins can also be accessed from icons on the home page, and where relevant, by right-clicking on an entity, such as a *Substance* or a *Dossier*.

1.4.6. Help

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

1.4.6.1. 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.

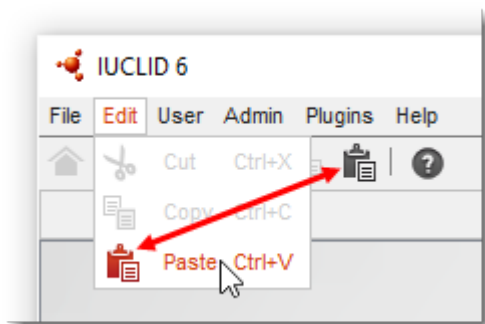
1.4.6.2. About

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 for the release of the application is shown at the bottom left of the first window.

1.5. Menu toolbar - upper

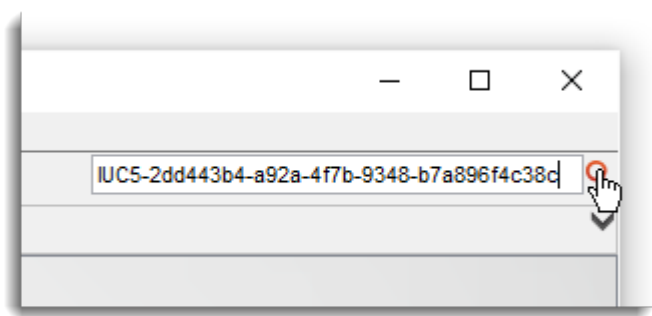
For user convenience, this menu contains links to frequently used functions that are also available via the main menu. An example is shown below in which the duplication of the link to *paste* is highlighted.

Figure 13: 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 14: 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*.

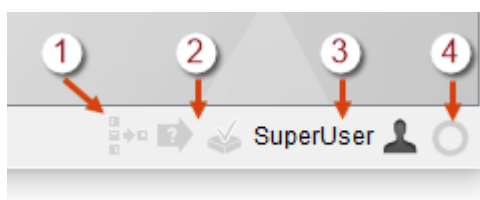
1.6. Message area

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 23 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 15: The lower menu toolbar

1.7.1. Inventory management

If the inventory manager is running, the icon is activated. Clicking on the icon whilst it is active, brings the window of the inventory management wizard to the front of the desktop of the operating system. More information is provided about inventory management in section 18 *Inventory management*.

1.7.2. Plugins

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


1.7.3. 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.

1.7.4. 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 at 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 4: The icons in the background jobs console



Icon	Meaning
	Cancel a running job.
	The job was completed successfully.
	A problem was encountered during the job. See the report for details.
	Clear, or close, the record of a completed job. It cannot be re-opened.
	Open the imported document in the data panel.
	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 <i>User</i> data, which can be done only from the background job.

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 three job records comprising, a bulk export of eight entities and two separate imports of a single entity. Two of the jobs were successful, as indicated by the green icon, , but for one of the imports, the red icon, , indicates that data was not imported. A Dossier could not be imported because it already exists in the database, and the feature *if newer than existing* was enabled in the import.



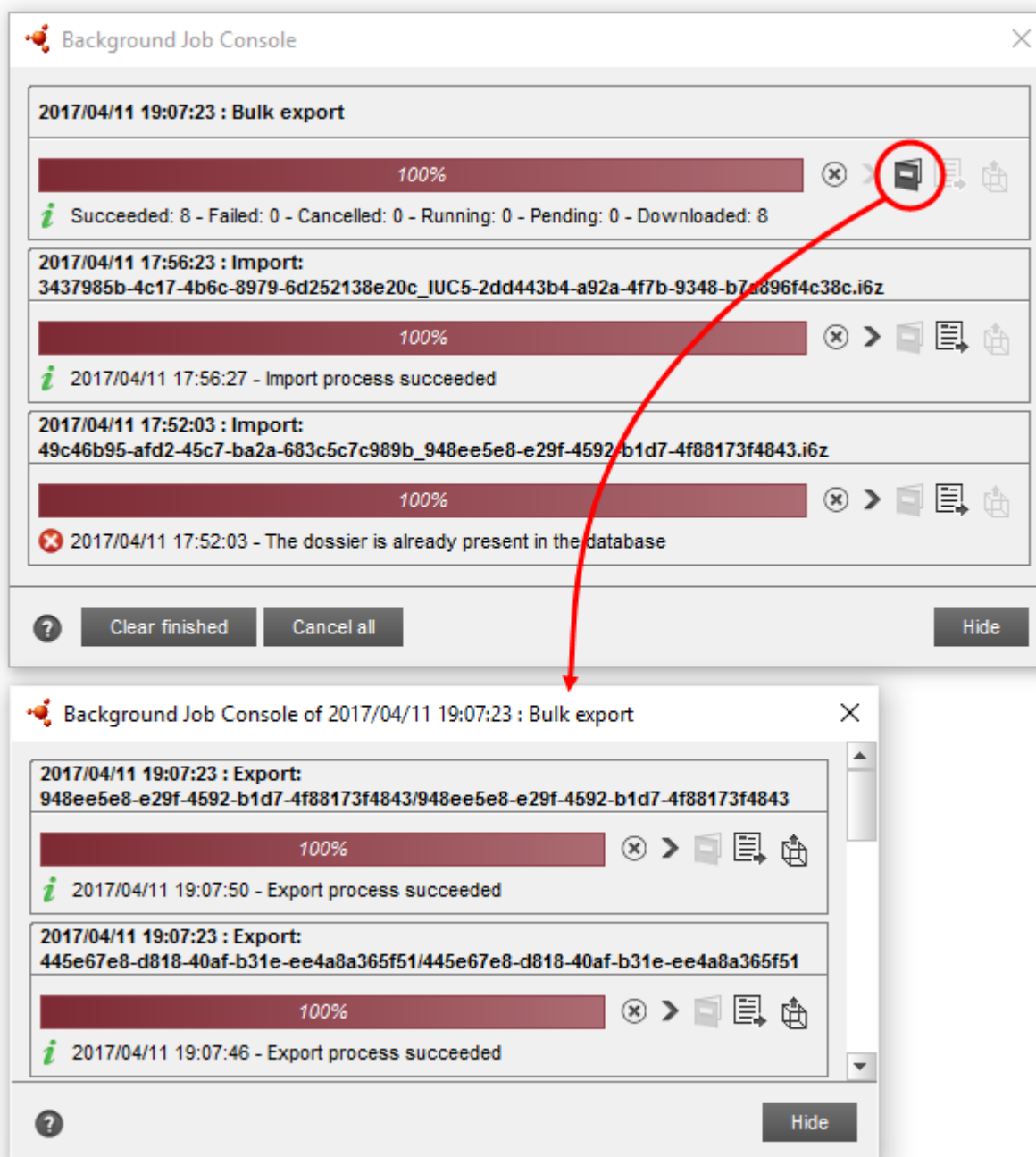
The record for the bulk export at the top of the list has 8 sub-jobs, whose records can be accessed individually by clicking on the icon for open document, , that is circled in red in the figure below. For bulk export, the icon for open, , is disabled because it is not relevant, but for the other entries it is active because the result of the job is a single entity in the database that can be viewed.


Figure 16: Example of records in the background job console



1.7.4.1. Background jobs for export

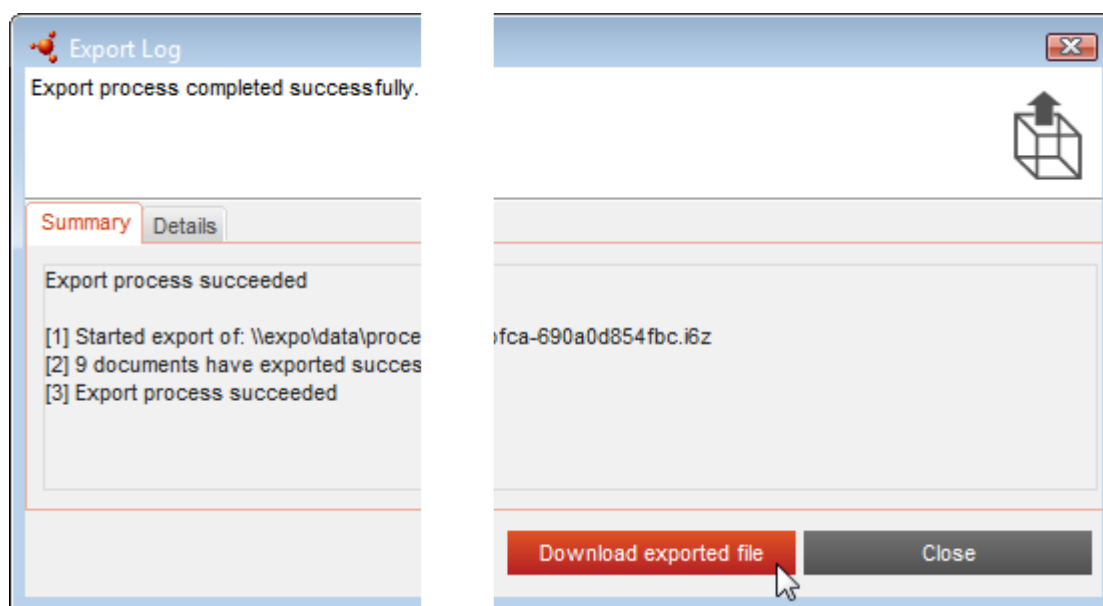
Exporting from the background job console is allowed only per sub-job. This can be seen in the example shown above where the export icon for the main job is disabled, but it is enabled for the sub-jobs. The data should already have been saved externally once while the background job ran, but this allows the save to be repeated, and to a different destination if required.

1.7.4.2. Reports for background jobs

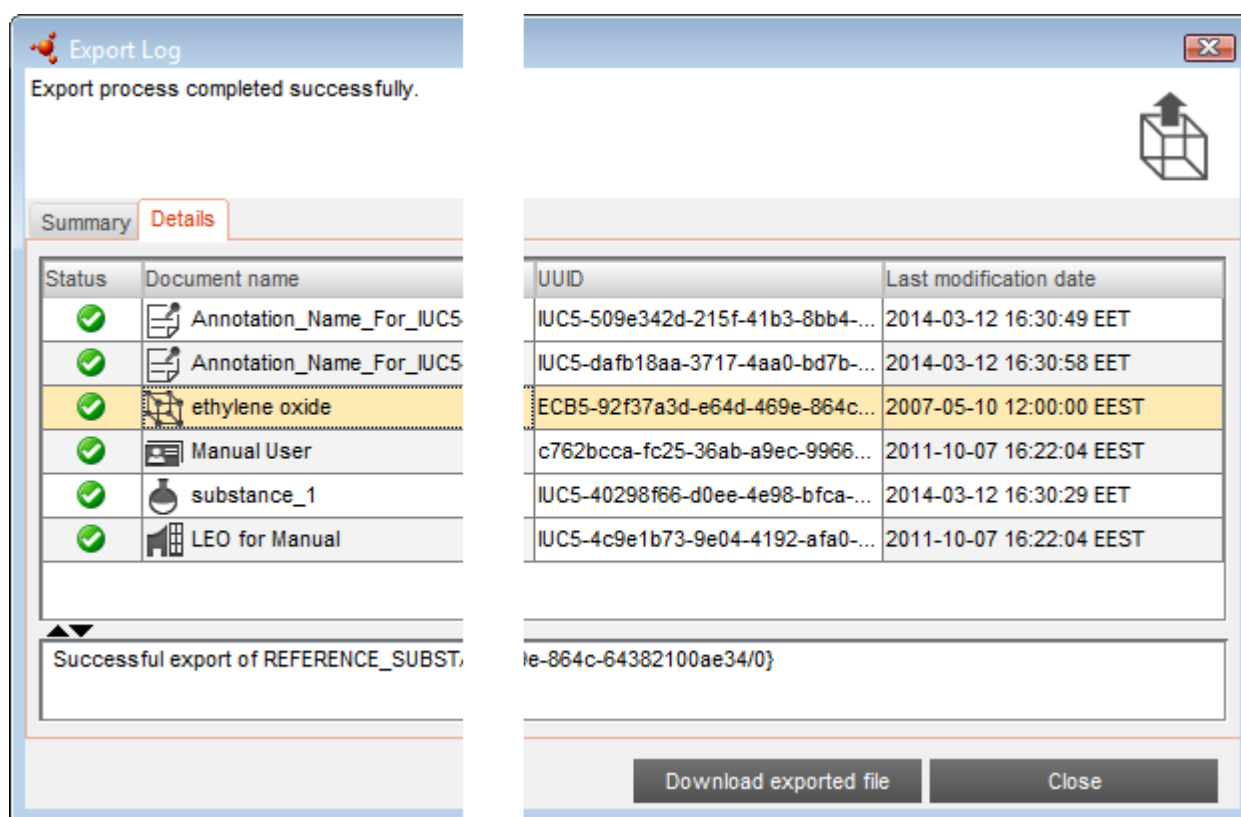
To obtain information about what happened in the job, click of the report icon . This opens a pop-up window that contains a detailed list of events that occurred during the job.

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 17: 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*.

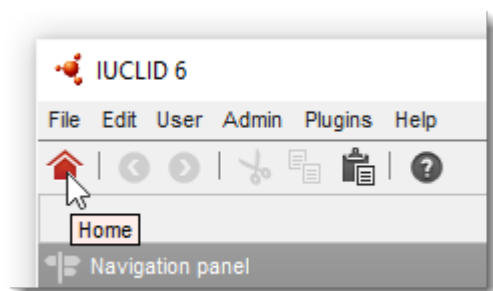
Figure 18: The details of a background job

1.7.4.3. Clearing background jobs

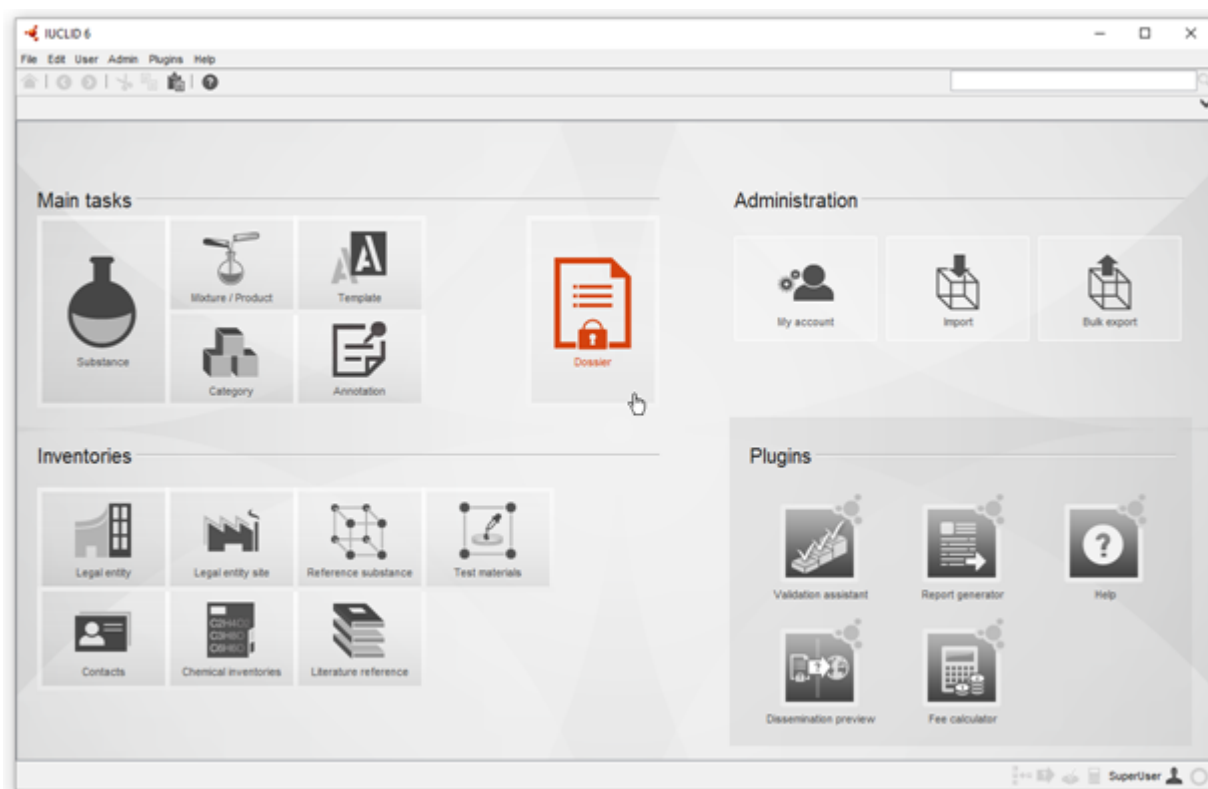
Do not clear a record of a job until you are sure that you no longer need the information it contains. Once cleared, or removed, the information is no longer available via the interface.

1.8. Home page

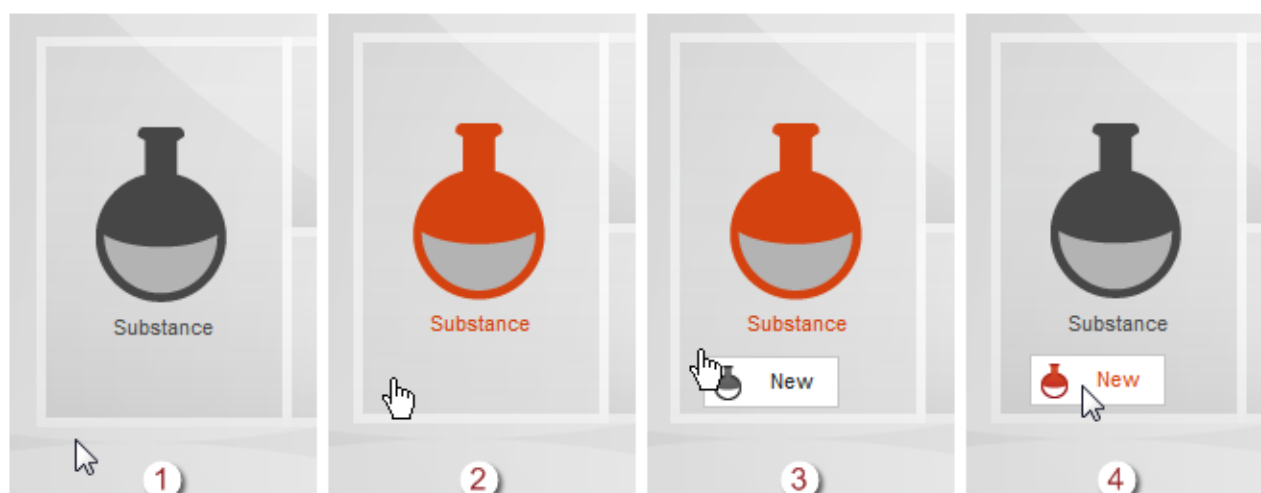
The home page is shown by default either when starting a desktop version of IUCLID 6, or when logging in to a server version. The home page can be viewed either by clicking on the house icon that is situated in the menu toolbar as shown below, or from the main menu Go / Home.

Figure 19: The icon for the home page

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

Figure 20: 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 21: Right-click on a panel on the home page to see its menu

Key for Figure 16:

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.

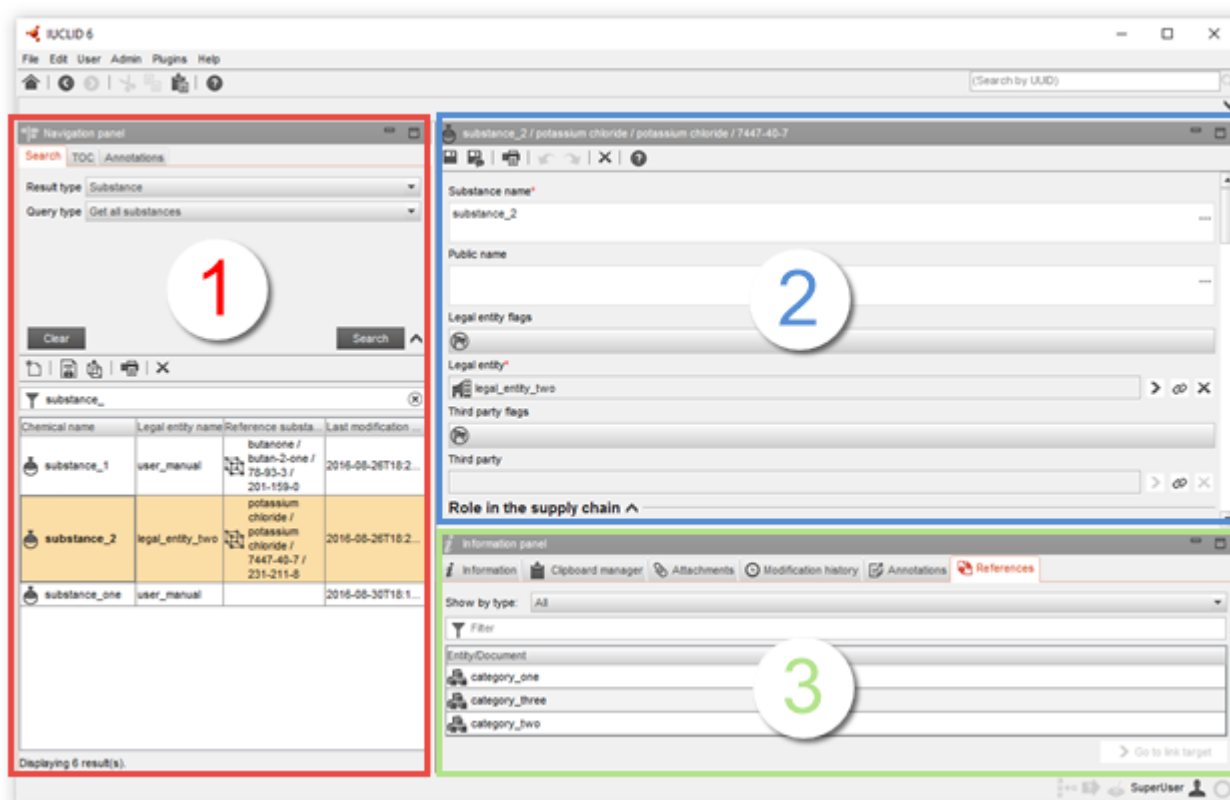
Main tasks contains links to entities in which a user enters data such as toxicological data, physicochemical data and information on uses that are specific to their own needs and circumstances. This data may be subject to change, for example during an evaluation process under a particular regulation.

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 22: 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 additional 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 23: Search for a substance by modification date

The screenshot shows the IUCLID 6 search interface. At the top, there is a 'Navigation Panel' with a 'Search' tab. Below it, the 'Result type' is set to 'Substance' and the 'Query type' is 'Find substances by creation/modification date'. The search criteria are: 'Creation date from' (empty) to (empty) and 'Last modification date from' 2016-04-04 to 2016-04-05. There are 'Clear' and 'Search' buttons. Below the search area is a toolbar with icons for document operations. A 'Filter' field is present above a table of results. The table has four columns: 'Chemical name', 'Legal entity name', 'Reference substance', and 'Last modification date'. Three results are shown. The third result, 'substance_3', is circled in red. A tooltip is visible over this entry, displaying the full name and reference substance: 'substance_3 / azacyclonol / diphenyl(piperidin-4-yl)methanol / 115-46-8' and 'Last modified Tue, 5 Apr 2016 19:02:56 +0300'. At the bottom, it says 'Displaying 3 result(s)'.

Chemical name	Legal entity name	Reference substance	Last modification date
substance_1	leo_for_manual	ethylene oxide / oxirane / 75-21-8 / 200-849-9	2016-04-05T18:03:43.10...
substance_2	oli_le	3-phenylpropionaldehy / 3-phenylpropanal / 104-53-0 / 203-211-8	2016-04-05T19:02:36.57...
substance_3	chem_le_01	azacyclonol / diphenyl(piperidin-4-yl) / 115-46-8 / 204-092-4	2016-04-05T19:02:56.02...

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.

To search for *Substances* by CAS number, use the field *Reference substance CAS number*.

1.9.1.3. *Ownership*

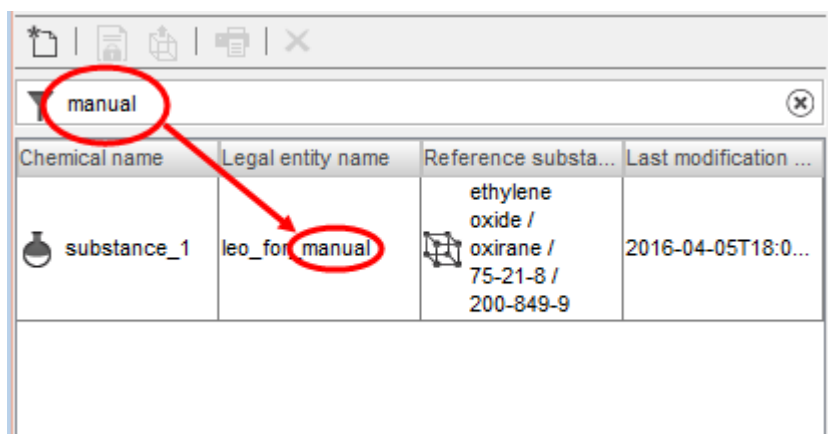
Ownership is shown as a criterion only if instance based security (IBS) is on, as described in section 15.2.2.5 IBS management.



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 24: Filter search results

Chemical name	Legal entity name	Reference substa...	Last modification ...
 substance_1	leo_for manual	 ethylene oxide / oxirane / 75-21-8 / 200-849-9	2016-04-05T18:0...

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.

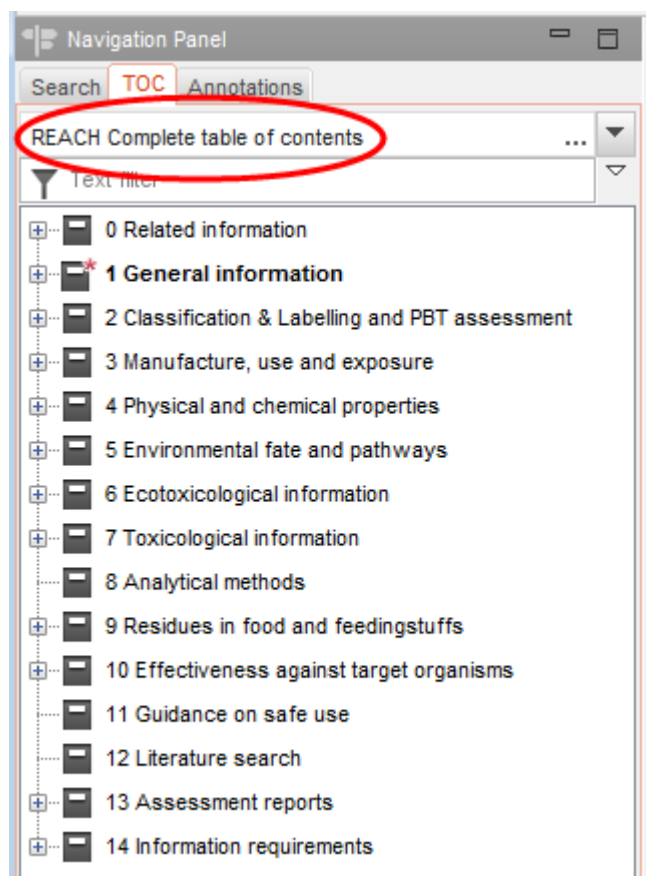
The search term can be cleared by clicking on the icon with a cross that is located at the right of the field.

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 in the figure below.

Figure 25: 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 26: Change the view in the TOC

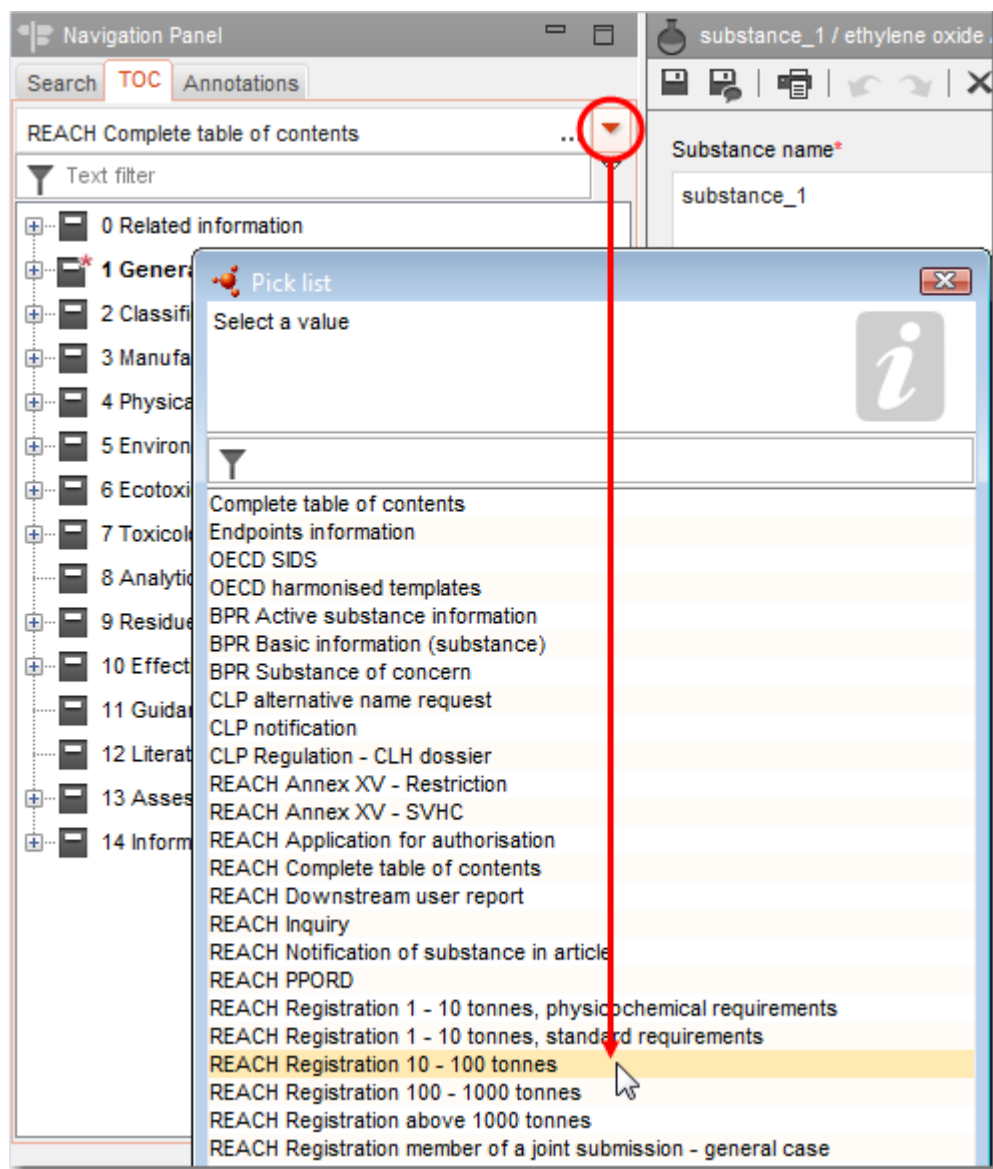
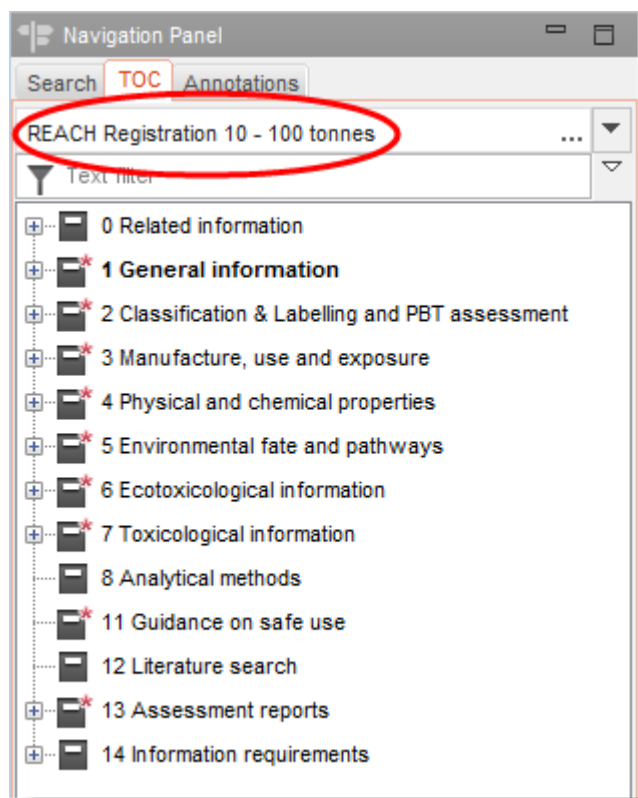
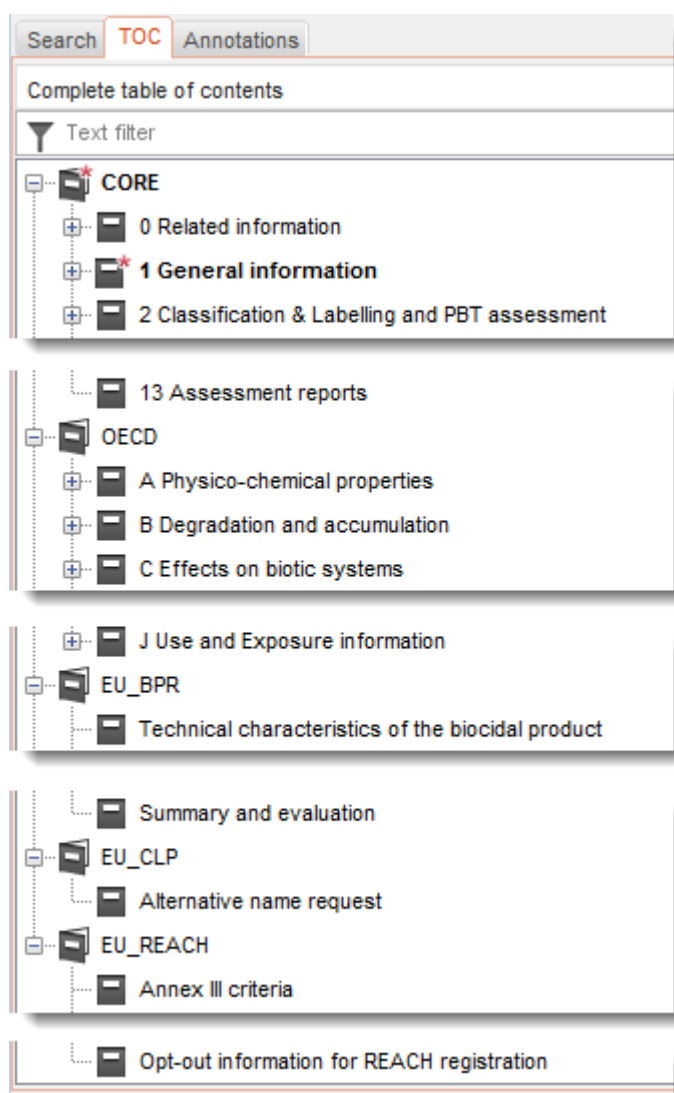


Figure 27: The TOC view: REACH Registration 10 - 100 tonnes

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 28: 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*.

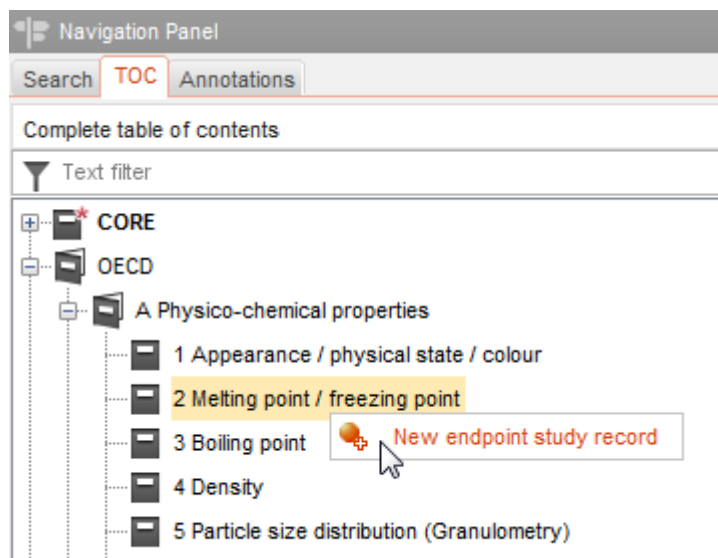
This means that under a legislation specific TOC view such as *REACH Registration above 1000 tonnes*, documents could have originated from either *CORE*, *OECD*, or *EU_REACH*. In addition, some documents can be shown together in the same section under TOC view for *REACH*, where under the TOC view *Complete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

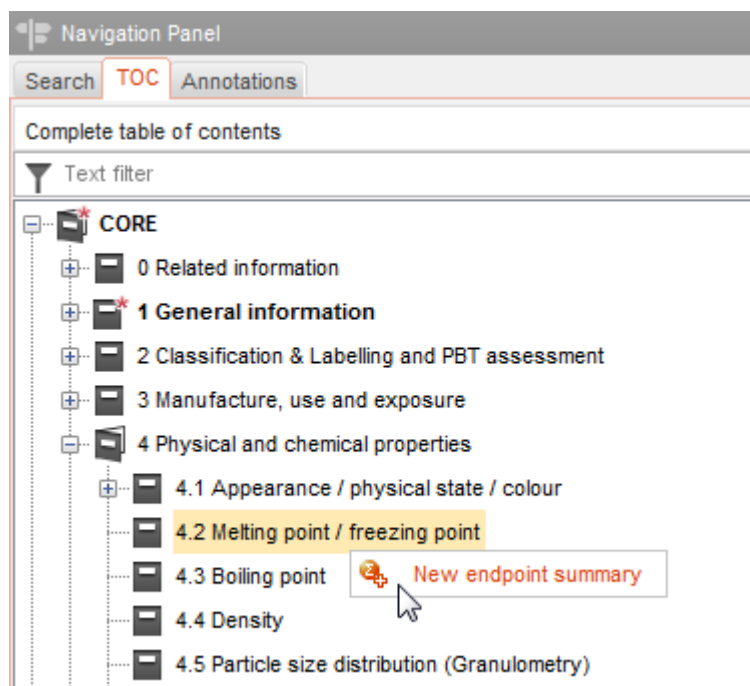
Figure 29: Creating an endpoint study record under OECD



1.9.2.2. Endpoint summary

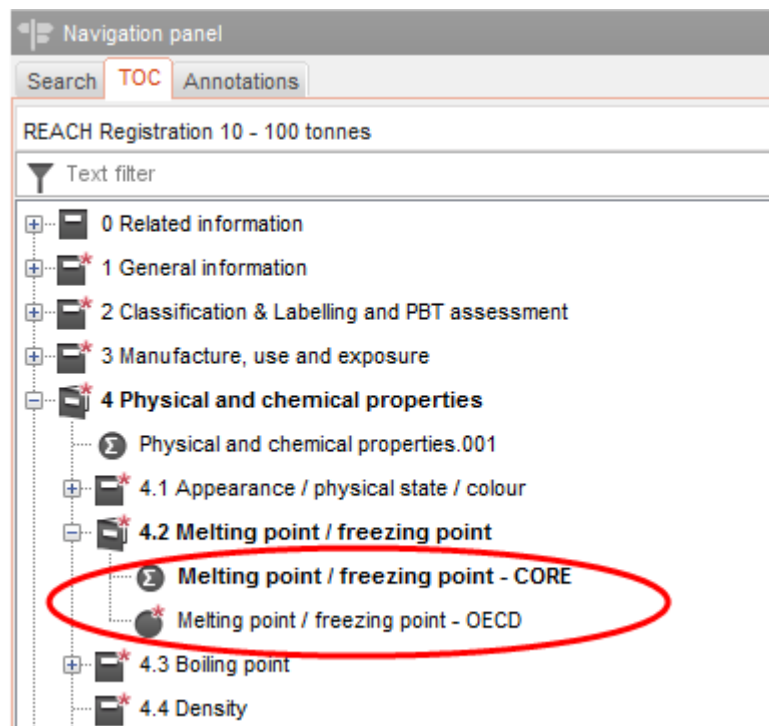
An *endpoint summary* provides a means of grouping *endpoint study records* and of providing further information about the grouping. An *endpoint summary* contains links to *endpoint study records* in the field *Link to relevant study records(s)*. To create a link, click on the button labelled *Add*.

Figure 30: 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.

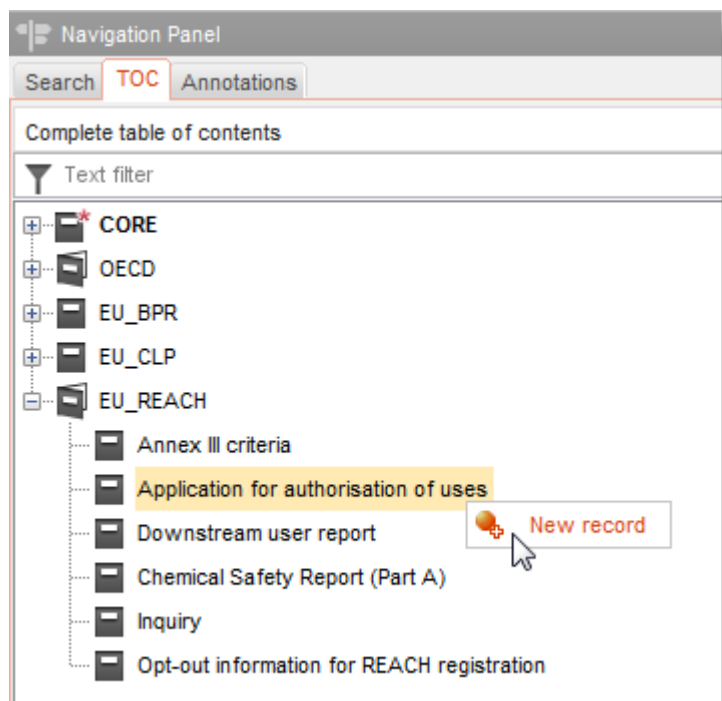
Figure 31: An endpoint summary and an endpoint study record shown together under a specific legislation



1.9.2.3. Record

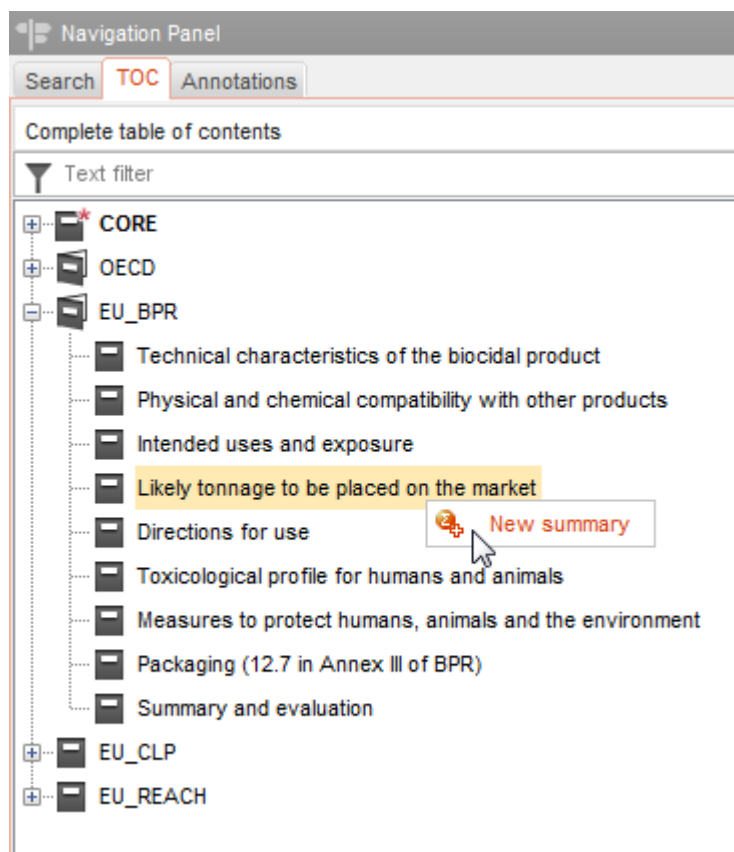
If a *record* contains data that cannot be described as an *endpoint study*, it is referred to just as a record.

Figure 32: 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 33: 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.

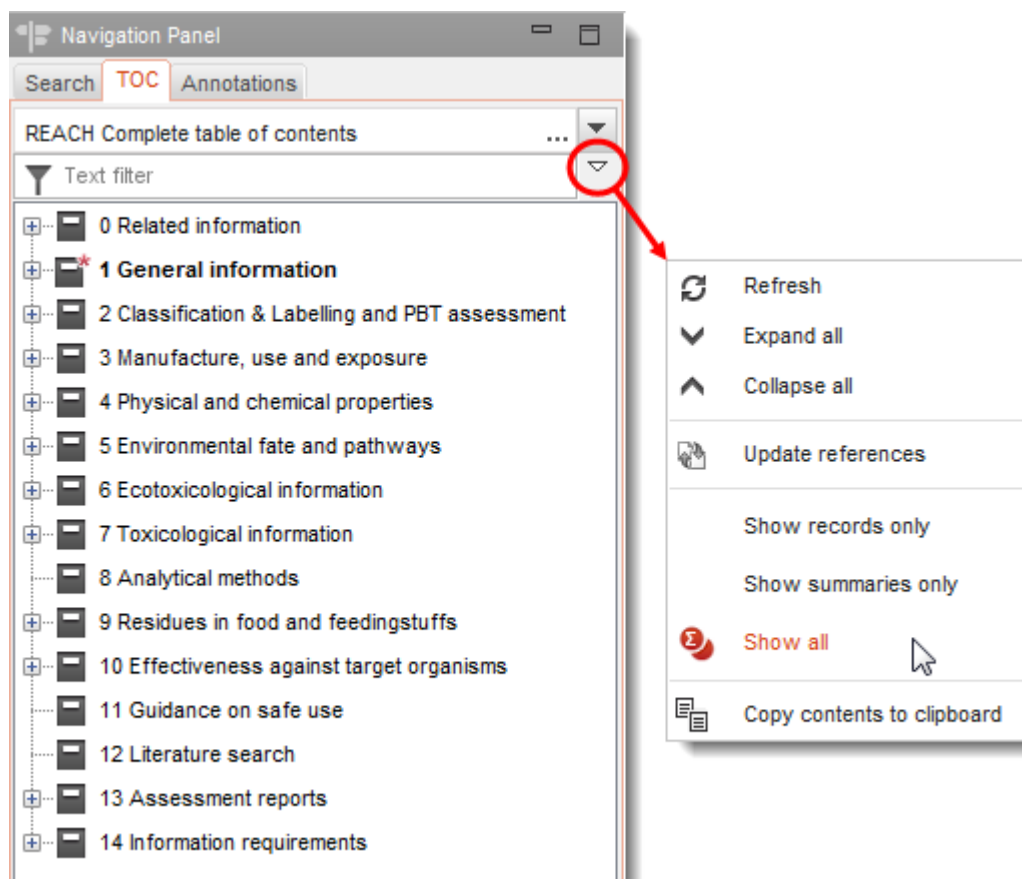
The example below shows filtering for section titles:

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 34: 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*.

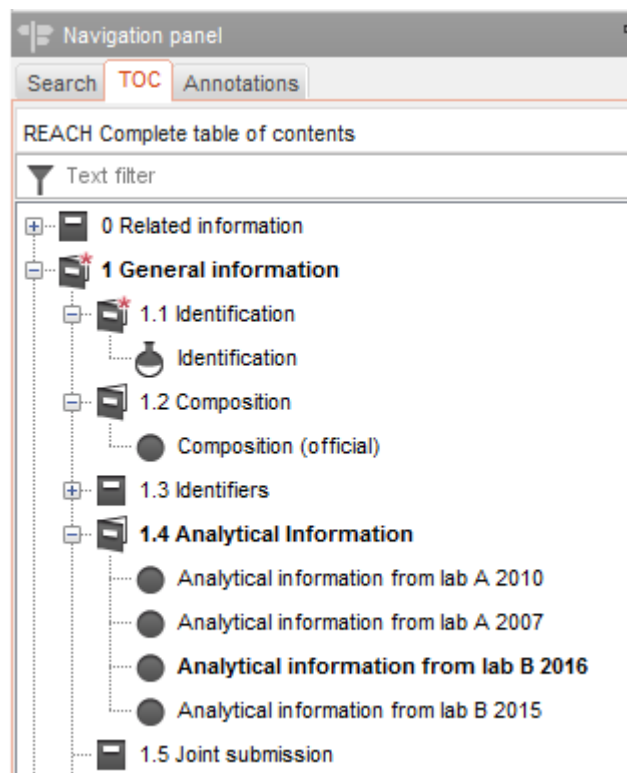
1.9.2.7.8. Copy contents to clipboard

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

1.9.2.8. The use of bold font in the TOC

The document currently displayed in the data panel has its name highlighted in bold in the TOC. Bold is used at each change in hierarchical level up the TOC tree, even when the TOC is collapsed. Thus the path to the document may be seen more easily by following the bold text. An example is shown below.

Figure 35: The use of bold font in the TOC



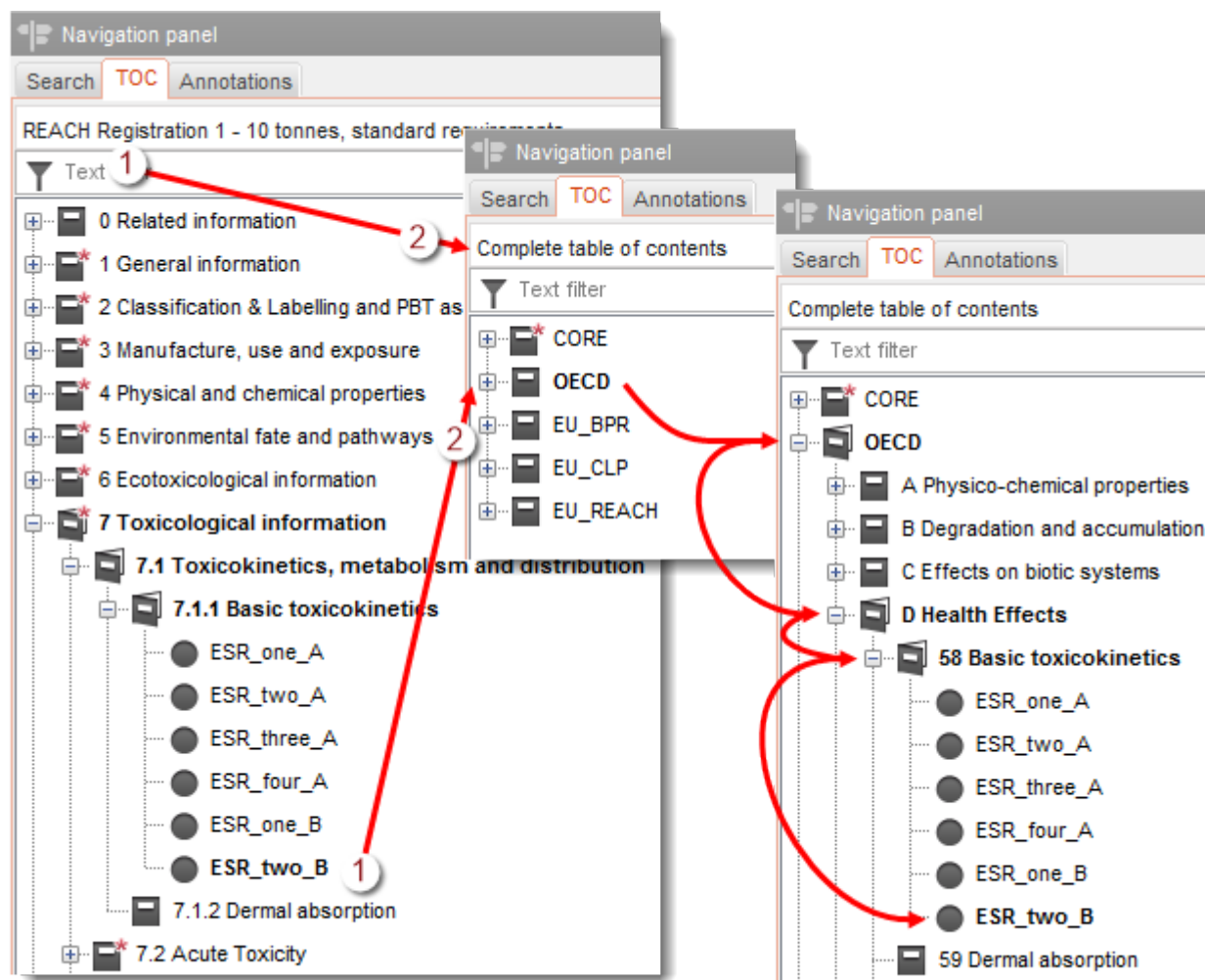
In the figure above, the document displayed in the data panel has the path shown below:

<https://iuclid6.echa.europa.eu>

General information \ 1.4 Analytical information \ Analytical information from lab B 2016

The highlighting in bold of the selected document can be used to help locate a document when switching between the different views in the TOC, as shown in the example below.

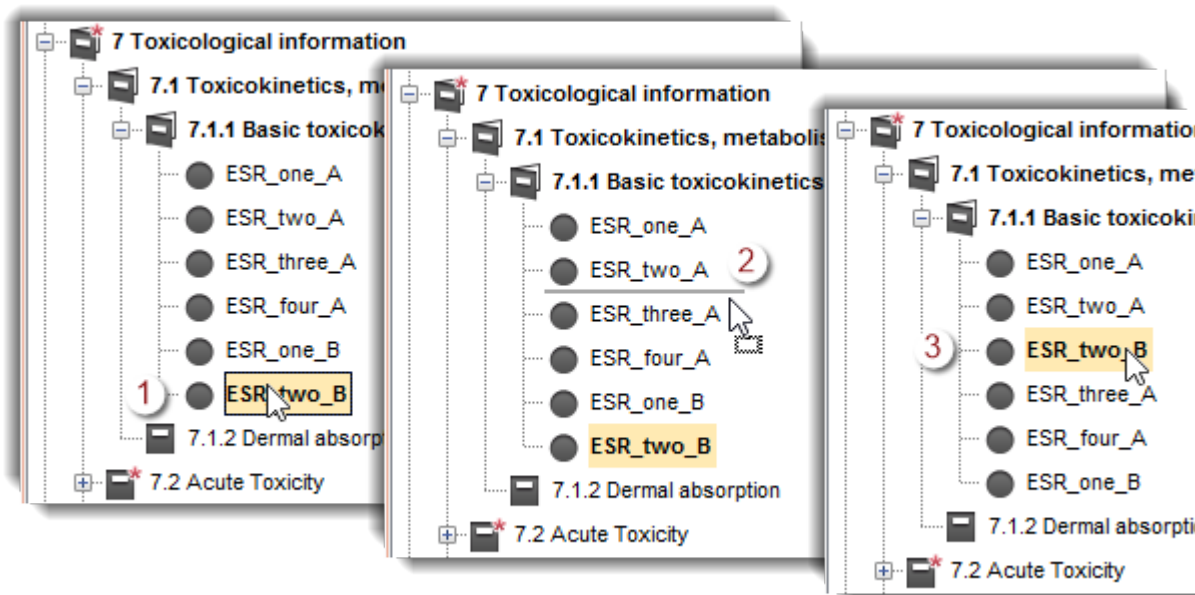
Figure 36: Using bold highlighting to navigate across different views in the TOC



In the example above, a document named *ESR_two_B* under the section *Basic toxicokinetics* is being viewed in the data panel. On the left, under a TOC view for *REACH*, the document can be seen to be in section 7.1.1. On going from the states numbered 1 to 2, the view has been switched to *Complete table of contents*, which has caused the TOC to collapse. The User can navigate back to the document in the TOC by opening the nodes highlighted in bold, which in this view leads to the section *OECD \ D Health Effects \ 58 Basic toxicokinetics*.

1.9.2.9. Ordering documents within a section of the TOC

The order in which documents are shown within a section of the TOC can be set manually by selecting and then dragging them, as shown in the example below.

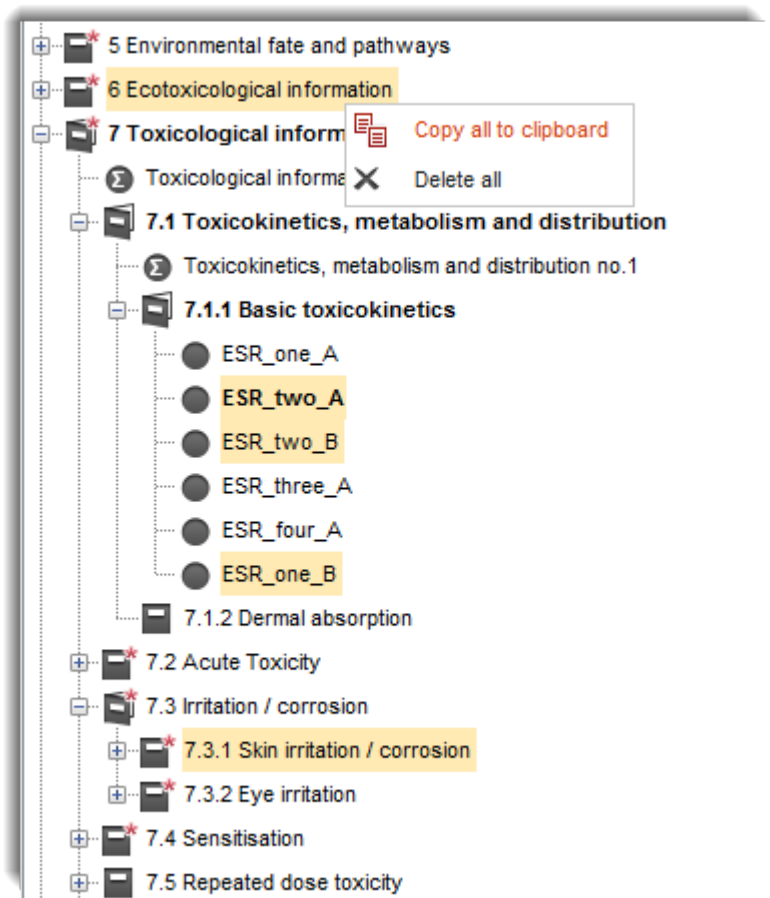
Figure 37: Ordering documents within a section of the TOC

Select a document (1). Move the grey bar to where you want the document to go (2), and then release the mouse button (3). This feature also works for a multiple selection of documents that have been preselected, as described in the next section.

1.9.2.10. *Selecting documents and sections in the TOC for bulk actions*

Multiple selections of documents and whole sections can be made in the TOC. The standard selection methods work, both within sections, and across boundaries between sections. If a section header is selected, this counts as a selection of all the documents below it in that section.

Once a selection is made, a function can be carried out on all the selected documents at once, using the right-click menu from anywhere within the selection. The functions available are *Copy all to clipboard* and *Delete*, as shown in the example below.

Figure 38: Multiple selection of documents within a section of the TOC

The above example, the function *Copy all to clipboard* is applied to all the documents in section 6, the individually selected documents in section 7.1.1, and all the documents in section 7.3.1.

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 entity or the document and its Universal Unique Identifier (UUID). If the entity or document is in a *Dossier*, the UUID of the *Dossier* is also given.

1.11.1.1. Origin

This indicates the version of *IUCLID* that was used to create the entity or document. Examples of the possible values are given below.

Table 5: Values of the field Origin

Origin	Version of IUCLID
IUC5	IUCLID 5
IUC6	IUCLID 6
IUC6-CLOUD-SME	IUCLID Cloud for SMEs

1.11.1.2. 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 39: Original document for a reference

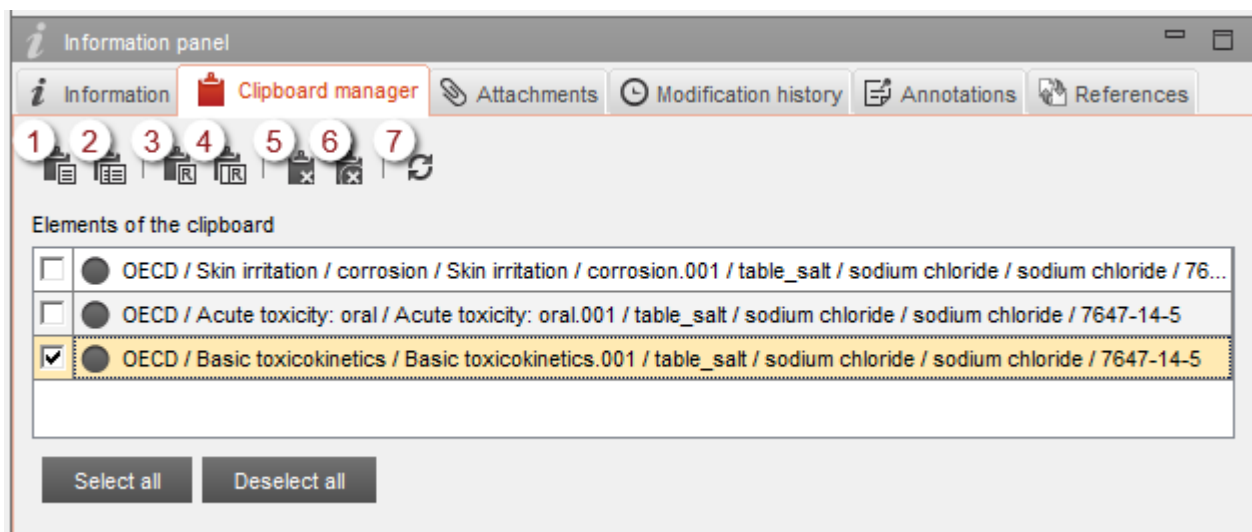
The screenshot shows the 'Original document' panel with the following content:

- Update referenced document** (button)
- Detach referenced document** (button)
- Reference**: CORE / Long-term toxicity to fish / Long-term toxicity to fish.001 / substance1 / formic acid
- Reference UUID**: 4ddb7460-ab7b-4b34-9878-ae5d4cfe799
- Reference dataset**: substance1 / formic acid
- Remarks**: pasted from clip board as a reference
- Version**: Thu, 10 Dec 2015 12:21:38 +0200

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 40: The clipboard manager



Key for Figure 31

1. Paste selected
2. Paste all
3. Paste selected as a reference
4. Paste all as a reference
5. Delete selected
6. Delete all
7. Refresh synchronises the clipboard with the most recent data in the database. For example, in a multi-user environment, if some other user deletes a document that is on the clipboard, clicking *Refresh* causes the document to be removed from the clipboard.

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.

On export and dossier creation a dynamic reference is replaced by a static copy of the document. This is done for export because it is not known whether the destination document of the link will always be present in the IUCLID database to which the dataset is exported. If it is missing, the link is broken. For a dossier, the dynamism of the link is removed because the content of a dossier cannot change.

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 shows the links to the current document that were made either via the chain-link icon, or by pasting as a link from the clipboard. A filter can be applied for the type of referencing entity/document. A referencing entity/document can be opened by selecting the reference, and then clicking on *Go to link target*.

If the current entity is an *Annotation*, there is no tab *Annotations*. In that case, the tab for *References* contains no filter for document type, and there is an additional feature *Unlink*, which allows an association to be removed.

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.

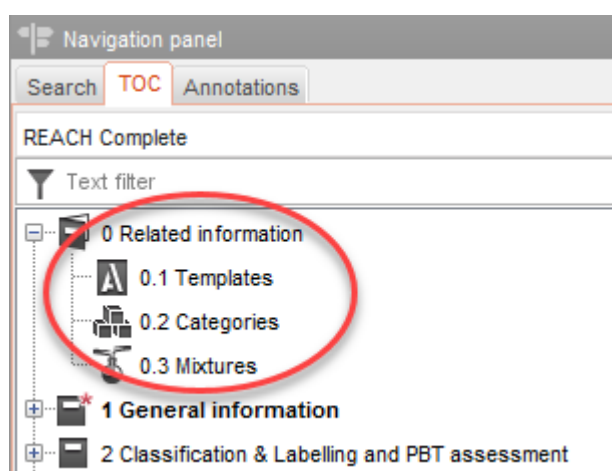
More detail can be provided about the *Substance* identity in section 1.2 *Composition*, where one or more compositions can be defined. A composition may contain the identities of *constituents*, *additives* and *impurities*, and their relative proportions. To define the identity of a *Substance* properly 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*, and *Mixture/Product*. The location in the TOC is shown below.

Figure 41: 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*.

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. To ensure consistency, 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.

Assessment entity is under section 1.10 of the tables of contents for REACH. There is a fixed record for the whole section, and four subsections under which multiple records can be created.

2.2.1. Assessment approach (assessment entities)

The fixed section under *Assessment approach (assessment entities)* has a default name of *Assessment approach*. It contains the following two fields.

2.2.1.1. Approach to fate/hazard assessment

Approach to fate/hazard assessment contains 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. Such a description provides the overall reasoning used in the creation of the *Assessment entities*.

2.2.1.2. Approach to fate/hazard assessment - public information

This is a specific field to provide a public description of the approach to fate/hazard assessment.

2.2.2. Types of assessment entity

The types of *assessment entity* that can be created are listed below:

1. Registered substance as such
2. Specific composition/form of the registered substance
3. (group of) constituent in the registered substance
4. Transformation of the registered substance

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

2.2.2.1. Assessment entity confidentiality claim

A flag can be set that applies to all of an individual *assessment entity* document. A flag is set from under the flag icon at the top of the document. For more details about flags, see section 1.3.2 *Flag*.

2.2.2.2. Assessment entity name

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.

2.2.2.3. Relation to the registered substance

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

2.2.2.4. *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*]

2.2.2.5. *Related Composition*

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 titled *How to prepare Registration and PPORD Dossiers*.

2.2.2.6. *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.

2.2.2.7. *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.

2.2.2.8. *Reaction schema*

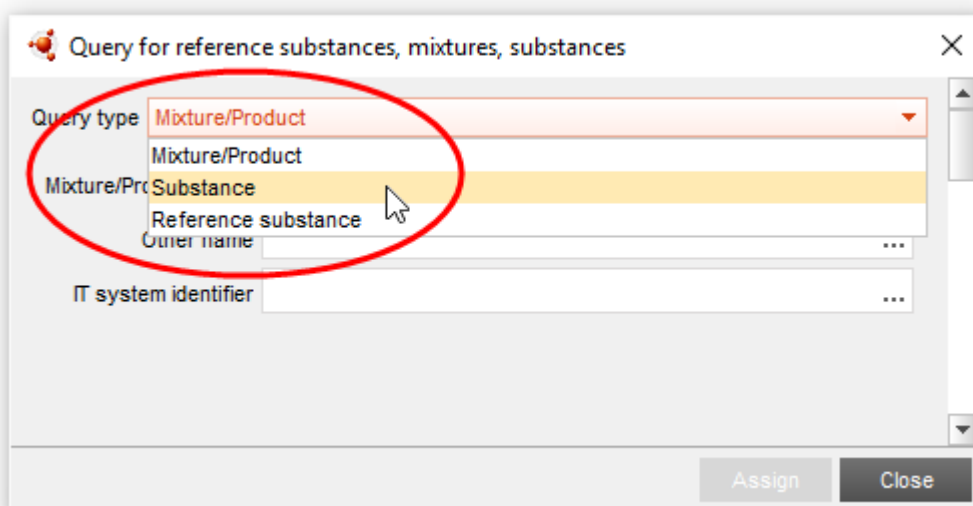
Upload the image of the reaction schema when needed [for *Transformation of the registered substance*].

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 42: 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 43: An example of a composition for a Mixture/Product

The screenshot displays the IUCLID 6 interface for editing a Mixture/Product. The window title is 'CORE / Composition / Composition.001 / mix_1'. The main content is divided into several sections:

- Administrative data:**
 - Mixture/product name:
 - Brief description:
 - Formulation type:
- Components:** A list of components with controls for adding, deleting, and reordering.

Component Name	Controls
substance1 / formic acid,	↓ ↑ + X
substance2 / "amyl nitrite", mixed isomers / 3-methylbutyl nitrite / 110-46-3,	↓ ↑ + X
- Impurities:**
- Additives:**


Paraffin waxes and Hydrocarbon waxes, chloro / 1,2,3,4,6,7,10-heptachlorododecane ...	↓ ↑ + X
---	-----------

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

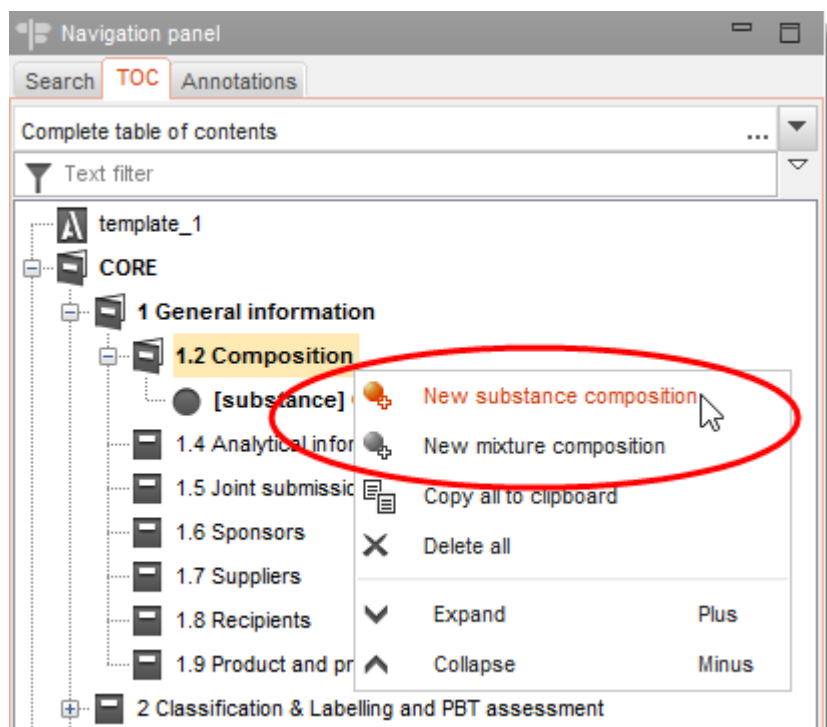
A *Template* is an entity that allows data from multiple sections to be inserted into a *Substance* or *Mixture/Product* entity all at once without having to manually recreate all the sections individually and re-enter data.

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

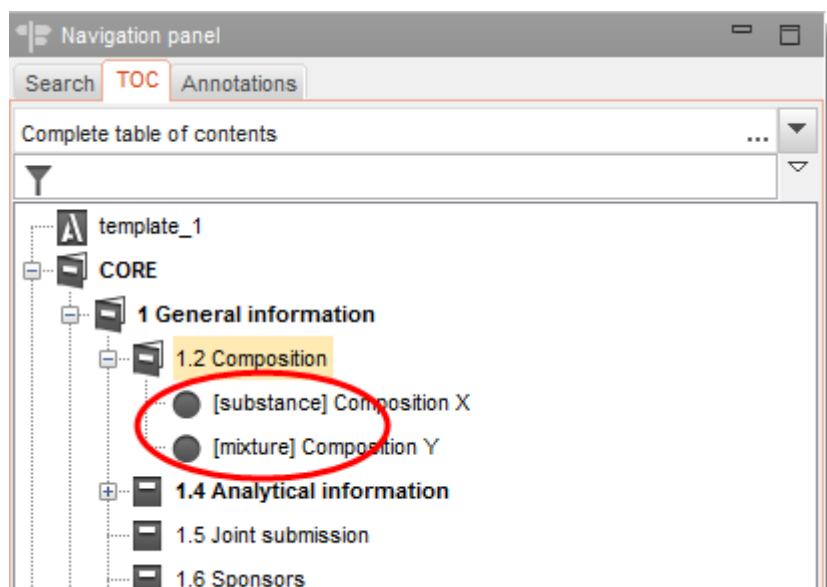
Section 1.2 *Composition* is different for *Substance* and *Mixture/Product*. Whilst editing a *Template*, if the TOC view is set to *Complete table of contents*, it is possible to create either type of *Composition*, as shown below:

Figure 44: Create a composition in a Template



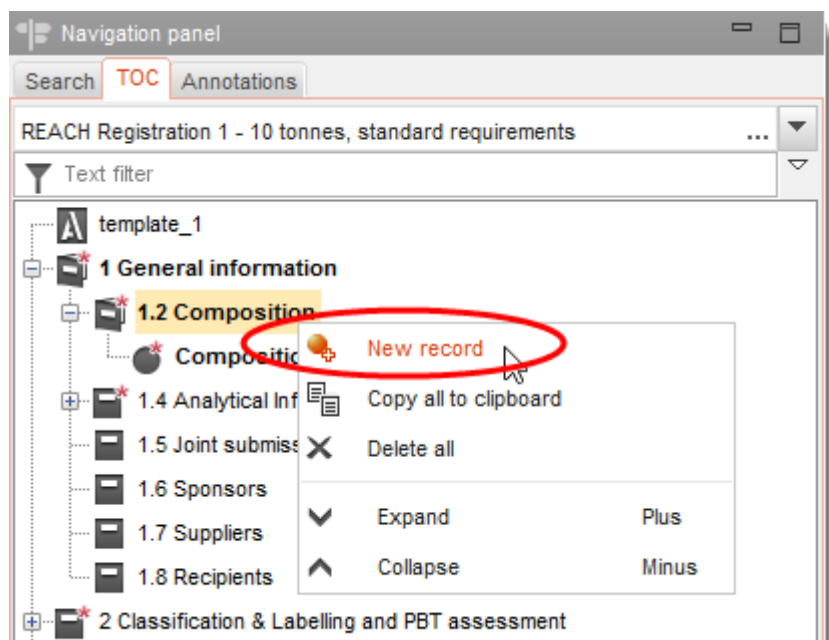
The names of the *Compositions* are prepended with their type, as shown in the example below:

Figure 45: 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:

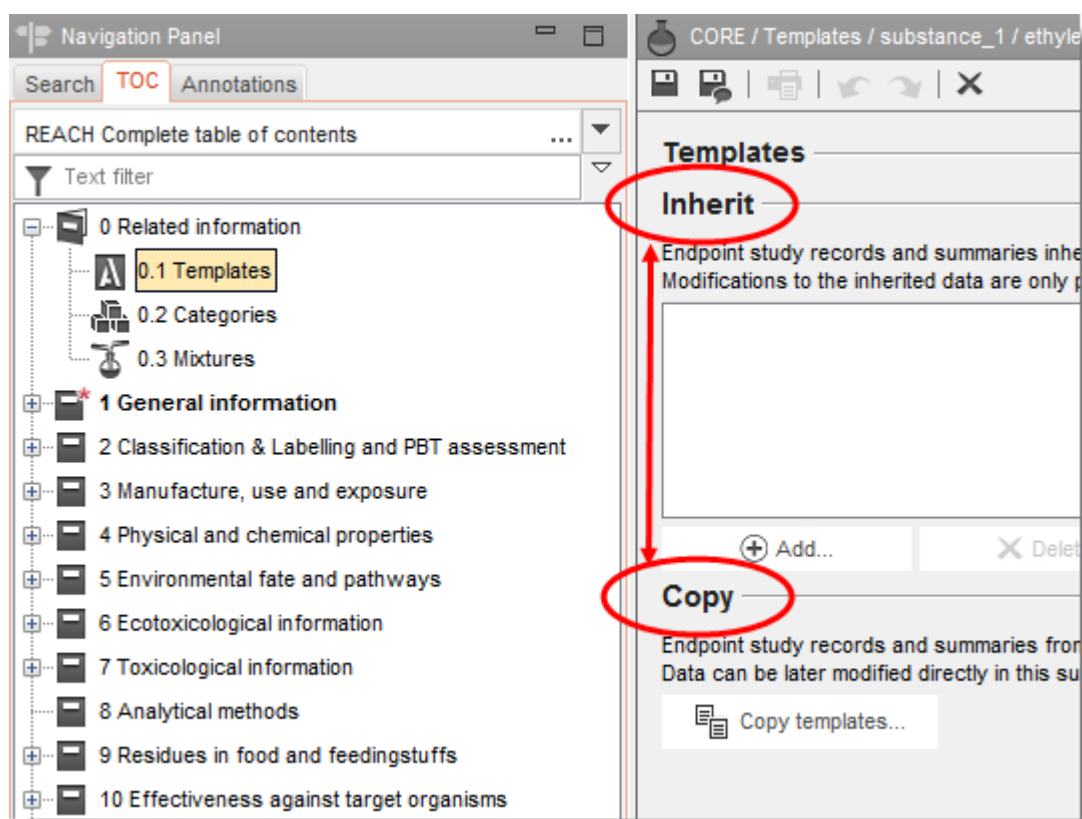
Figure 46: Creating a Composition with the TOC set to a view specific to the REACH Regulation



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 47: Attach a Template as copy or inherit

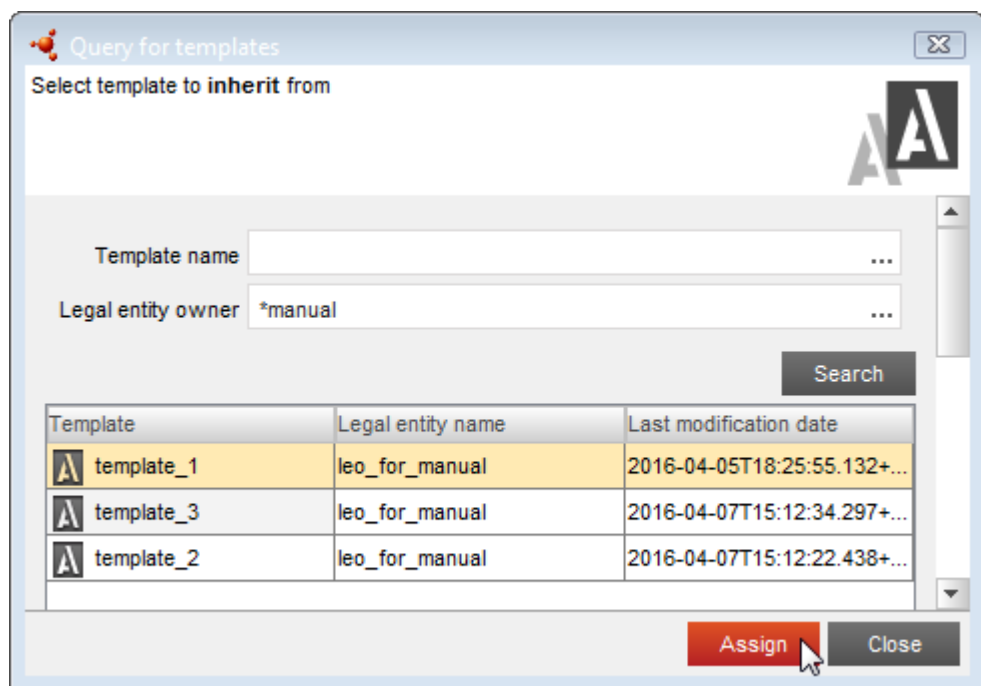
A *Template* can be attached in one of two different ways, *inherit* or *copy*.

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*.

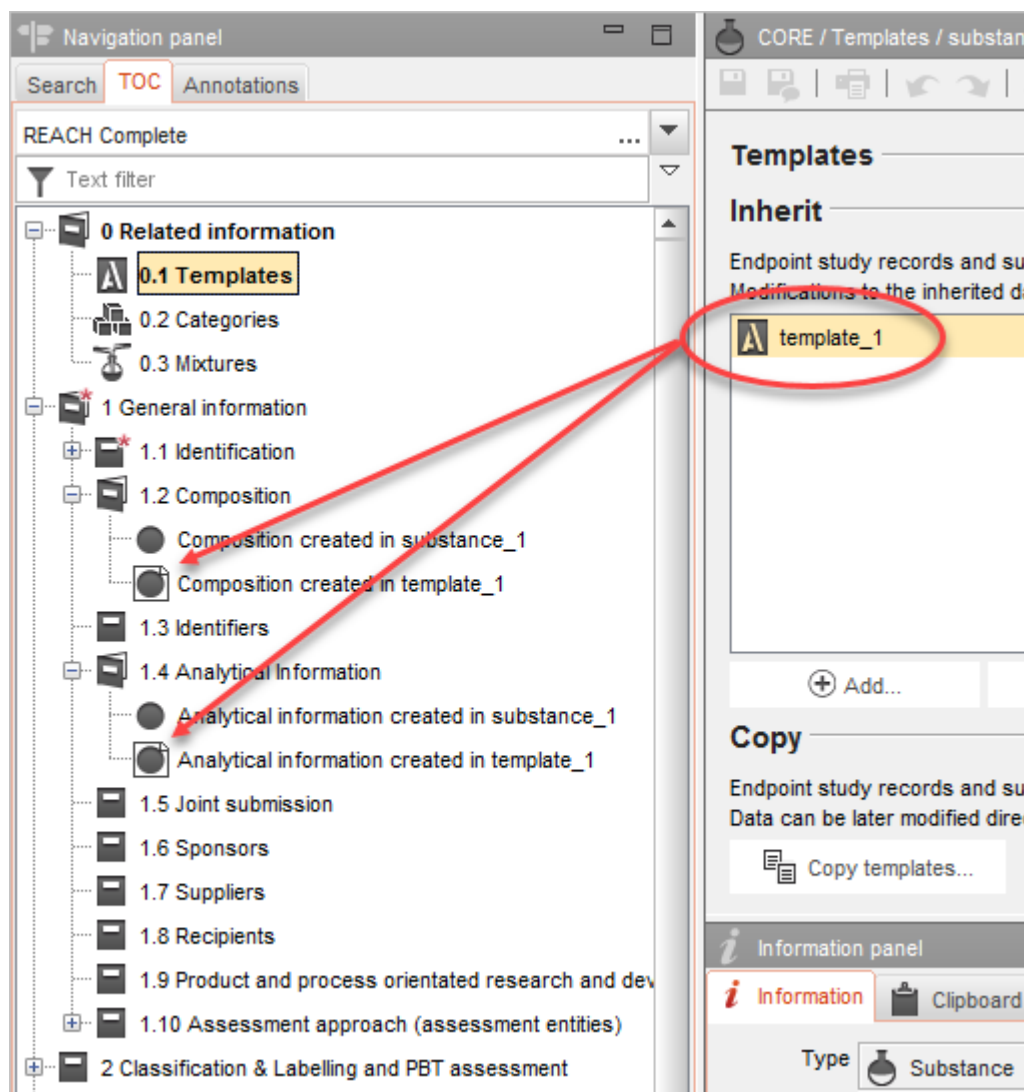
Copy adds a copy of the documents in the *Template* to the *Substance* or *Mixture/Product*. There is no link. A document copied in this way can be modified in the *Substance* or *Mixture/Product* to which it was copied. Even if the *Template* is completely deleted, the data in the *Substance* or *Mixture/Product*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

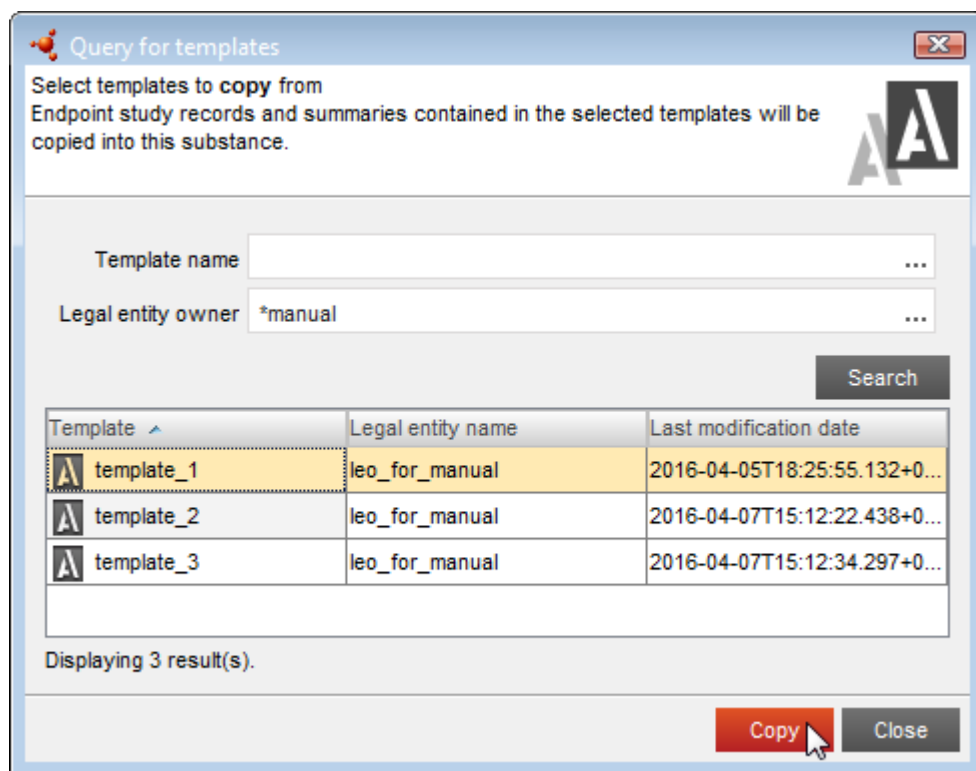
When you have decided between using *inherit* or *copy*, in the *Template* management window, click on either *Add* or *Copy templates*. In the example shown above, the pointer is hovering over the function *Add* ready to create a dynamic link to the currently open *Substance*. Clicking on *Add*, opens 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 48: Select a Template from which to inherit

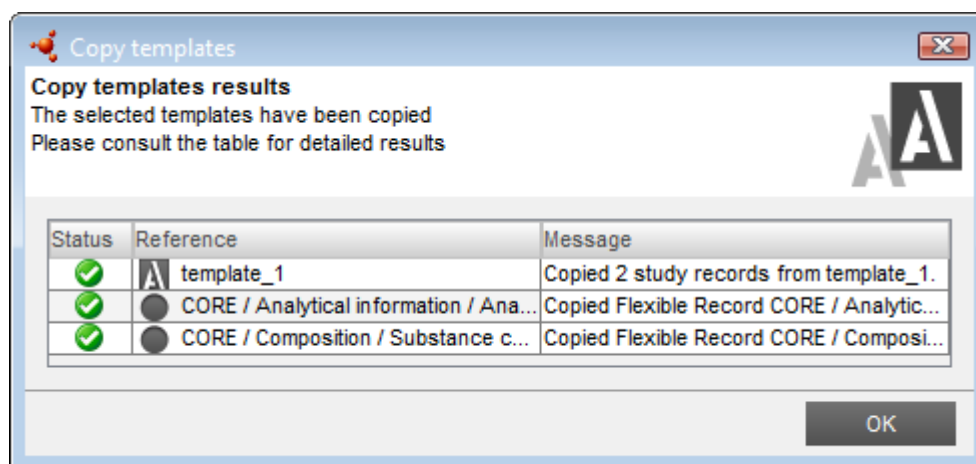
After assignment, the *Template* is added to the list of *Templates* that were attached using *inherit*. *Templates* on the list can be re-ordered and deleted from the list. Deletion from the list does not affect the *Template* itself; it just removes the data provided by the *Template* from the *Substance* 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 49: Documents in a Substance inherited from a Template

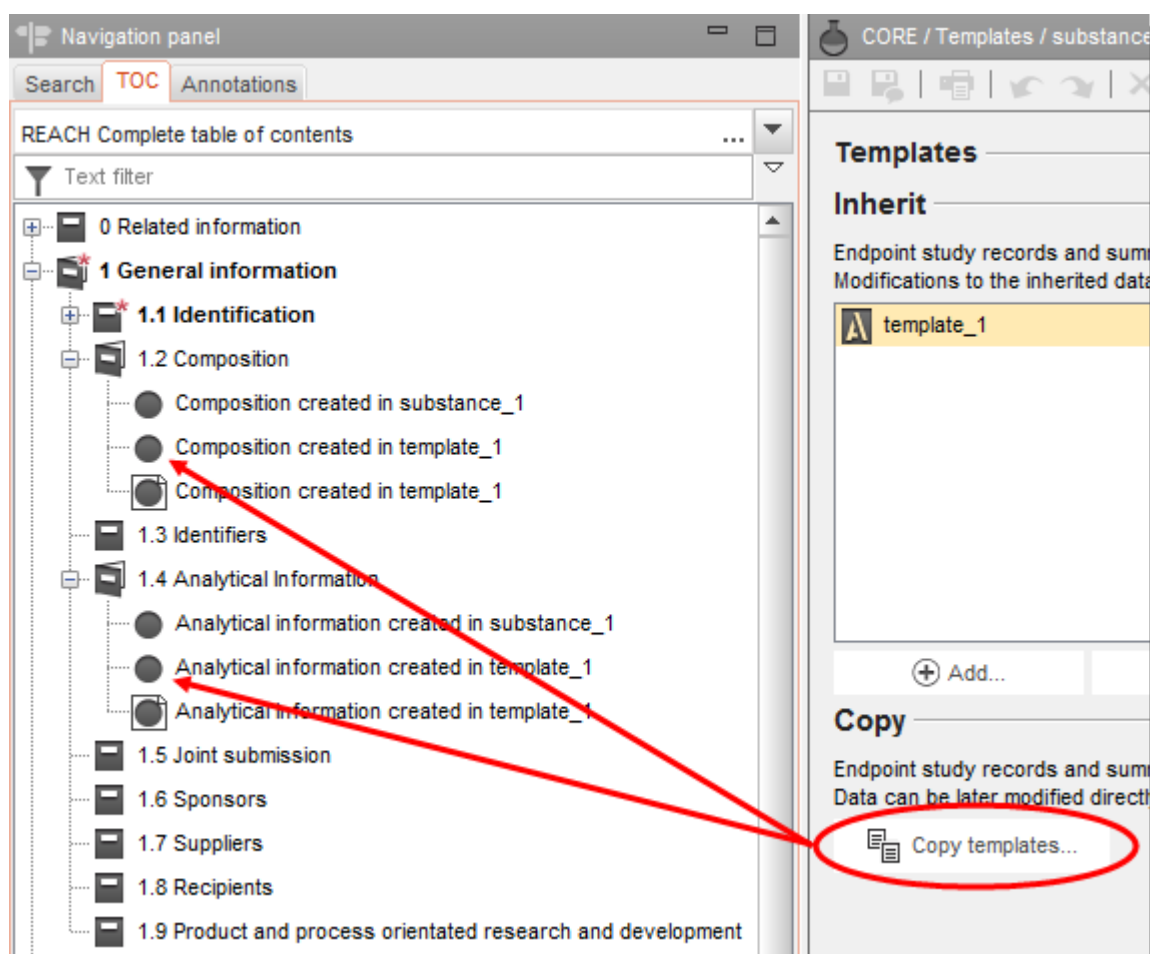
To copy documents from a *Template*, click on *Copy templates* in the *Template* management window. This opens a pop-up window in which a *Template* can be searched for and assigned. In the example shown below, all the *Templates* whose Legal entity name ends in "manual" have been found using the wild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

Figure 50: Selecting a Template from which to copy documents

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

Figure 51: 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 52: 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 an 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 53: The mandatory fields in a Category

The screenshot shows a web interface for creating a category. At the top, there is a header with a folder icon and the text 'category_1'. Below this is a navigation bar with two tabs: 'Category Information' (active) and 'Matrix'. The main content area contains the following fields:

- Category name***: A text input field containing 'category_1'.
- Public name**: An empty text input field.
- Legal entity***: A dropdown menu showing 'legal_entity_1'.
- Regulatory purposes**: A dropdown menu showing 'OECD: CoCAP'.
- Remarks**: An empty text area.

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

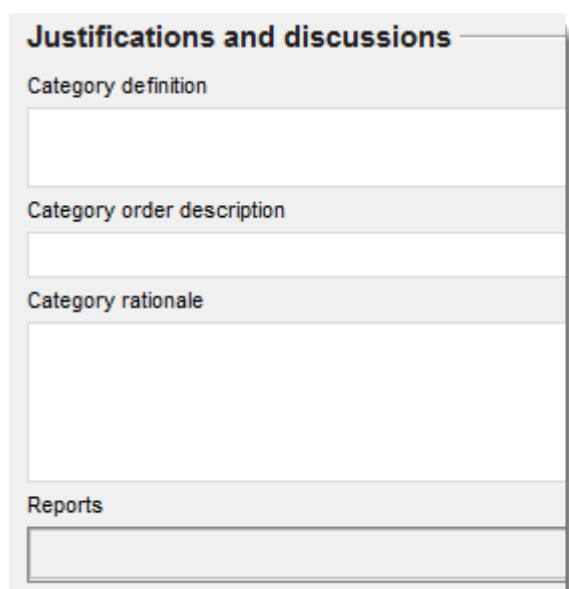
Provide in the field *Category definition* a summary of the common features of the category members.

In the field *Category order description*, describe the order of the substances grouped in the category including a brief explanation, if the properties of the category members follow a certain pattern.

Under *Category rationale*, describe why the category can be formed (e.g. common functional group(s), common precursor(s)/breakdown product(s), common mechanism(s) of action, trends in properties and/or activities) and summarise how available experimental data verify that the category is robust (i.e. category hypothesis and justification). Furthermore, describe here the set of inclusion and/or exclusion rules that identify the ranges of values within which reliable estimations can be made for category members (i.e. applicability domain of the category). Use the text template available for this field to ensure that you address the relevant points.

Under *Reports*, you can attach supporting documents to describe the category.

Figure 54: Justifications and discussions for a Category



Justifications and discussions

Category definition

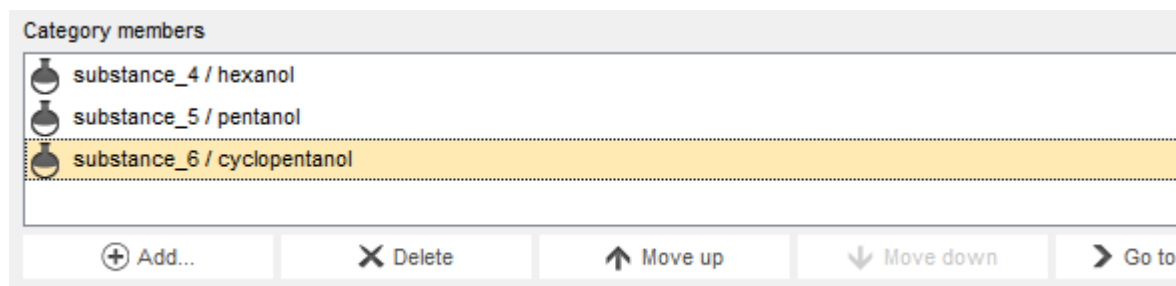
Category order description

Category rationale




Reports

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 55: Managing the members of a Category



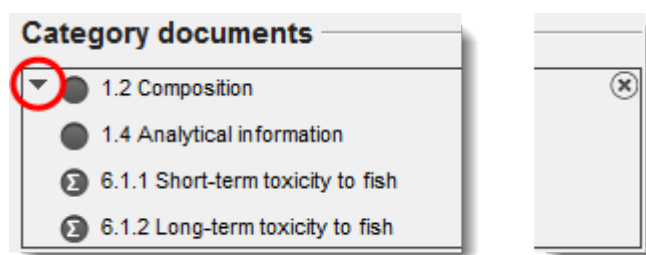
Category members

 substance_4 / hexanol
 substance_5 / pentanol
 substance_6 / cyclopentanol

+ Add... X Delete ↑ Move up ↓ Move down ➤ Go to

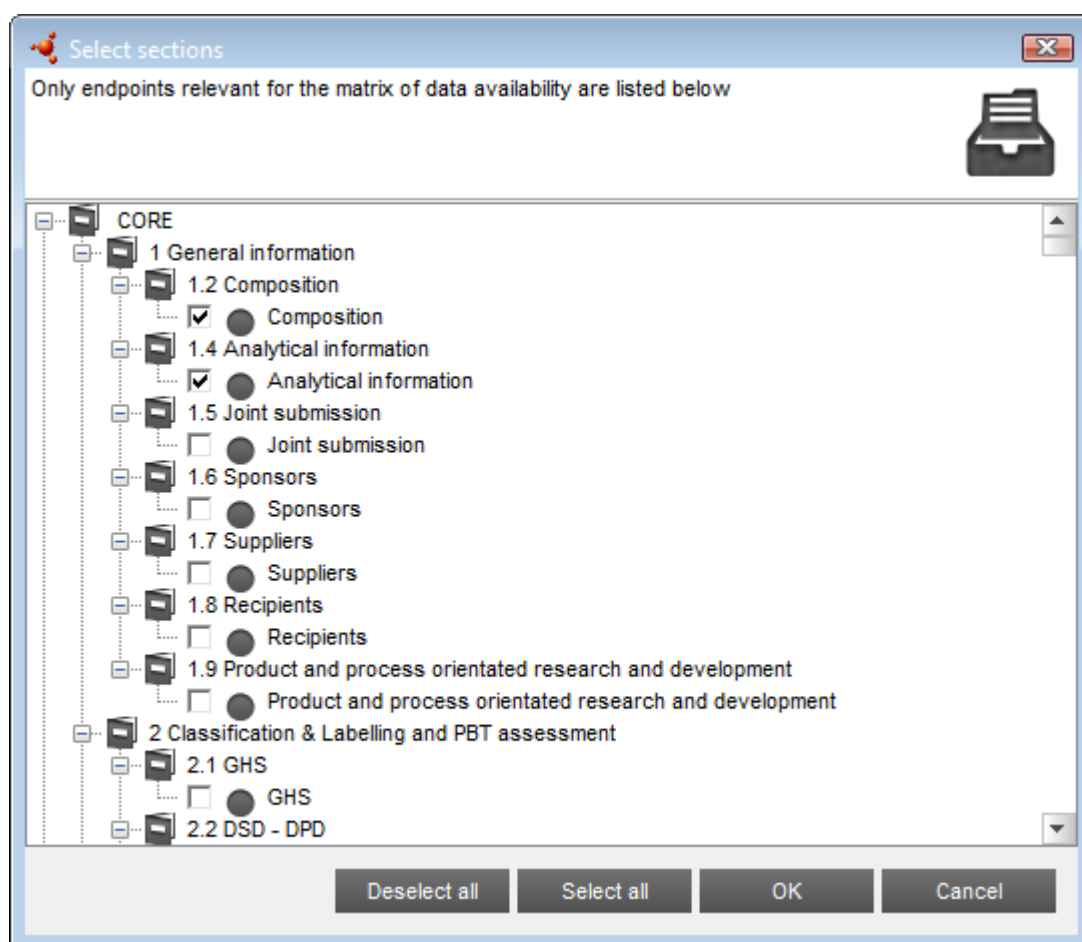
The category matrix shows the documents in the sections selected in the field shown below. Click on the downward facing arrow to open the selector.

Figure 56: The sections available in the matrix view for a Category



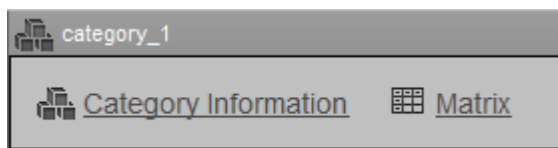
The selector for sections is shown below.

Figure 57: 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 58: Toggle between the matrix and the category management window

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

Figure 59: The main page of the matrix

 A screenshot of the 'Matrix' interface. At the top, there is a toolbar with 'Category Information' and 'Matrix' buttons. Below the toolbar, the word 'Matrix' is displayed next to a grid icon. The main area contains a table with the following structure:

	substance1	substance2	substance3
CORE			
1.2 Composition	3 ●	1 ●	
1.4 Analytical information	3 ●		
6.1.1 Short-term toxicity to fish	2 Σ		1 Σ
6.1.2 Long-term toxicity to fish	1 Σ		

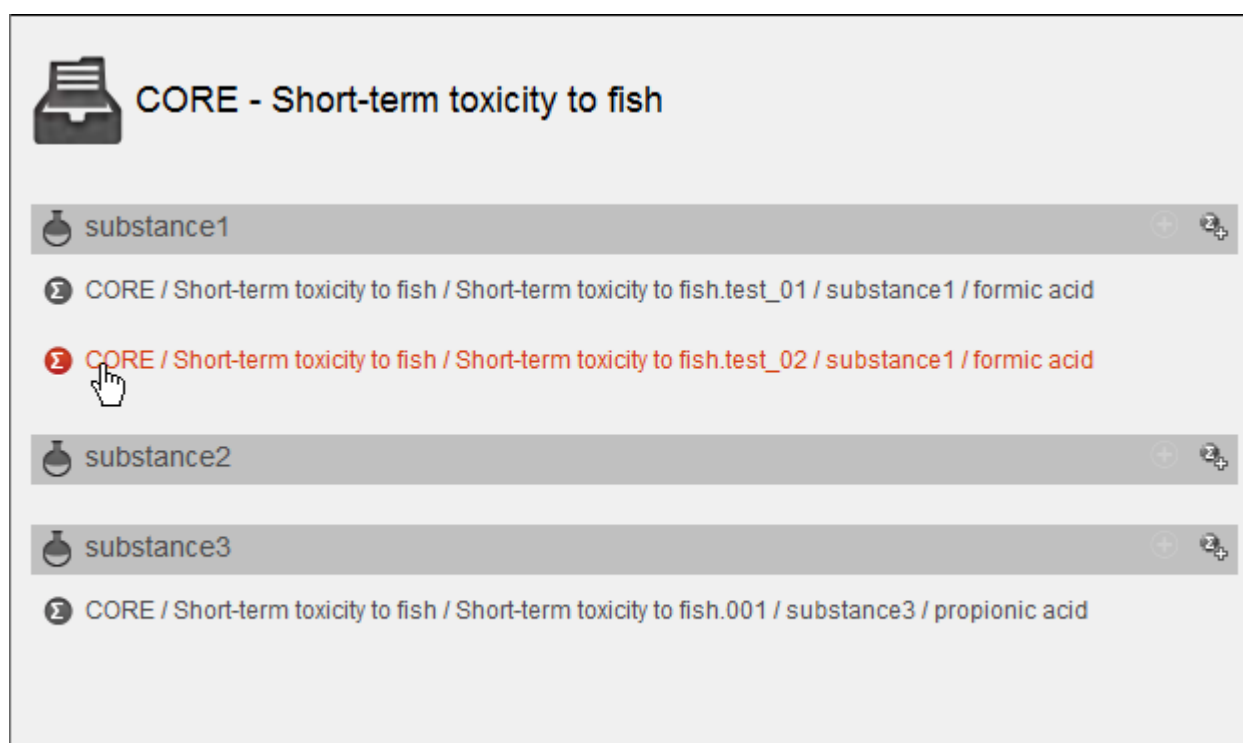
 A tooltip is visible over the '1 Σ' cell in the '6.1.1' row, showing a list of document paths:

- > CORE / Short-term toxicity to fish / Short-term toxicity to fish.test_0
- > CORE / Short-term toxicity to fish / Short-term toxicity to fish.test_0

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 60: The documents in a Category for a particular section

A new summary can be 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, **A**. 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

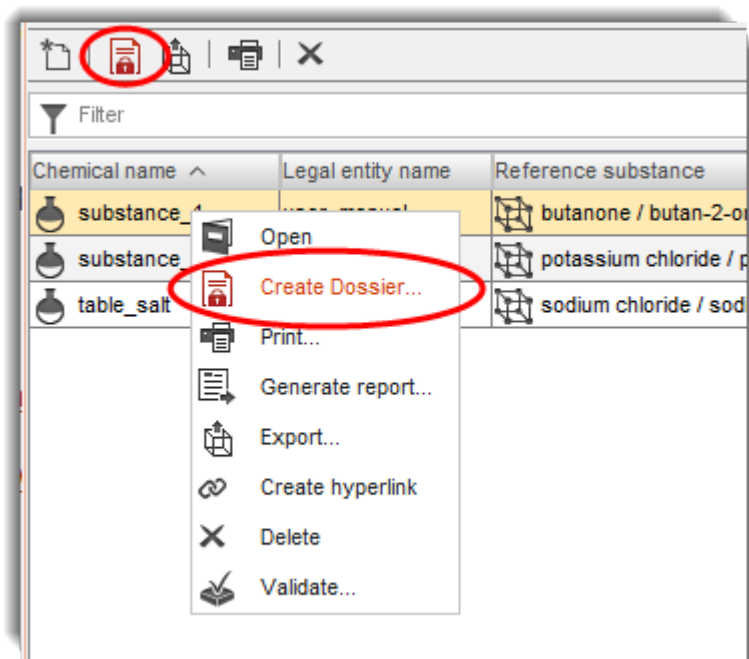
A *Dossier* is a write-protected copy of the data stored in a *Substance*, a *Category* or a *Mixture/Product*. Typically, a *Dossier* is used to submit data to a regulatory authority to satisfy a legal obligation arising from a legislation, for example REACH.

7.1. Dossier creation

Before creating a *Dossier*, ensure that at least all the required data is in the dataset 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 6 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 in the header of the search results, or right-click and then select *Create Dossier*, as shown in the figure below.

Figure 61: Starting the Dossier creation wizard

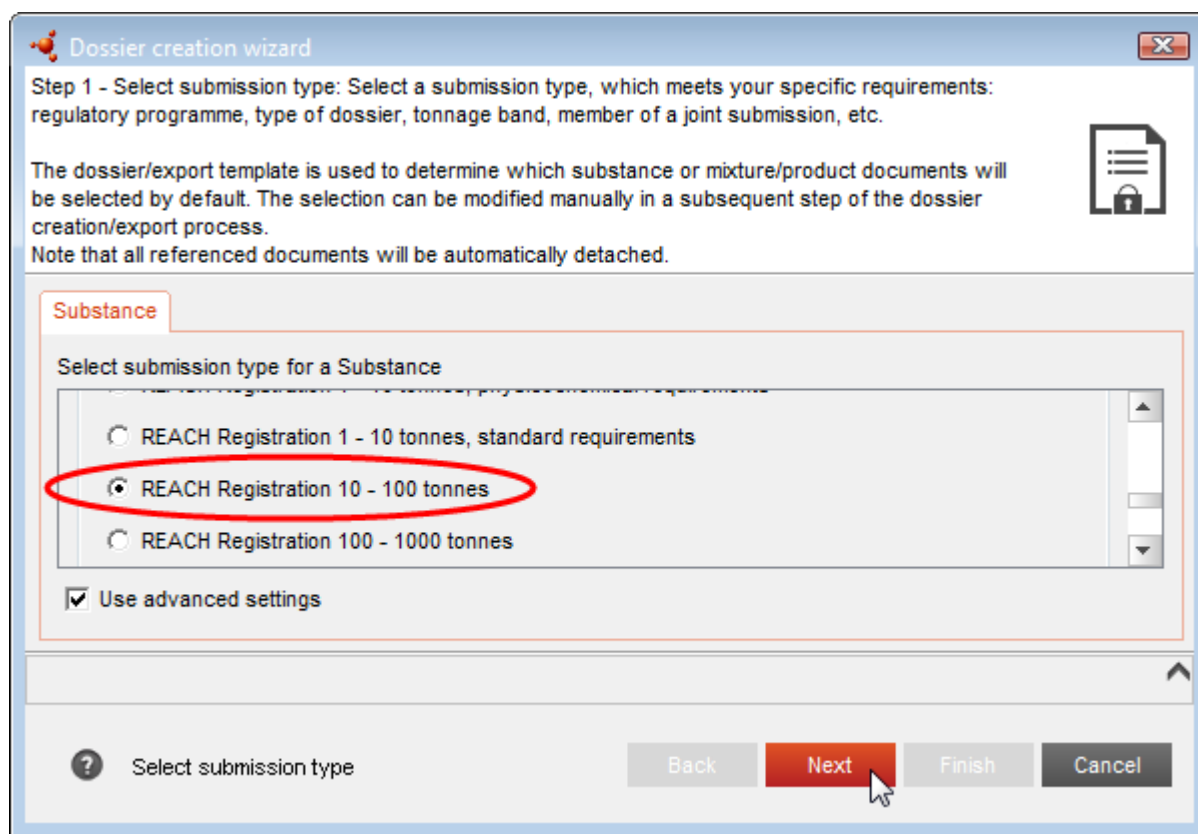


The wizard opens in a pop-up window. In the header of the window there are some instructions on how to fill-out the wizard. In the footer, there is an indicator of the current step in the process. If there is a problem with the data entered, a message is shown in the footer.

7.1.1. Selecting the Dossier type

On the first page of the wizard, under the tab *Substance*, 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 62: Select the type of Dossier



7.1.1.1. Use advanced settings

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 the option *Use advanced settings* is ticked, the next pages of the wizard are described in section 7.1.3 *Advanced settings for excluding and including data from the Dossier*.

If all the available data required for the Dossier type is to be placed in the *Dossier*, the box can be left unticked, in which case, the next page of the wizard is that described in section 7.1.47.1.4 *Administrative data to be placed in the Dossier header*.

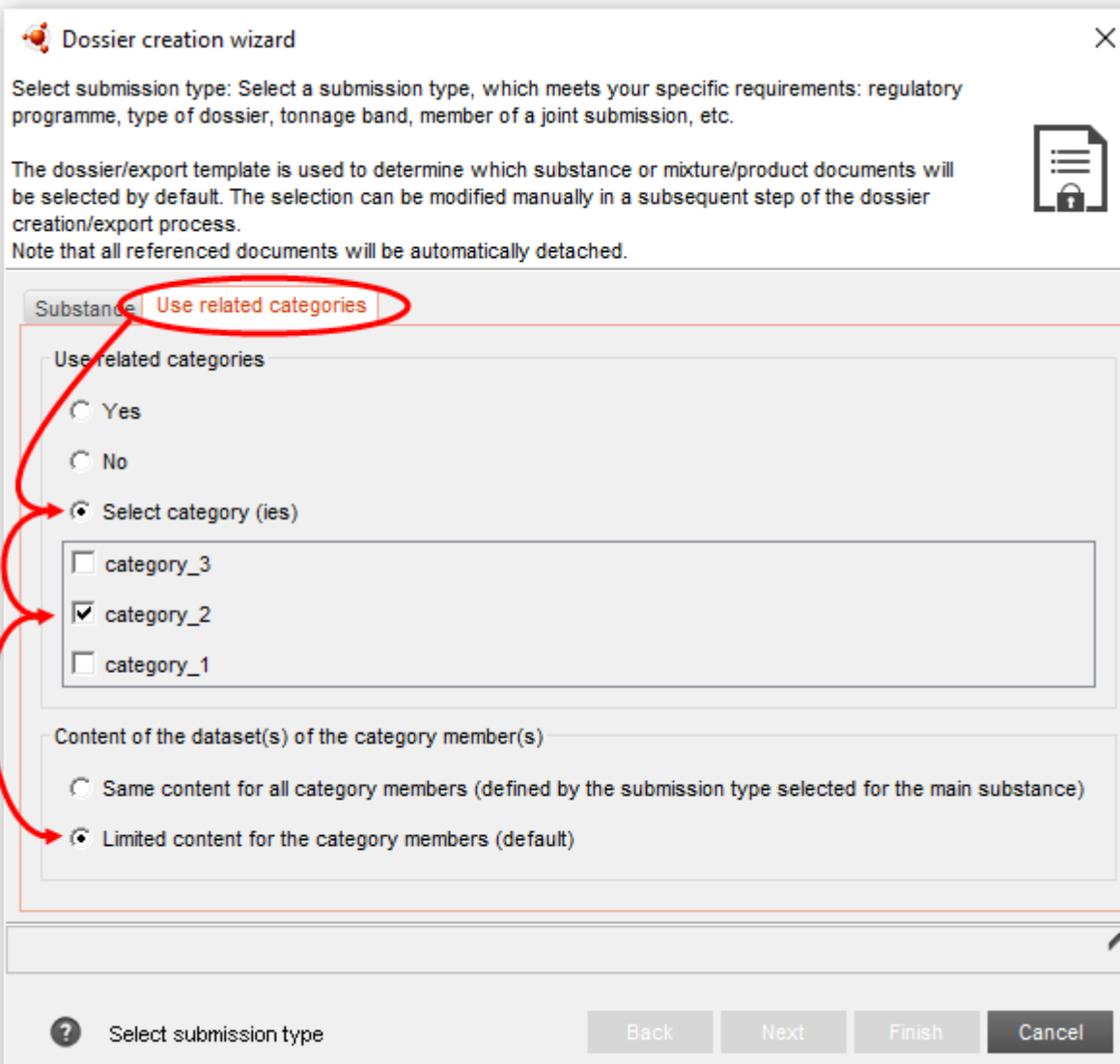
If a tab labelled *Use related categories* is visible, the dataset from which the *Dossier* is being created is in a *Category*. See the next section for more information of the inclusion of data from a *Category*.

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

7.1.2. Use related categories

If the *Substance* 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*. In addition, either a subset or, none of the *Categories* may be selected. An example is shown below in which only the *Category* named *category_2* is included in the *Dossier*.

Figure 63: Including a Category in a Dossier



The screenshot shows the 'Dossier creation wizard' window. The 'Use related categories' tab is selected and highlighted with a red circle. Below the tab, there are three radio button options: 'Yes', 'No', and 'Select category (ies)'. The 'Select category (ies)' option is selected. Below this, there is a list of categories with checkboxes: 'category_3' (unchecked), 'category_2' (checked), and 'category_1' (unchecked). Below the list, there are two radio button options for the content of the dataset(s): 'Same content for all category members (defined by the submission type selected for the main substance)' and 'Limited content for the category members (default)'. The 'Limited content for the category members (default)' option is selected. At the bottom of the window, there are navigation buttons: 'Back', 'Next', 'Finish', and 'Cancel'. A question mark icon is next to the text 'Select submission type'.

7.1.2.1. Content of the datasets(s) of the category members(s)

In *Export* and *Dossier creation* from a *Substance*, these fields may be used to reduce the scope of the data that is outputted from the member *Substances* of the selected *Category(ies)*. It can be used to avoid including large amounts of unnecessary data, thereby using the system resources of

IUCLID 6 more efficiently. The *Substance dataset* from which the *Export* or *Dossier creation* is launched is referred to below as the *main Substance*.

Limited content for the category members

Members of categories other than the main Substance have a filter applied to remove all documents except those in sections 1.1, 1.2, and 4 to 7. The field in the *Category(ies)* named *Category documents* is not used in the filtration process. In effect, the entity *Category* is used only to define a group of *Substances*. The only documents that are included from outside sections 1.1, 1.2, and 4 to 7, are those from the *main Substance* that are required by the *Dossier* type. This is the default setting.

Same content for all category members (defined by the submission type selected for the main Substance)

The type of *Dossier* determines which documents are included for both the *main Substance*, and all the members of the *Categories*. The field in the *Category(ies)* named *Category documents* is not used as a filter. In effect, the entity *Category* is used only to define a group of *Substances*.

After configuring the use of *Categories*, to proceed with *Dossier creation*, click on the tab *Substance*, and then click on the button *Next*.

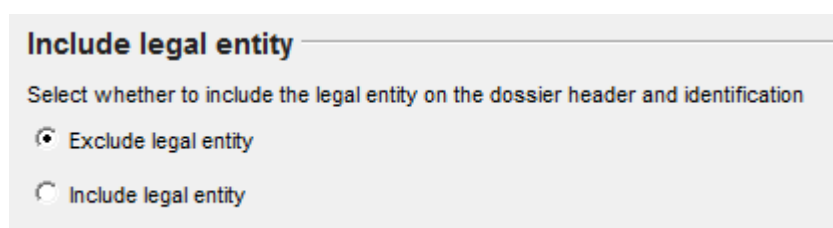
7.1.3. Advanced settings for excluding and including data from the Dossier

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*.

7.1.3.1. Include legal entity

Either exclude or include the *Legal entity* that is attached to the *Substance* or *Mixture/Product*. Unlike the other fields, the default is to **exclude**.

Figure 64: Include/Exclude legal entity from a dossier



Include legal entity

Select whether to include the legal entity on the dossier header and identification

Exclude legal entity

Include legal entity

7.1.3.2. Detail level of document fields

Unticking the box labelled *Detailed fields*, excludes from a *Dossier* the fields that are labelled as being confidential by having the word *confidential* in the name of the field, and a grey warning icon to the right of the field name. Note that these fields are handled completely separately from fields for which flags may be set.

Figure 65: Detail level of document fields, to be included in a dossier

Detail level of document fields

Content of the documents to be included: by default the basic fields are included, please select if you want to include:

- Detailed fields (e.g. needed for robust study summaries)
- Fields marked "(confidential) ⚠"

Example

The figure below shows an example of a field that can be excluded. It is part of *Test materials*.

Figure 66: Example of a field marked as confidential but with no flag

Other characteristics

Test material form

solid: crystalline ... Other

Details on test material

⚠ | X

Confidential details on test material ⚠

⚠ | X

0.1 % EDTA

7.1.3.3. 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 67: Automatically exclude fields from a Dossier

Flags for confidentiality

1 Select information that will be included 2

3

▼ Data for which a confidentiality flag may be set, but it is not. [x]

CBI	CBI: Information must not be provided to other companies or disseminated to public
IP	IP: Information should only be provided to other companies when they are trusted
no PA	no PA: Information can be provided to other companies but must not be disseminated to public

Flags for regulatory programme

Select information that will be included

▼ No regulatory purposes [x]

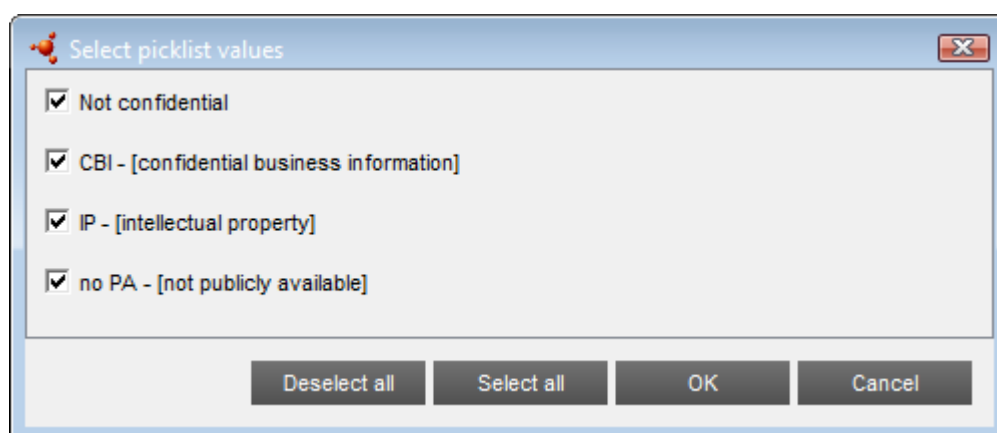
- EU: BPD or EU: BPR
- EU: CLP
- EU: PPP
- EU: REACH
- CA: CEPA
- CA: PCPA
- JP: CSCL
- OECD: CoCAP
- US: EPA HPVC
- US: FIFRA
- US: TSCA
- Any other

Key for Figure 67

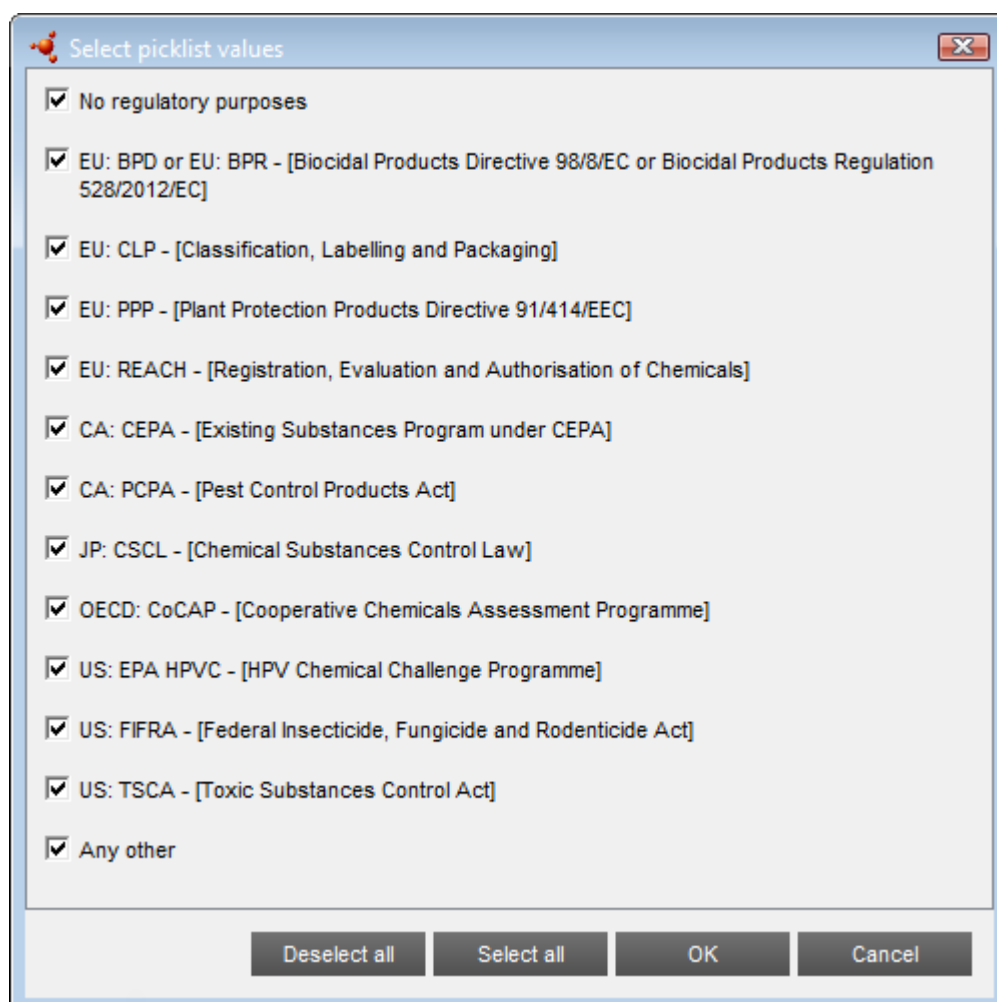
1. Open the pick lists that are shown in the figures below
2. Get some tips on what the abbreviations used here mean.
3. Untick all the options in one go, and collapse the field.

Clicking on the black triangle opens a pick-list. Unticking a box 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 68: Automatic exclusion of fields from a Dossier according to the values of confidentiality flags

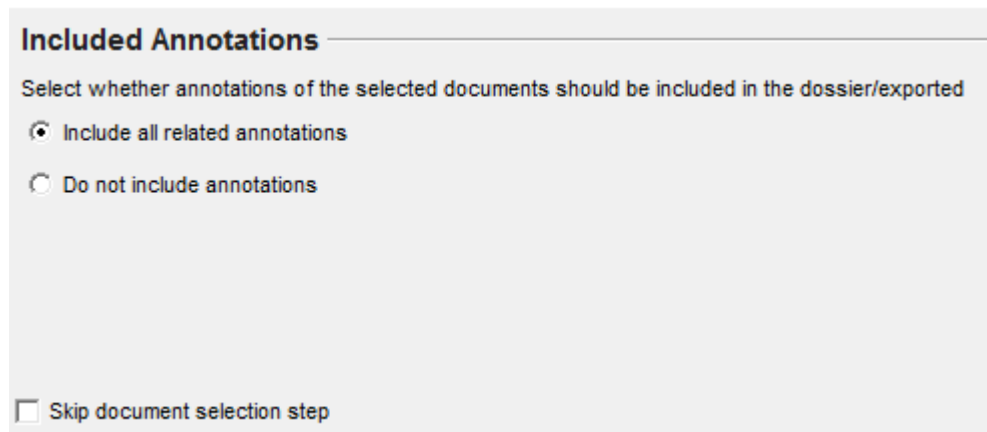
The pick-list for regulatory flags is shown in the figure below. For example, if the box for EU: CLP were unticked, all fields flagged with EU: CLP would be automatically excluded from the Dossier.

Figure 69: Automatic exclusion of fields from a Dossier according to the values of regulatory flags

7.1.3.4. *Include Annotations*

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

Figure 70: Exclusion of Annotation entities



Included Annotations

Select whether annotations of the selected documents should be included in the dossier/exported

Include all related annotations

Do not include annotations

Skip document selection step

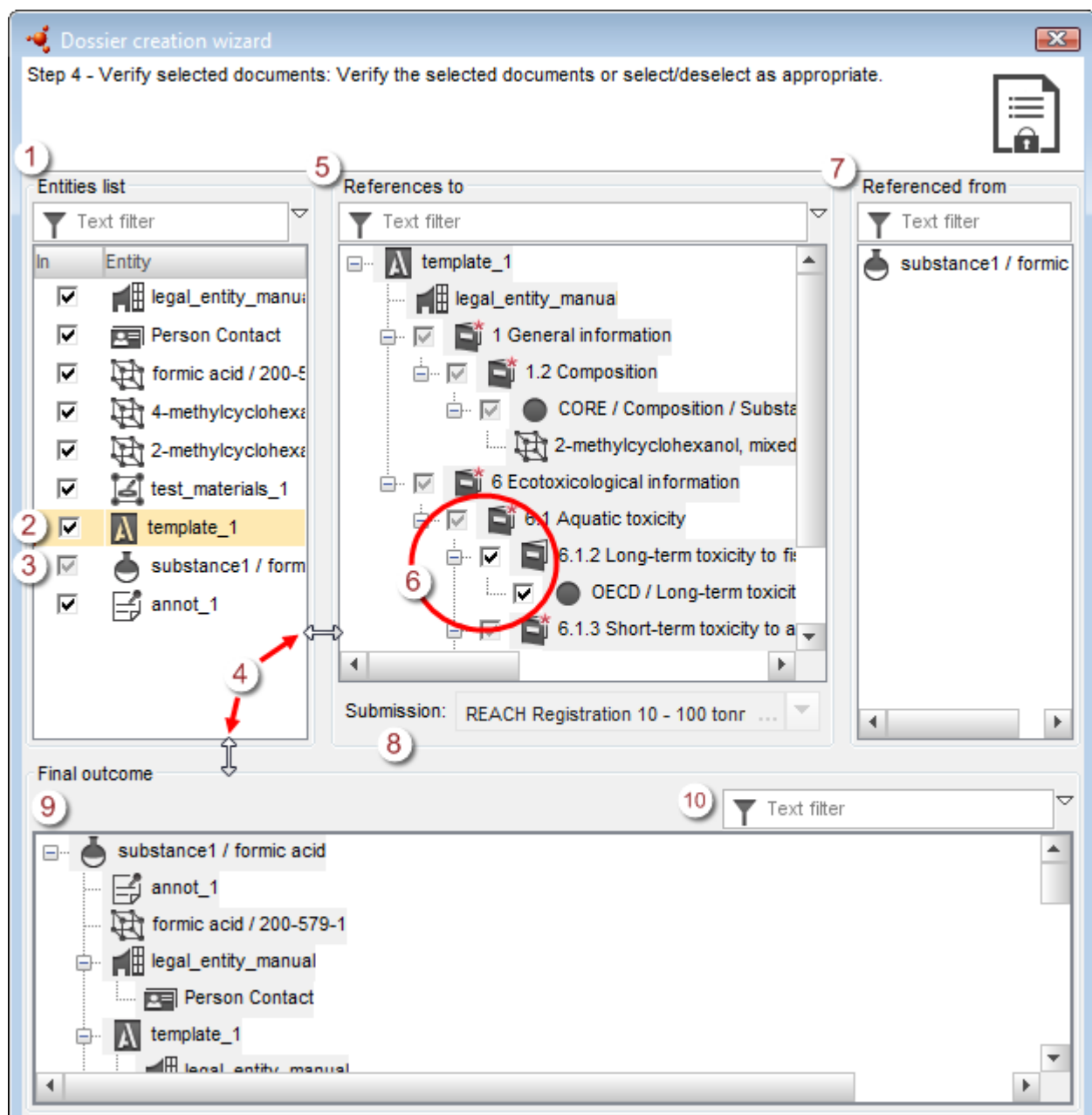
7.1.3.5. *Skip document selection*

If all the documents in the substance dataset are to be included in the dossier, tick the option *Skip document selection*. This misses out the next step in the wizard, and jumps straight to the entry of administrative data in to the dossier header.

7.1.3.6. *Document selection*

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 71: Manual selection of documents in a Dossier

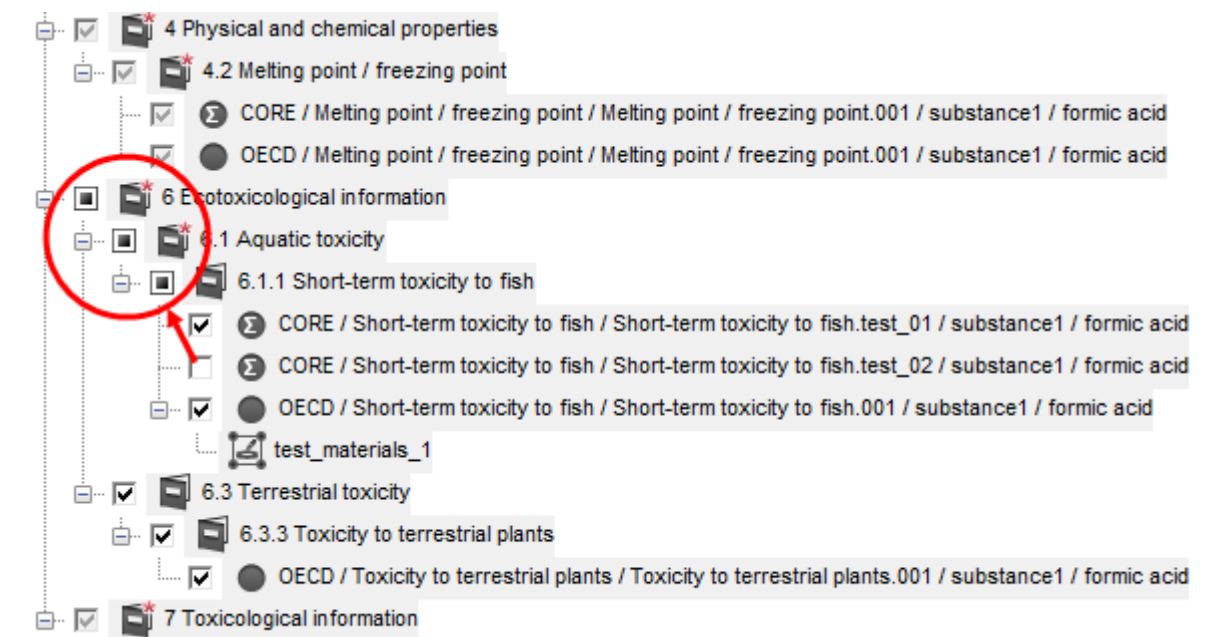


Key for Figure 71

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.

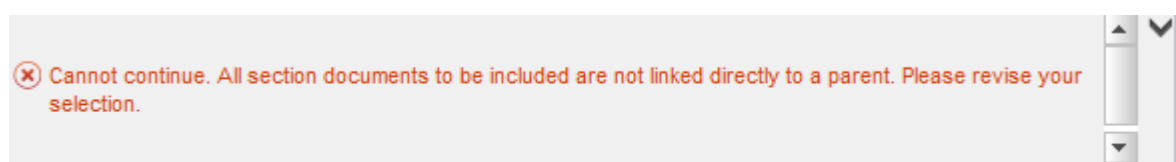
- The upper middle pane contains a tree view of the entity currently selected in the upper left pane.
- Within the entity tree view in the upper middle pane, some sections and documents can be excluded by unticking their boxes, but some cannot. This is because IUCLID is applying the rules for which sections 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 72: Section with excluded documents in Dossier creation



- The right-hand upper pane shows documents that refer to the selected entity.
 - The type of *Dossier* is stated here, under the upper middle pane.
 - The expected final outcome of what the *Dossier* will contain, is shown in the lower pane.
 - 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 73: Error message on exclusion of an essential entity from a Dossier



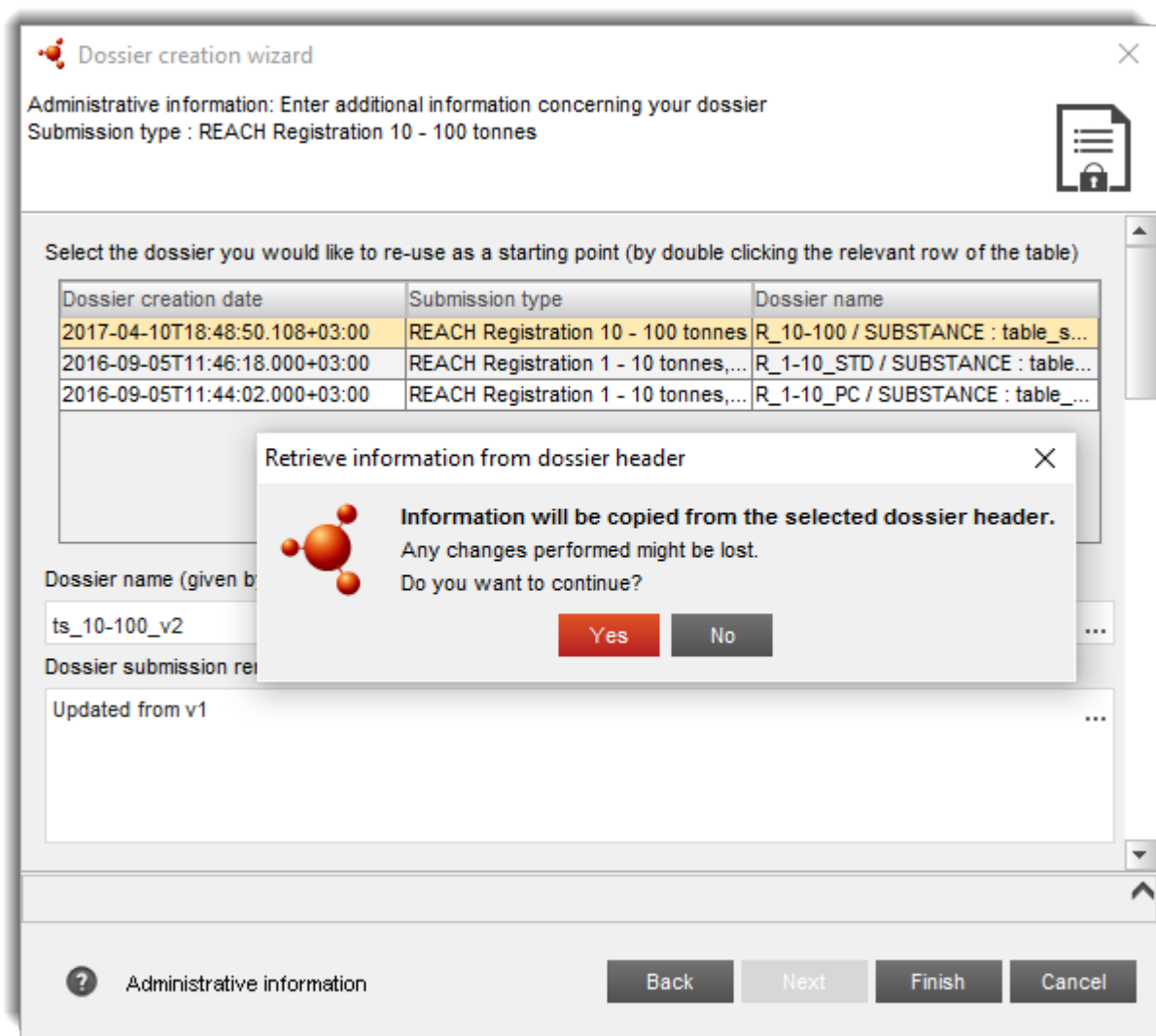
After making any exclusions of documents required, go to the next step of the wizard where administrative information is entered.

7.1.4. Administrative data to be placed in the Dossier header

The information entered on this page is recorded in the header of the *Dossier*.

If the IUCLID 6 database contains at least one Dossier that was created from the same Substance dataset as the current Dossier, there is an option to copy all the information from the header of such a Dossier. To perform the copy, double-click on the entry in the list for the required Dossier. All the values in the Dossier header are copied over, including empty fields. Therefore, where an empty field is copied, any value in the header being edited is deleted. The feature of copying a header is particularly useful when preparing an update to a regulatory submission. After copying a Dossier header, remember to edit the copied values, where necessary, so that they are correct for the Dossier being created.

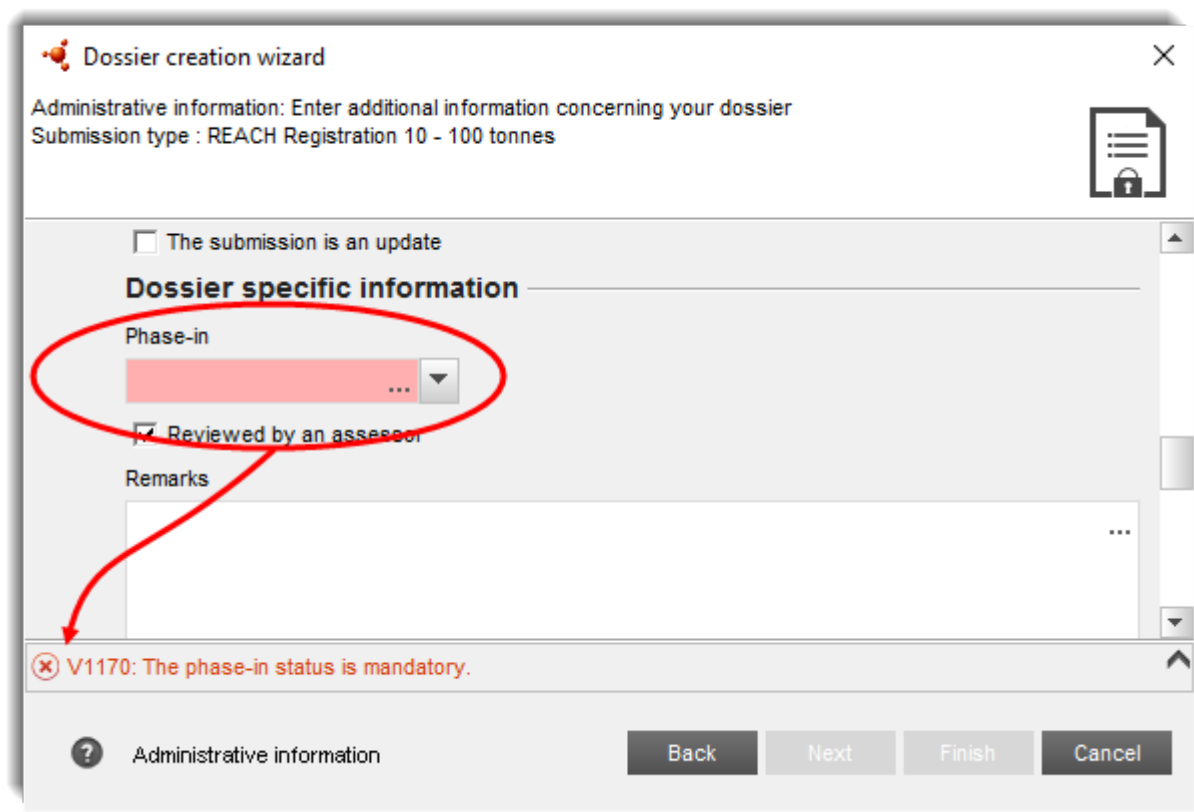
Figure 74: Copy data from the header of a Dossier that was created from the same Substance dataset



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, the background of the

field is coloured in pink, and a brief explanation is provided 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 75: Data validation in the Dossier header

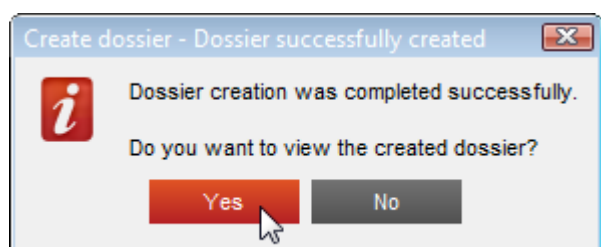


The screenshot shows the 'Dossier creation wizard' window. The title bar reads 'Dossier creation wizard'. Below the title bar, it says 'Administrative information: Enter additional information concerning your dossier' and 'Submission type : REACH Registration 10 - 100 tonnes'. There is a checkbox for 'The submission is an update' which is unchecked. Below this is a section titled 'Dossier specific information'. The 'Phase-in' field is highlighted with a red oval and is currently empty, with a dropdown arrow on the right. Below it is a checkbox for 'Reviewed by an assessor' which is checked. There is a 'Remarks' text area below that. At the bottom of the window, there is a red error message: 'V1170: The phase-in status is mandatory.' Below the error message, there is a navigation bar with a question mark icon, the text 'Administrative information', and four buttons: 'Back', 'Next', 'Finish', and 'Cancel'.

7.1.5. 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 76: Dossier created successfully



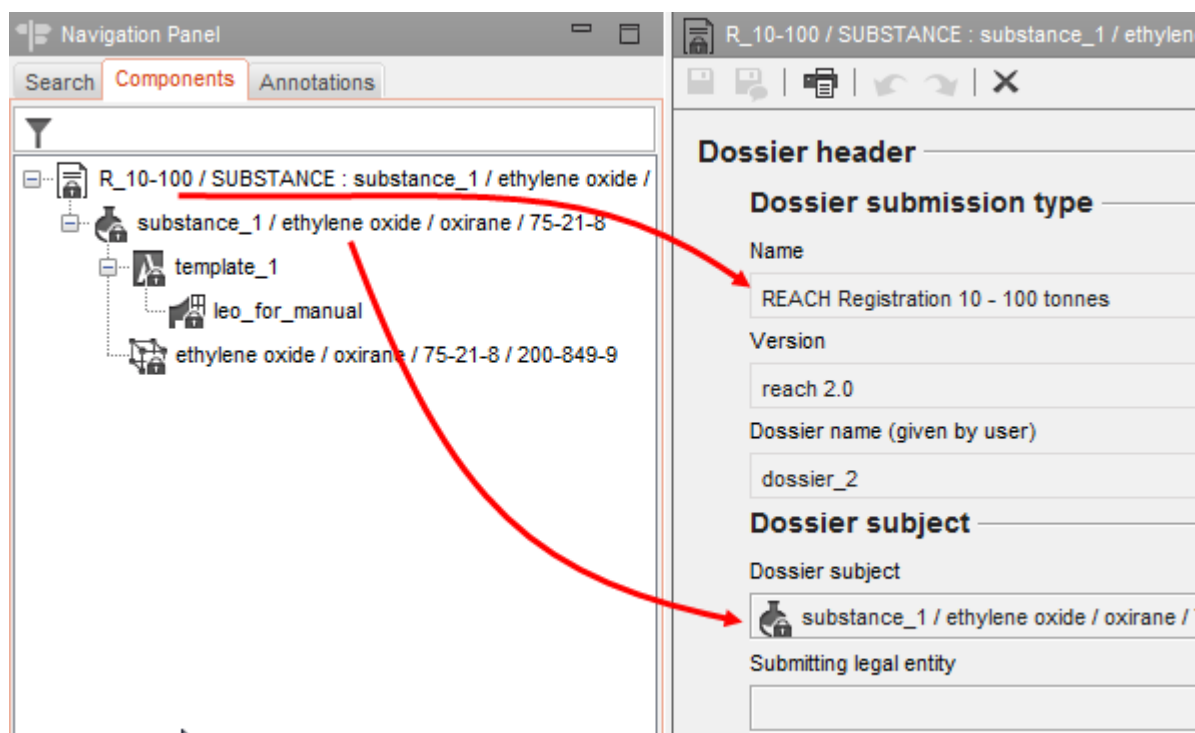
To view the content of the *Dossier*, first click on *Yes*, and then browse through the tree structure shown in the tab *Contents*. The structure of a *Dossier* is described in the next section.

If you do not need to view the *Dossier*, but you want to check it straight away using one of the plugins, for example the *Fee calculator*, first click on the tab *Search*, which shows the *Dossier* as a single search result. Next, right-click on the record of the *Dossier*, and select the required function.

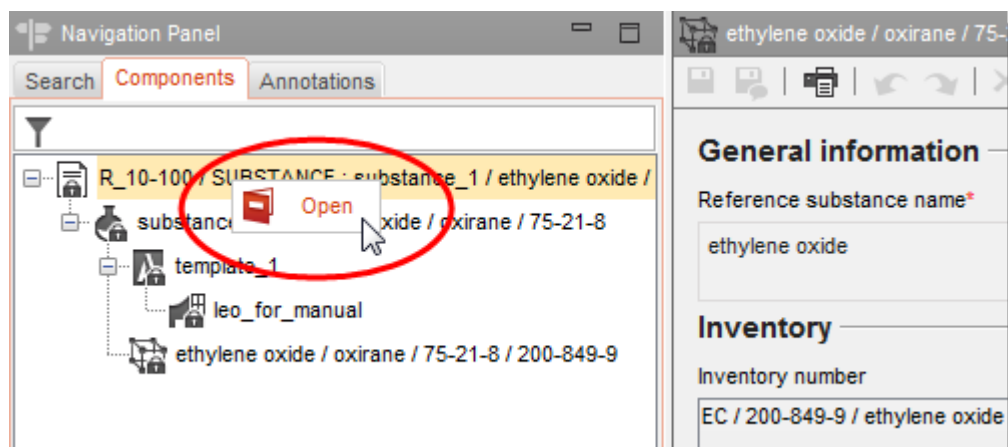
7.2. The structure of a Dossier

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.

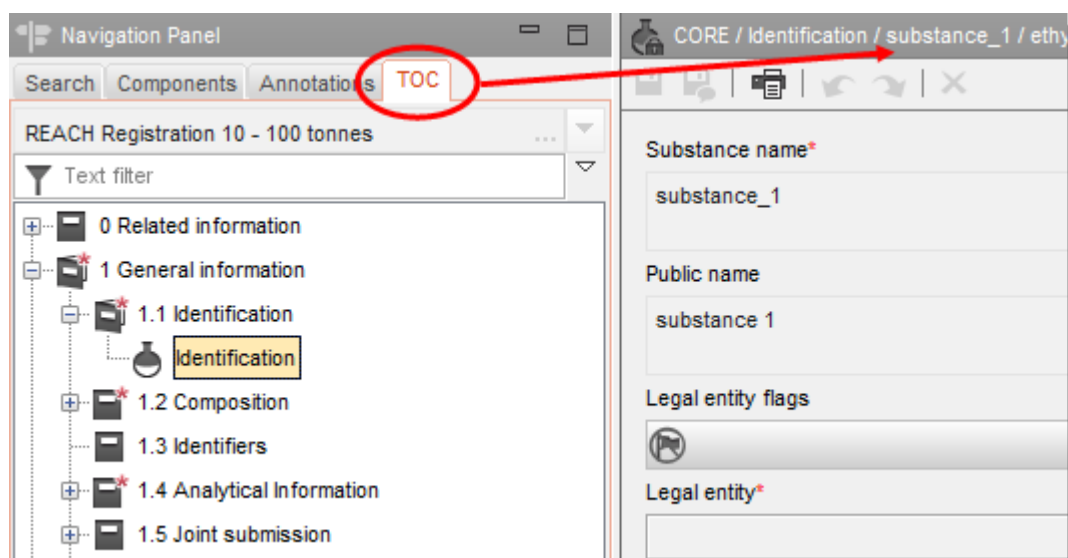
Figure 77: Top-level entities under the component tab and in the Dossier header



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 78: How to display the Dossier header

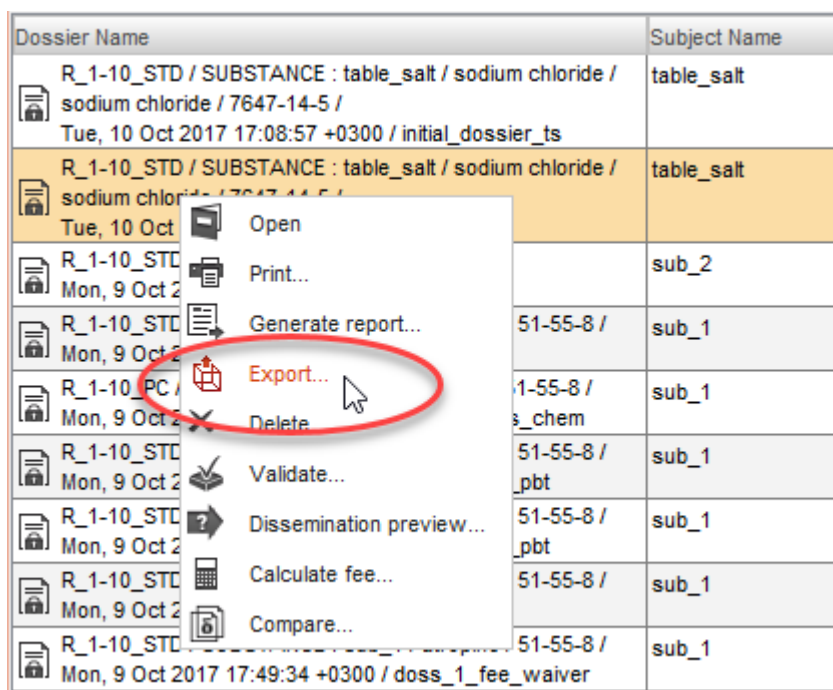
Opening a *Substance* entity displays its TOC under a new tab. The TOC of the *Substance* can be browsed in the usual way, in read-only mode.

Figure 79: 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 80: Export a Dossier



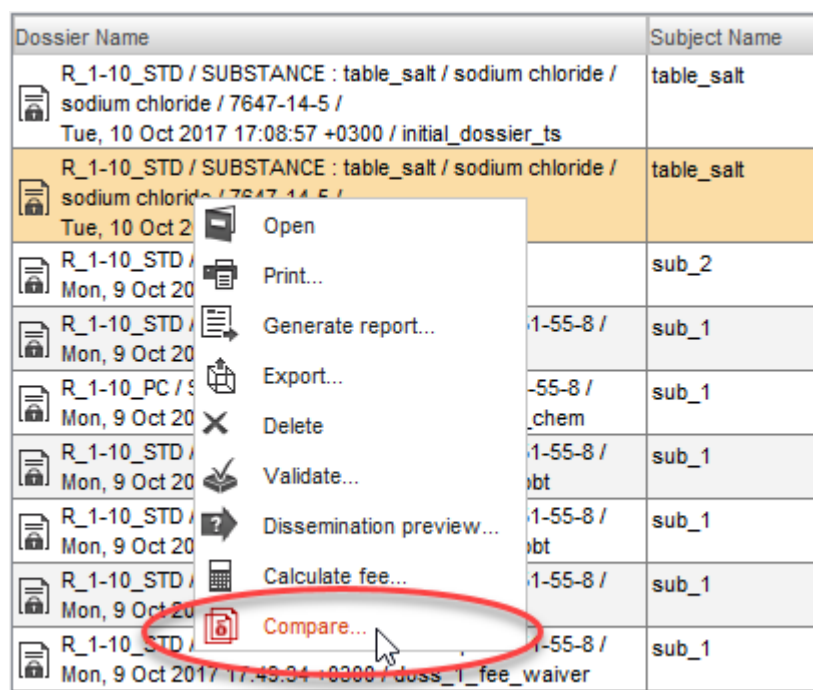
7.4. Compare Dossiers (Available only in the web interface)

The function *Compare* provides a means of viewing all the differences between the data contained within two Dossiers.

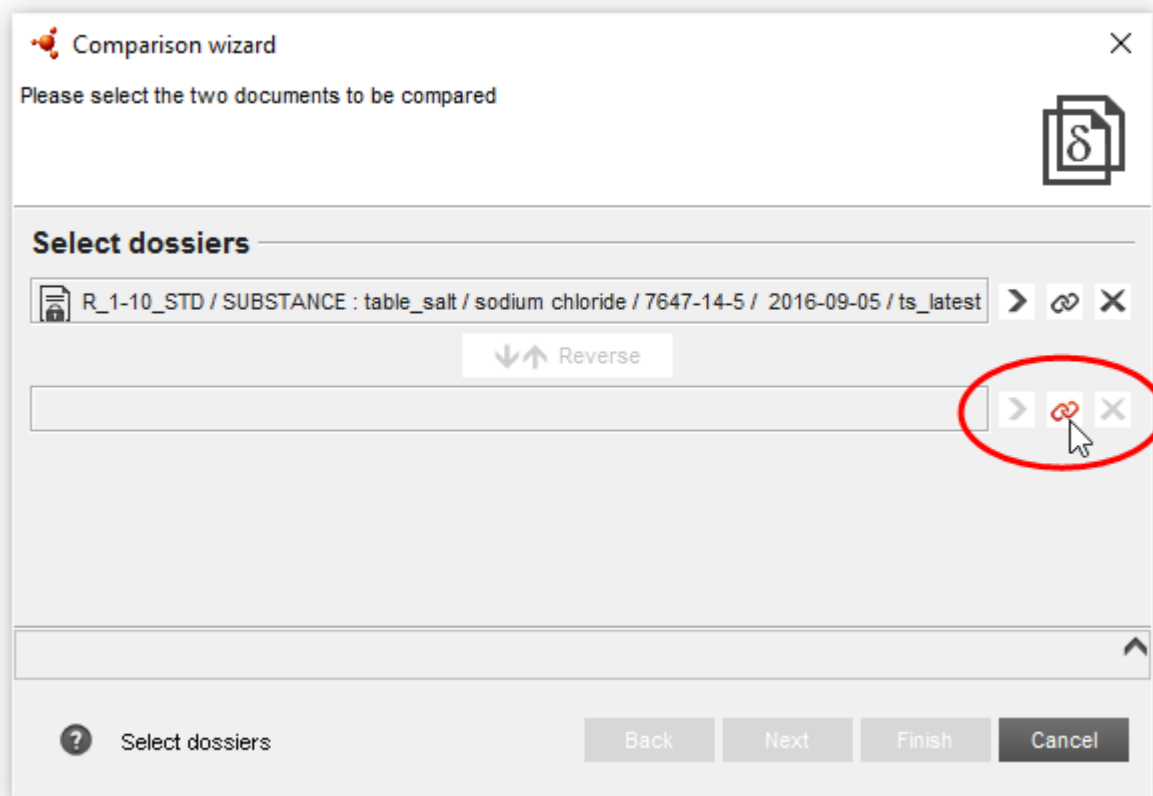
7.4.1. Selecting Dossiers to compare

To compare any two Dossiers, right-click on one of them in the search results, and then select *Compare*, as shown below.

Figure 81: Starting the Dossier comparison wizard from a single Dossier

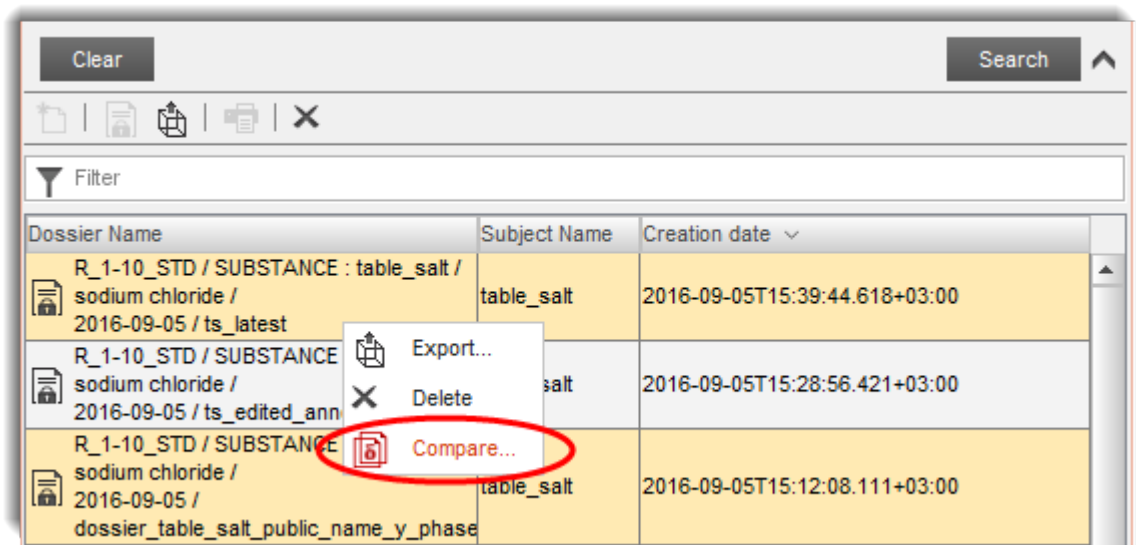


This opens the Dossier comparison wizard in a pop-up window. An example is shown below.

Figure 82: Selecting Dossiers for comparison, and the order of comparison

The selected Dossier is shown in the upper field. To select the other Dossier, in the lower field, click on the link icon and then search for the Dossier. The order in which the Dossiers are compared may be reversed by clicking on the button that is between the two fields.

If both Dossiers are visible in the results of the search window, and both are selected, the Dossier comparison wizard may be opened from either Dossier record, in which case both Dossiers appear in the comparison wizard, and in the same order as in the search results. An example of the selection of Dossiers in the search window, and right-clicking an entry is shown below:

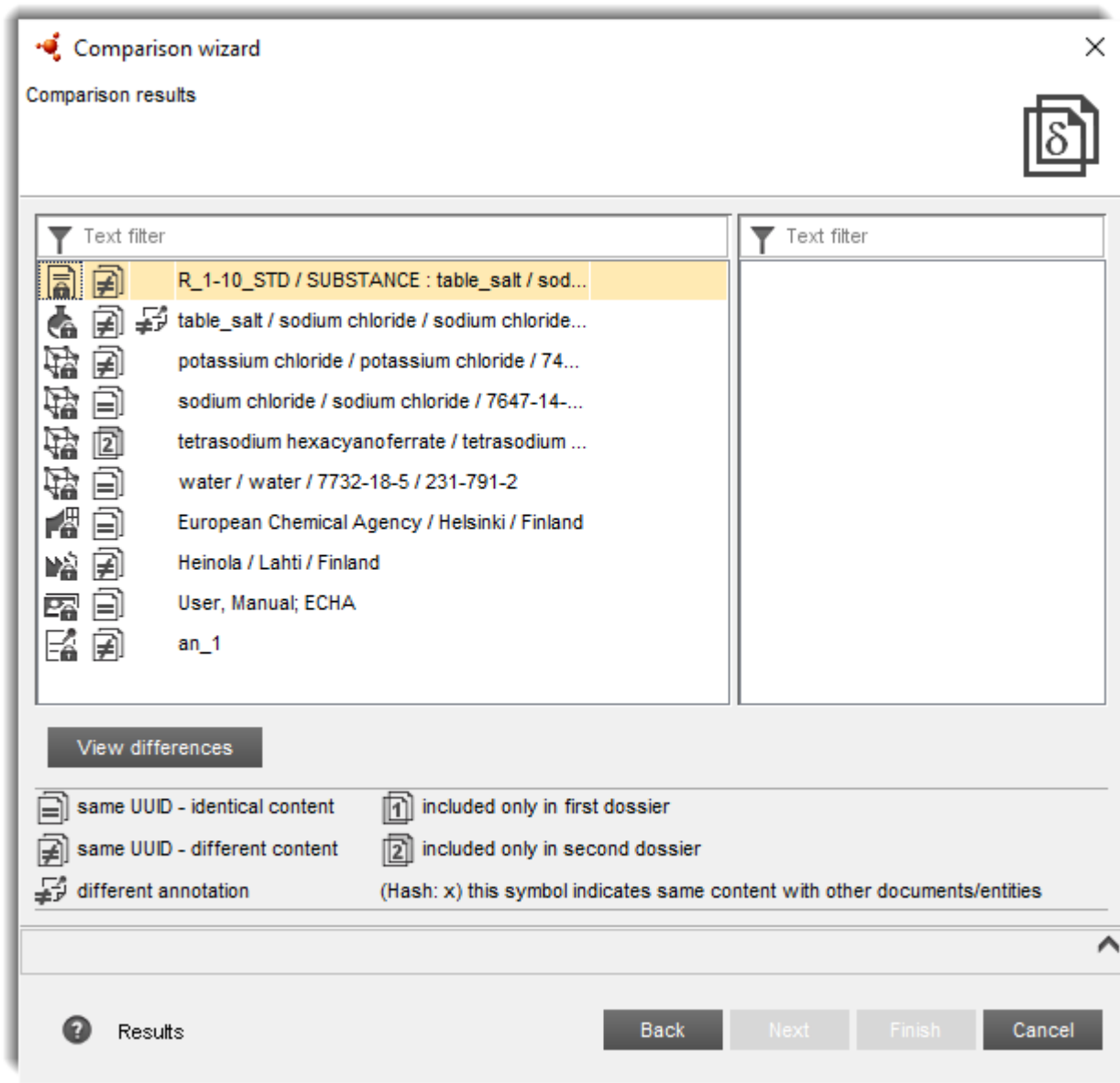
Figure 83: Select two Dossiers for comparison from within the search results

7.4.2. The summary view in Dossier comparison

When you are sure that you have selected the correct Dossiers in the required order, click on the button, *Next*. The wizard shows a high-level summary of the comparison; with the compared entities listed on the left. An example is shown below in which the differences between the Dossiers are:


- 1) The names of the Dossiers given in the Dossier headers are different;
- 2) The Annotation *an_1* that is attached to the Substance was edited;
- 3) Information was added to the Reference substance named *Potassium chloride*;
- 4) The Legal entity site named *Heinola* was edited;
- 5) A new Reference substance was included in the second Dossier, named *tetrasodium hexacyanoferate*;
- 6) Data was added to the Substance in an endpoint study record in the section on *Basic toxicokinetics*.





Figure 84: Page two of the dossier comparison wizard



In the first column, icons are used to indicate the type of entity. In the second and third column, icons are used to indicate the results of the comparison, as described in the table below.

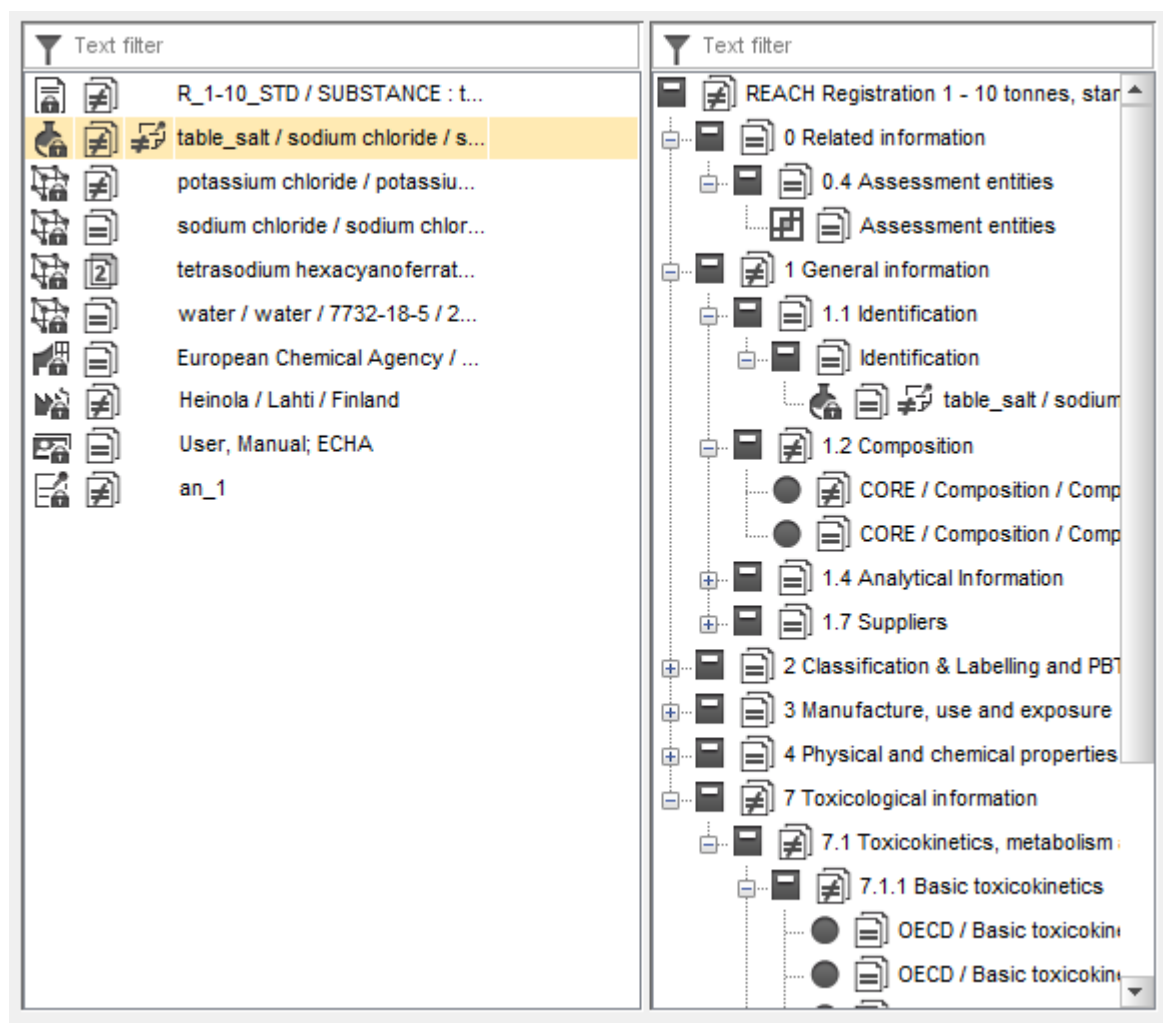
Table 6: Key for the icons in the Dossier comparison wizard

Icon	Label in interface	Description
	Same UUID - identical content	The entity or document is exactly the same in both Dossiers.

Icon	Label in interface	Description
	Same UUID - different content	The entity or document has the same UUID in both Dossiers, but different content. For example, this could happen for an endpoint study record if the Dossiers being compared were created from the same Substance that contained it, and the endpoint study record were edited after the creation of the first dossier. This can occur during the process of providing updated data under a regulation, for example under REACH.
	Different annotation	There is a difference in the content of the Annotation, even if the UUID is the same in both Dossiers.
	Included only in first dossier	The numbers 1 and 2 refer respectively to the upper and lower fields on the first page of the comparison wizard.
	Included only in second dossier	The numbers 1 and 2 refer respectively to the upper and lower fields on the first page of the comparison wizard.

If the selected type of entity contains other entities or documents, as is the case for Substance, selecting it in the left panel causes a hierarchical table of contents to be shown in the right panel.

An example of the table of contents shown on the right, for a Substance, is given below.

Figure 85: Viewing the table of contents of a Substance in the Dossier comparison wizard

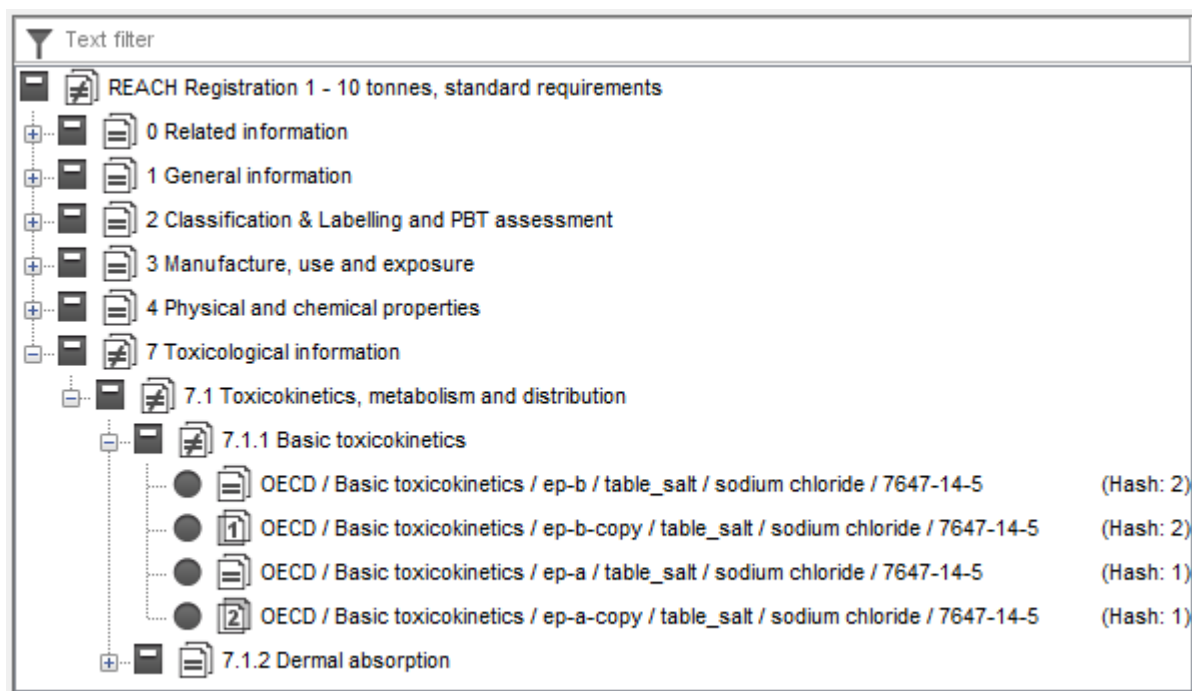
Difference is indicated in an upwards direction through the hierarchy of the table of contents. For example in Figure 71 above, a difference is indicated for *1 General Information*, but not for *0 Related information*.

7.4.3. Hash: x

If two or more entities or documents in a single Dossier have identical content, but different UUIDs, a label of the form (*Hash: x*) is appended to the entry in the tree view shown on the right. The number *x* is unique to the duplicated content. It starts at 1 and increments by 1 for each document/entity that contains unique identical content.

Example

An example is given below in Figure 72, where there are two sets of repeated content, one with an entry ending in (*Hash: 1*), and another with an entry ending in (*Hash: 2*).

Figure 86: Entities/documents with content duplicated within a Dossier

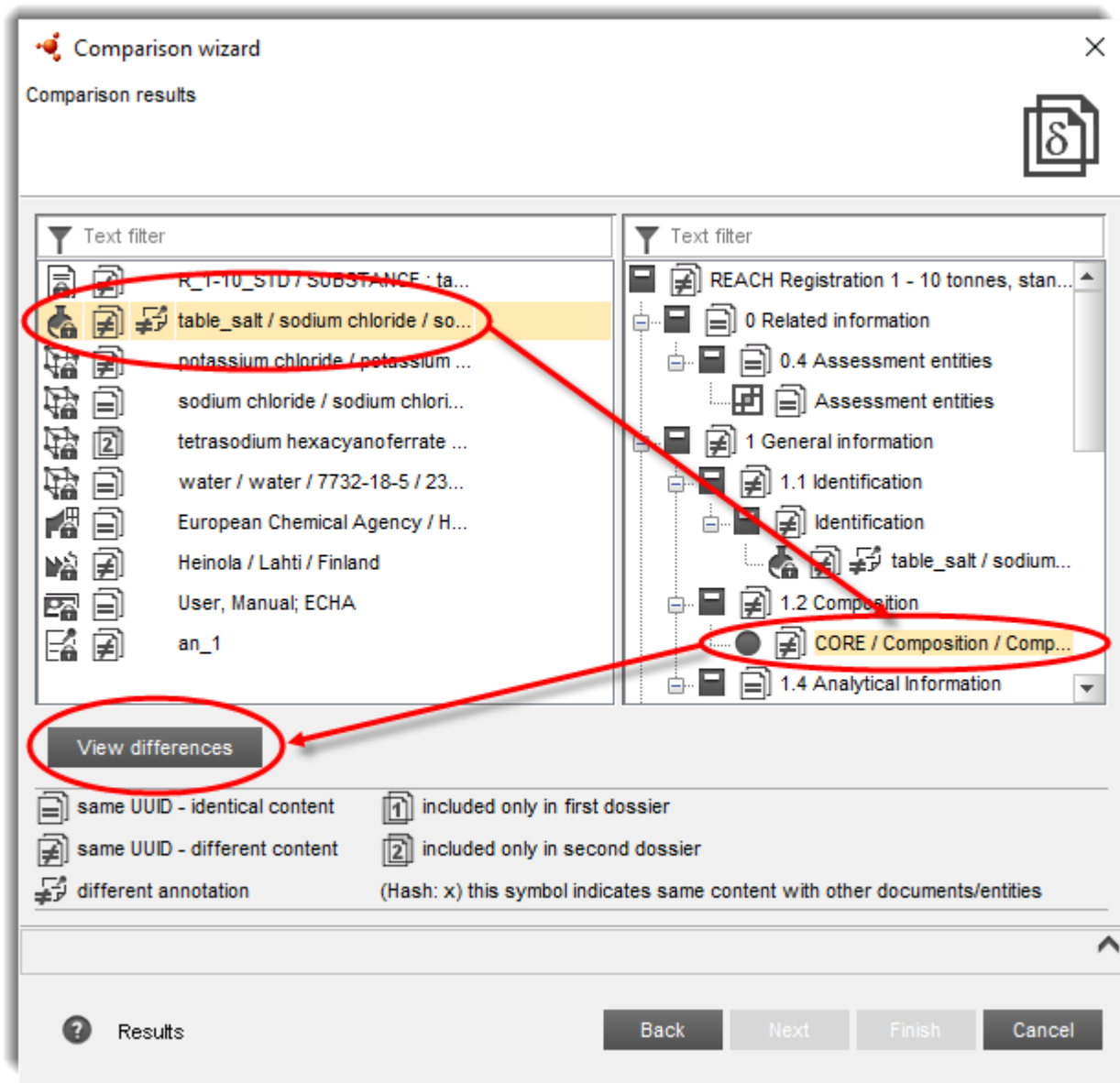
In Dossier 1 there are two endpoints with identical content and different UUID: *ep-b* and *ep-b-copy*. In Dossier 2 there are two endpoints with identical content and different UUID: *ep-a* and *ep-a-copy*. The endpoints *ep-a* and *ep-b* are in both Dossiers. Endpoint *ep-a-copy* is in only Dossier 2 and endpoint *ep-b-copy* is in only Dossier 1.

7.4.4. View difference

The button *View difference* is active on selection of a row in either the left or right panels for which a difference is indicated, and the row represents either a document or an entity at the lowest level in the hierarchy. In the left panel, this includes the top row, which represents the Dossier header, and some other entities such as Legal entity site, and Reference substance.

An example of the table of contents shown on the right, for a Substance, is given below. Various differences have been found in the Substance. In this case, the view on the right of the page is being used to select a *Composition*.

Figure 87: Viewing the table of contents of a Substance in the Dossier comparison wizard



Whilst the button *View difference* is active, clicking on it opens a page that lists the differences within the document or entity. An example of the window is shown below for the selection made in Figure 70. The difference indicated is for the Dossier header, where the names of the Dossiers are *initial_dossier_ts* and *update_dossier_ts*.

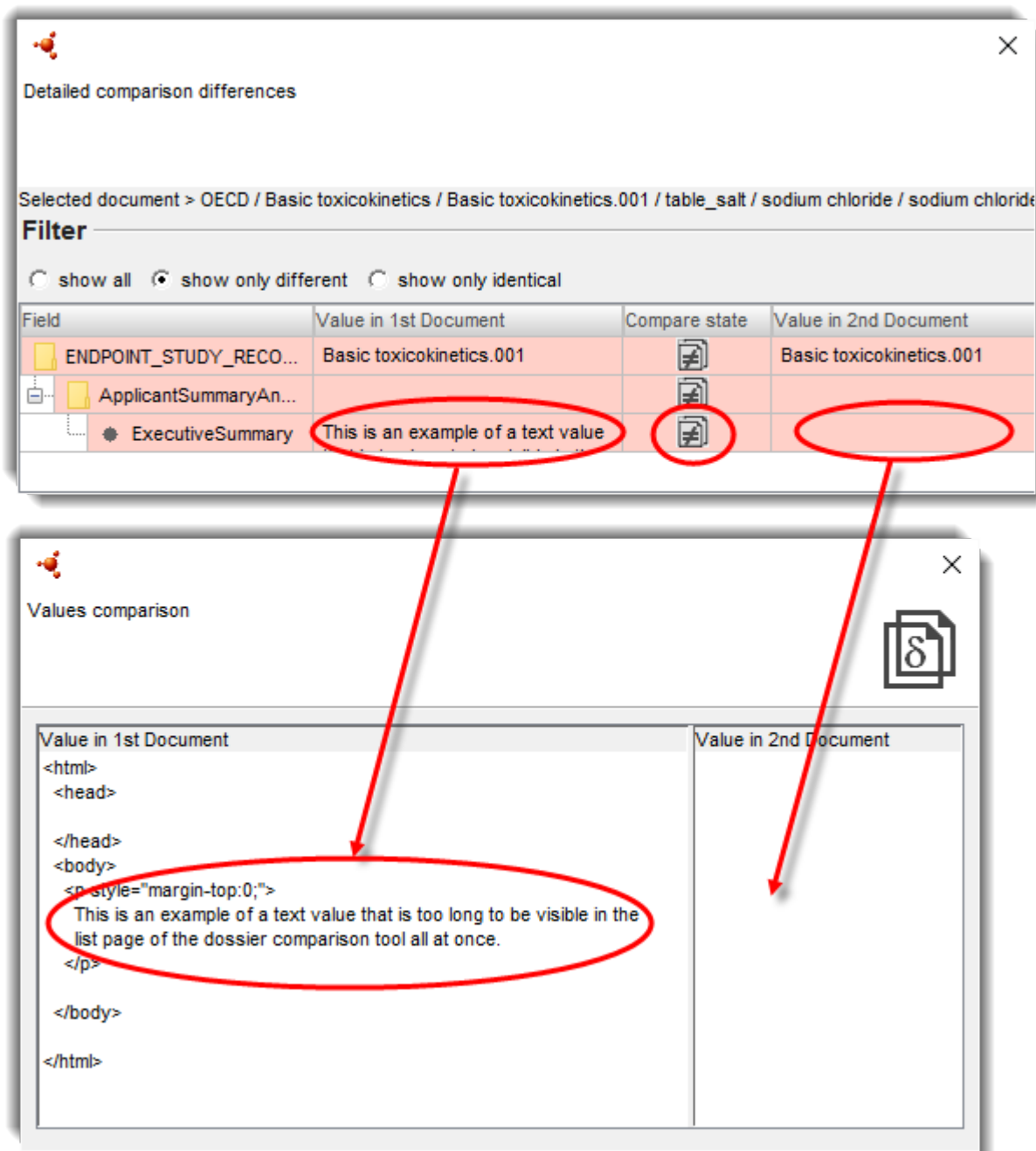
Figure 88: A list of the differences between the headers of two Dossiers

Field	Value in 1st Document	Compare state	Value in 2nd Document
DOSSIER.R_1-10_STD	initial_dossier_ts		update_dossier_ts
DOSSIER.R_1-10_STD	initial_dossier_ts		update_dossier_ts
SubmissionType			
JointSubmission	false		false
InformationProvidedByLead			
ChemicalSafetyReport	false		false
GuidanceOnSafetyReport	false		false
ReviewedByAssessor	false		false

This view has three types of filter: *show all*, *show only different*, and *show only identical*. The locations of differences are emphasised using a red background, as opposed to green where the data are identical. The tree view may be collapsed or expanded as required. The compared values are shown in the columns *Value in 1st Document* and *Value in 2nd Document*.

If a value is too large to be seen all at once in the list view, or if you need to copy the value to the clipboard, open the side-by-side comparison view, by clicking on the icon in the column for *Compare state*. An example is shown below for a rich text field in an endpoint study record. For a field of type rich text, the HTML code for the field is shown.

Figure 89: Show side by side, the values for a field in two different dossiers



7.4.4.1. Comparing the headers of Dossiers

To view the differences between Dossier headers, select the top row on the second page of the comparison wizard, and then click on the button *View differences*. An example of the selection is given in Figure 70. All the fields in the Dossier header are shown, for example, the phase-in state, and whether the Dossier is marked as an update.

If there are two icons for Dossier, this means that the Dossiers were created with different submission types; for example, *REACH Registration 1 - 10 tonnes, standard requirements* and *REACH Registration 1 - 10 tonnes, physicochemical requirements*.

8. Legal entity

In IUCLID, a *Legal entity* is used to store information about a party or person that is involved in the life-cycle of a chemical substance, mixture or product. A *Legal entity* can be used to identify the party that is responsible for a certain activity, such as the manufacturing or import of a substance. The *Legal entity* does not have to be created by the person or party it represents. For example, a manufacturer can create a *Legal entity* to store information on a third party representative of the substance, or an only representative can create *Legal entities* to identify their suppliers.

A *Legal entity* 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: import it, create it, or if applicable, obtain access to it from your system administrator. The administration of the access to *Legal entities* is described in section 15.2.2.4.2 *Assign Legal entities to users*.

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

Figure 90: Data window for Legal entity

legal_entity_1

General information Identifiers Contact information Sites

Legal entity name*

legal_entity_1

Legal entity type

consultant ... Other

Remarks

Free text can be entered here.

Other names

Flags	Name
[CB] EU: CLP	another_name

+ Add... Edit... Delete Move

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, a new *Contact* is created in IUCLID 6 for each set of contact information in IUCLID 5.

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 1.7.4 *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

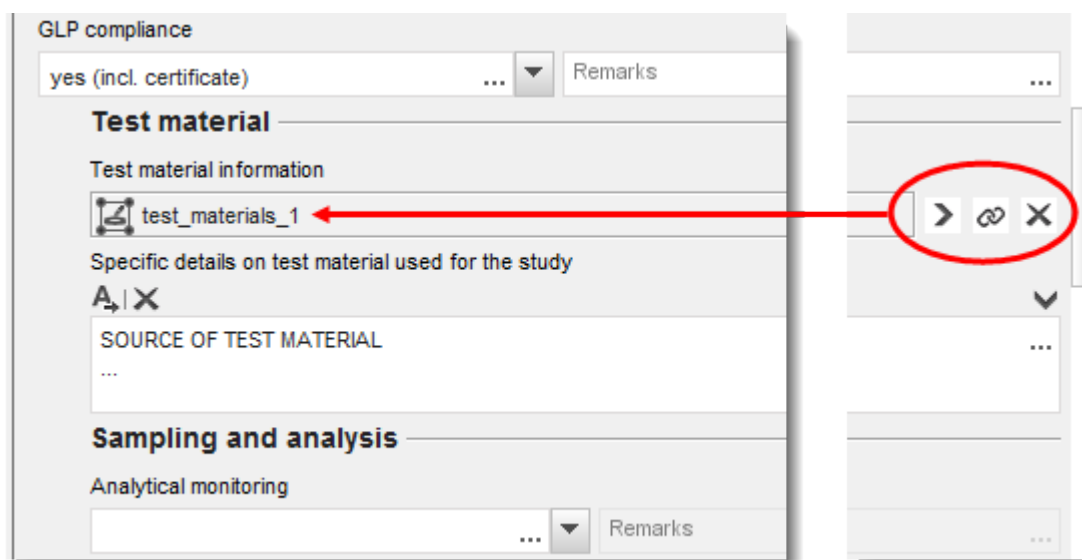
A *Literature reference* is an entity that identifies a particular document that contains information on a *Substance* or a *Mixture/Product*. The only mandatory field is the title, but there are also various other fields that allow a reader to find the document outside IUCLID. A link may be made to 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 91: 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.

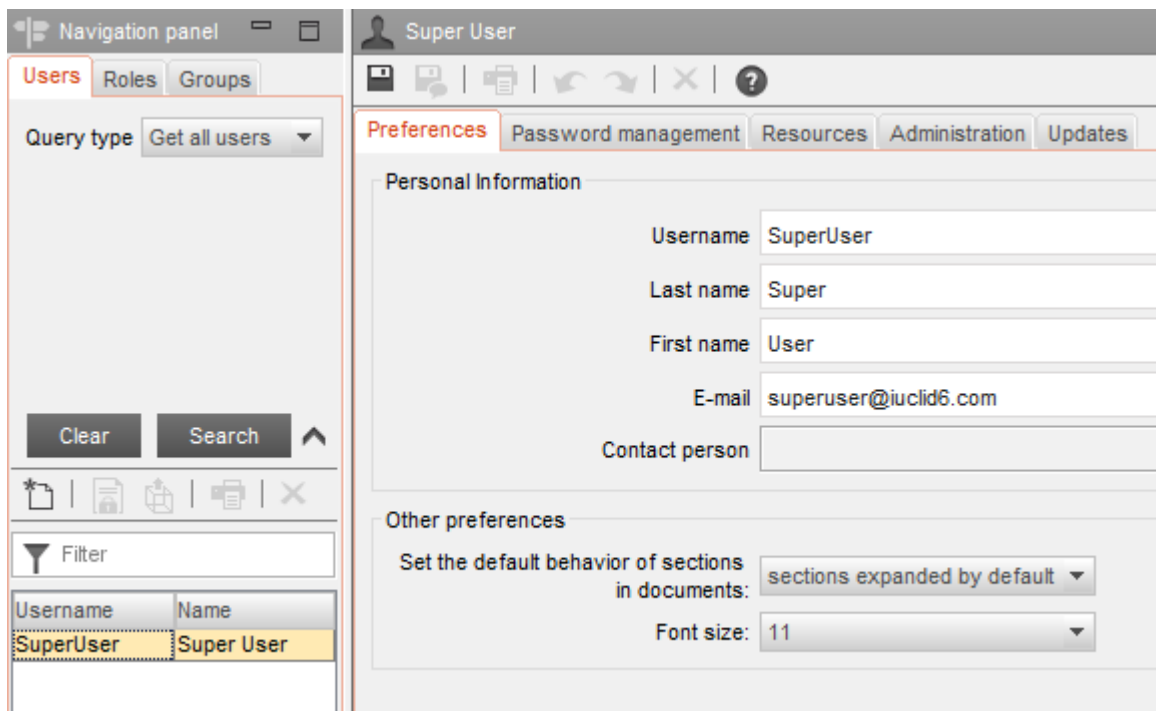
By default, the rules that govern the authentication of the *User* *SuperUser* are the same as those for all the other *Users*. This means that it is possible for the *User* *SuperUser* to become locked as described in section *User management / Administration / General 15.1.2.4.1*. The locking of *SuperUser* 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 92: User management

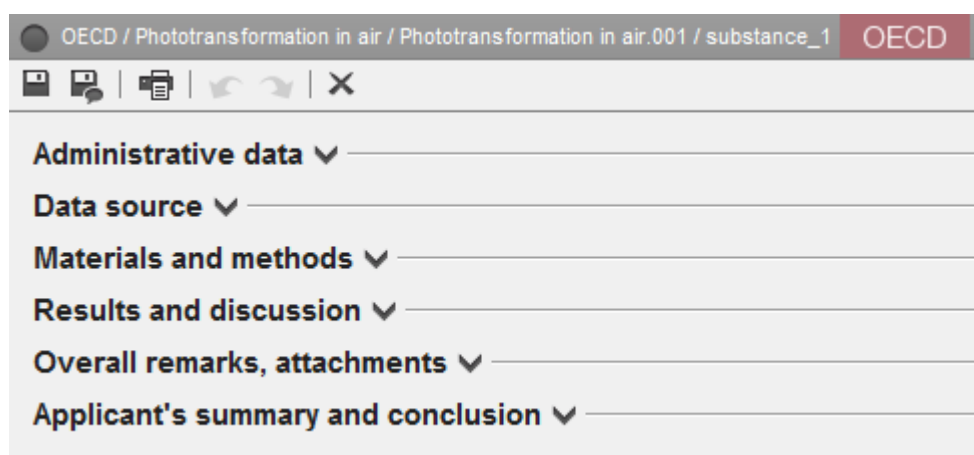
A *User* with user management rights can see all the other *Users*, except those with either the right *Security Management* or *System Configuration*, which includes SuperUser. Therefore, if a *User manager* does not have administrator rights, it cannot see the SuperUser in the interface. A *User* without 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*.

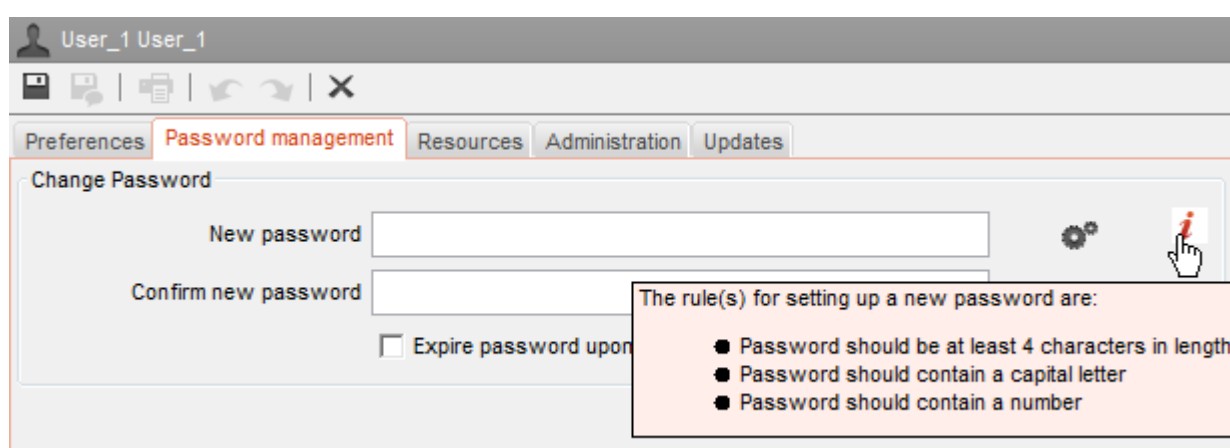
The field *Set the default behaviour of sections in documents* determines whether by default all the sections shown in the data panel are either expanded or collapsed. An example of an endpoint study record with all sections collapsed is shown below:

Figure 93: An example of an endpoint study record with all sections collapsed

The field *Font size* is used to set the size of the font that is used throughout the interface of IUCLID 6 to display the labels of fields and text values. The default value is 11. A change in the setting takes effect immediately on saving the new value. The setting is valid per *User*, so in a multi-*User* environment, different *Users* can have different font sizes. In fields where text can be entered in rich text format, the font and its size can be changed independently of the value set here.

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 94: Password management


Key for Figure 80:

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*.

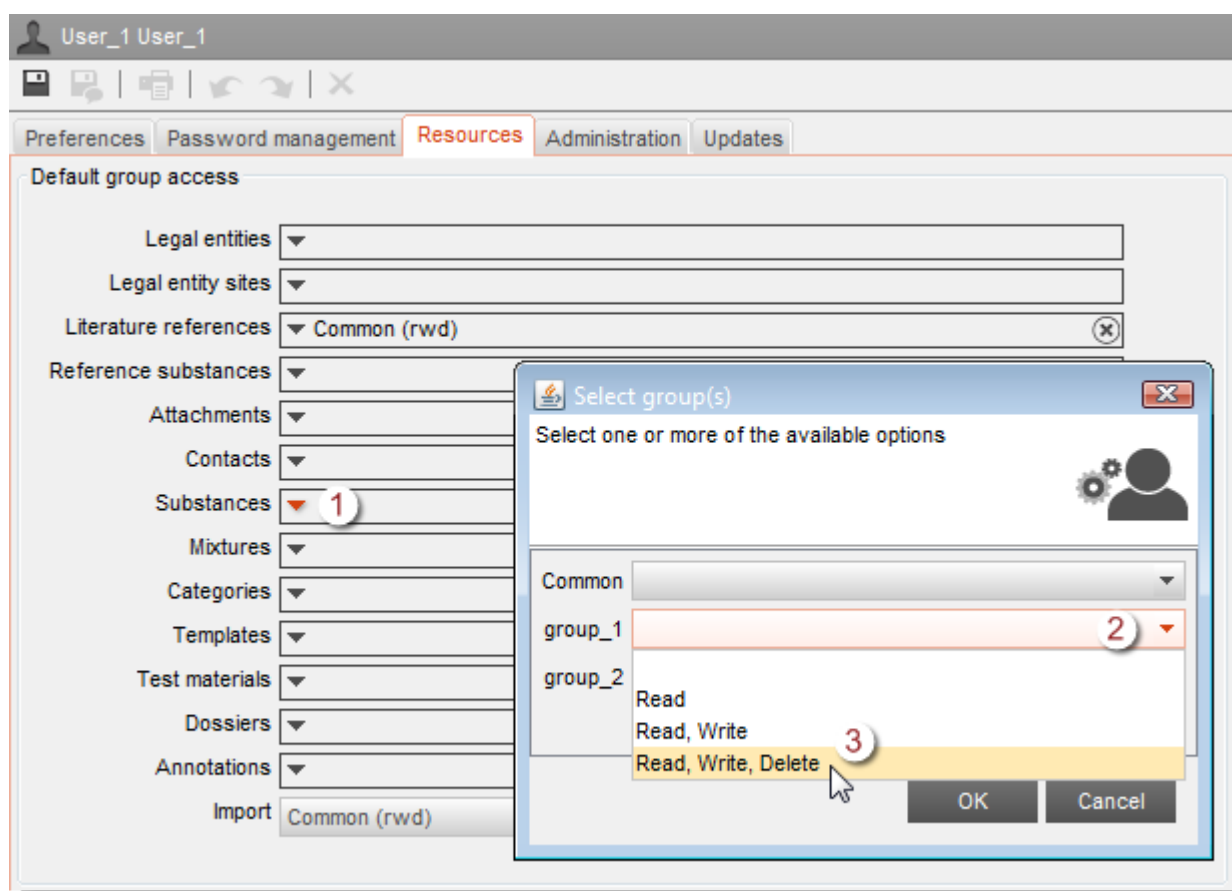
15.1.2.3. Resources

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.

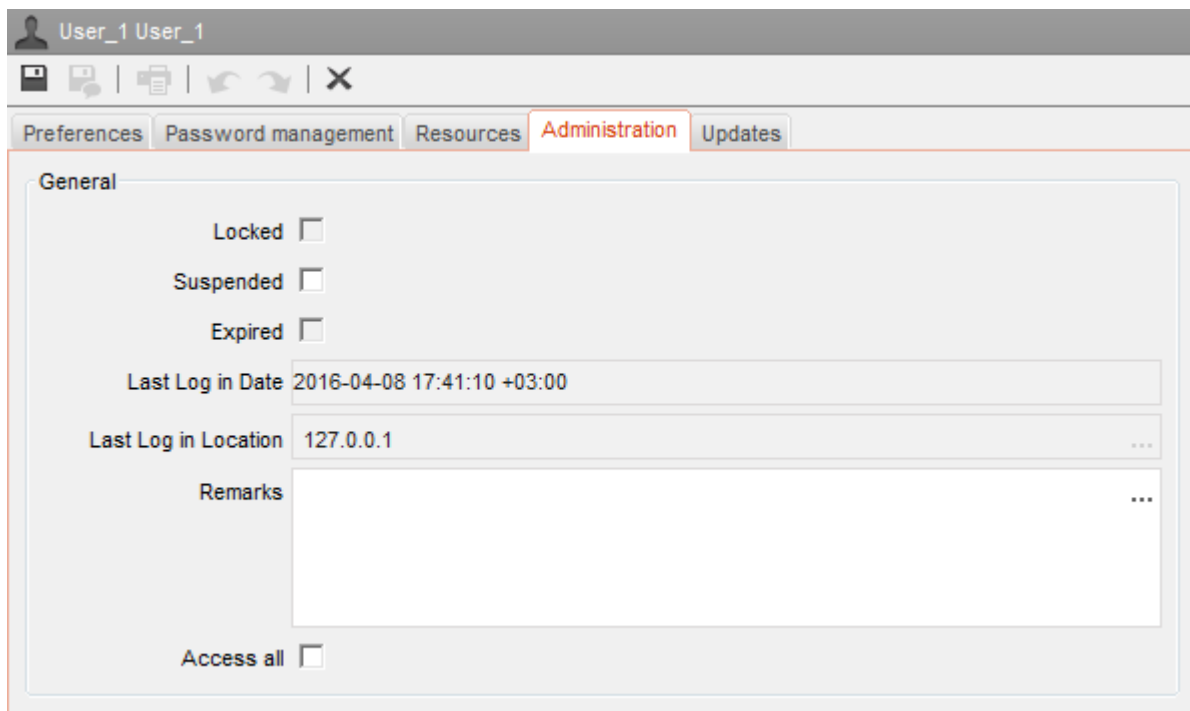
Figure 95: Resources for a User

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 96: 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*.

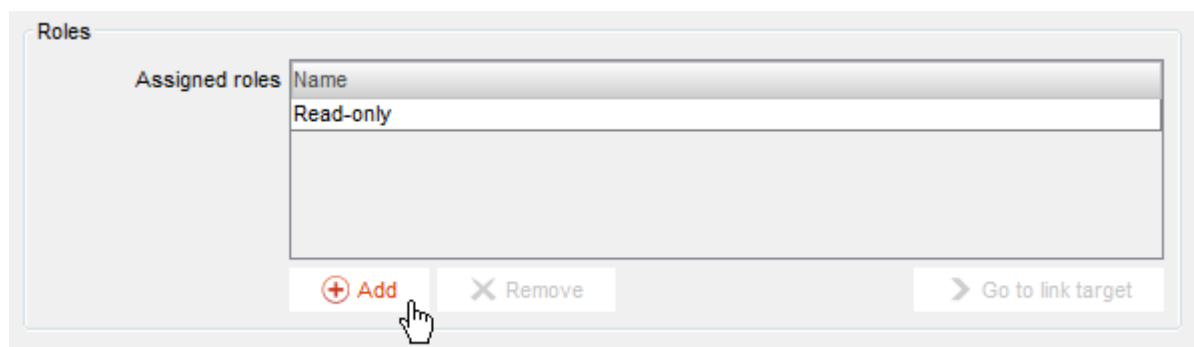
The *last log in location* states the IP address of the computer from which the most recent previous log in occurred for the *User*. For the desktop type of installation, this value will be that for localhost (127.0.0.1).

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 and functionality. 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

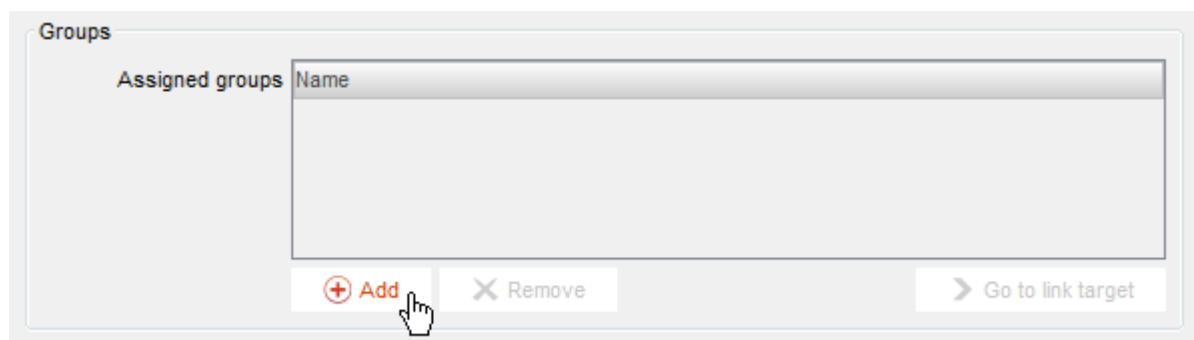
Figure 97: Adding a Role to a User under User management / Administration / Role



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 98: Adding a User to a Group under User management / Administration / Group

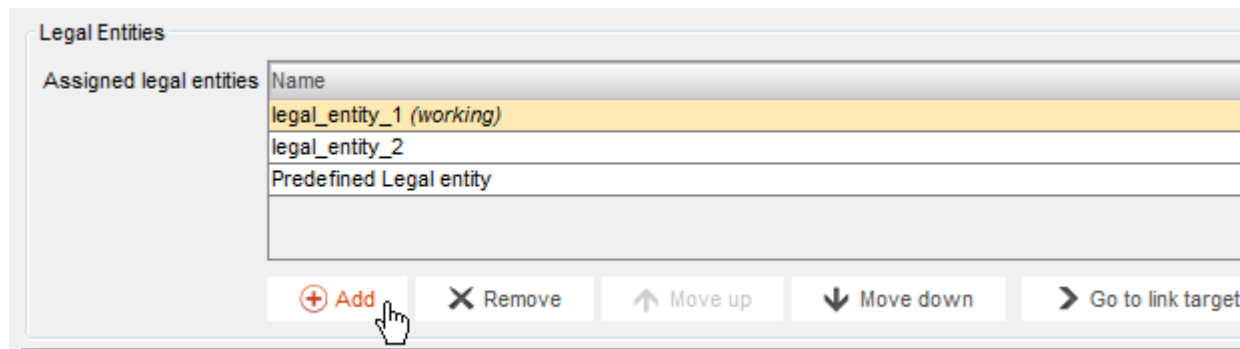


This field is shown only when instance based security (IBS) is on. For a description of IBS, see section 15.3 Instance based security (IBS).

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 99: 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.

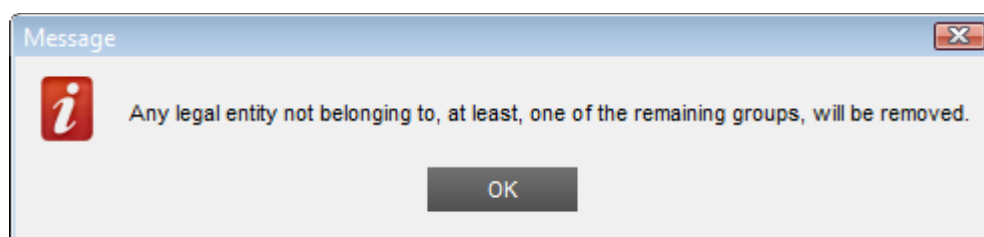
To set a *Legal entity* as the working one, move it to the top of the list using the buttons labelled *Move*.

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

If you cannot see or assign a legal entity you want, see the description of access in section 15.2.2.4.2 *Assign Legal entities to users*.

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 100: 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.

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.

Figure 101: Notification of updates to the IUCLID 6 application

The screenshot shows the 'Updates' configuration window in the IUCLID 6 application. At the top, the user is identified as 'Super User'. The window has a navigation bar with tabs for 'Preferences', 'Password management', 'Resources', 'Administration', and 'Updates'. The 'Updates' tab is active. Below the navigation bar, there are two main sections: 'Check for updates' and 'Proxy settings'. In the 'Check for updates' section, there are four radio button options: 'Every hour', 'Every day', 'Every week' (which is selected), and 'Never'. In the 'Proxy settings' section, there are two radio button options: 'Automatically detect settings' (selected) and 'Manual proxy configuration'. Below these are input fields for 'Host', 'Port', 'Username', and 'Password'. There is also a checkbox for 'Proxy requires authentication'. At the bottom left, it says 'Last checked for updates: 2016-08-22 16:41:34'. At the bottom right, there is a button labeled 'Check now for updates'.

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.

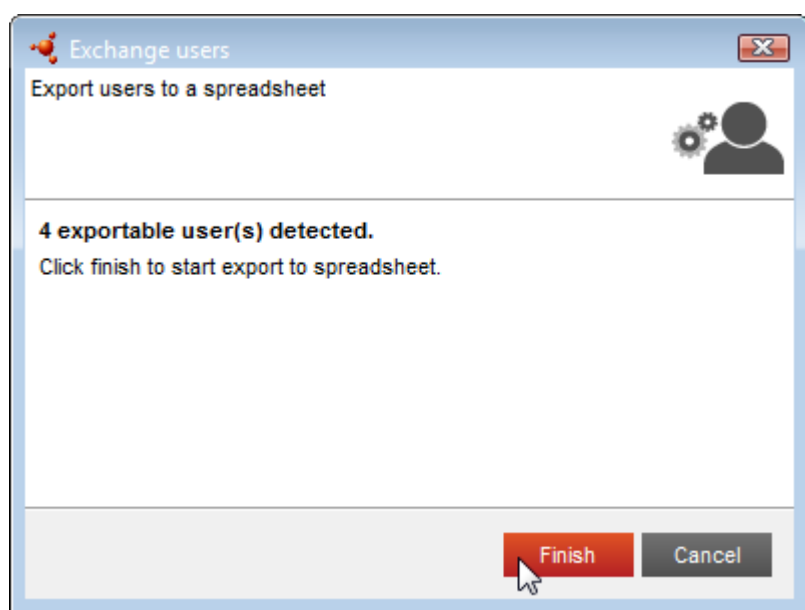
If an attempt to make a check gives an error message, check the internet connection, and ensure that any proxy settings entered into IUCLID 6 in to the fields shown above are correct for the host computer and the network.

Note that the update process updates both the application and its plugins. Plugins do not require separate updates.

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 102: Export users pop-up window



Click finish to start the export. The export is carried out as a background job, as described in section 1.7.4 *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 7: The fields in the text file for the functions *Export users* and *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 <i>Suspended</i> . This can be used to suspend and to unsuspend existing <i>Users</i> . [Yes No]
Remarks	Free text with a maximum of 32,768 characters.

Roles*	Name(s) of user <i>Role(s)</i> 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 <i>User</i> . 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 <i>Group(s)</i> 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. Where IBS is not used, the Group “Common” is required.
Delete*	Delete a pre-existing <i>User</i> on import. [Yes No]
E-mail	The email address associated with the <i>User</i> .
Contact	UUID of the <i>Contact</i> assigned to the <i>User</i> . 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 above in section 15.1.2.6. 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 1.7.4 *Background jobs*.

If there is an error message about file formatting, check the file against the format described in section 15.1.2.6. 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 the import.

Technical tip 1: The character encoding of an imported file must be *UTF-8 without BOM*. An attempt to import non-ASCII characters, e.g. ö, ä, in an encoding other than *UTF-8 without BOM* results in a file format error. If you need to import non-ASCII characters, check the character encoding before importing, for example, using an appropriate text editor such as Notepad++.

Technical tip 2: 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 particular types of entity and document 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.

Restrictions in access to data that are applied by *Instance based security (IBS)* are applied in addition to restrictions applied by *Roles*. For example, a *User* may have a *Role* that permits writing to all *Substances*, but cannot write to particular *Substances* because settings in *Instance based security (IBS)* forbid it. *Instance based security (IBS)* is described in section 15.3.

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*.

The access that *Users* have to *Legal entities* is organised in a tree structure with the built-in *User SuperUser* at the root. This means that *SuperUser* has access to all *Legal entities*. A *User* can assign only *Legal entities* that have been assigned to it. Therefore, for *SuperUser* to delegate the assignment of a *Legal entity*, *SuperUser* must first assign the *Legal entity* to the delegate *User*. The process of assignment is described in section 15.1.2.4.4 *Legal entity*.

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.

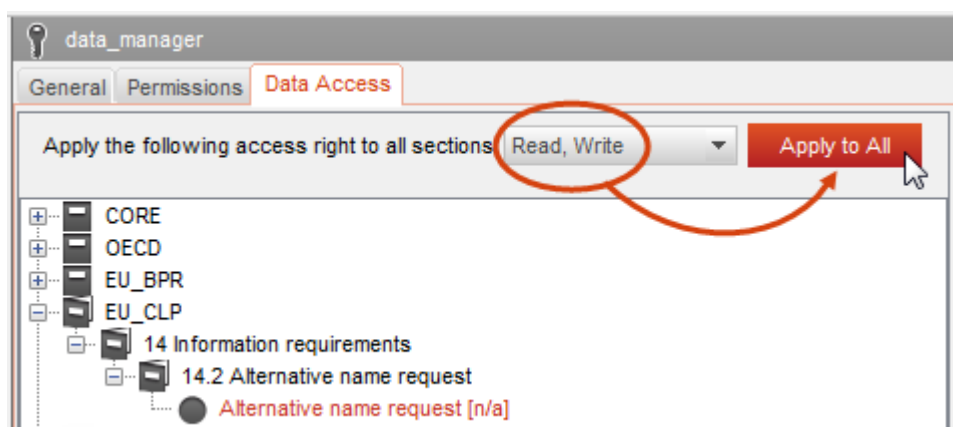
15.2.2.6. Plugin configuration

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

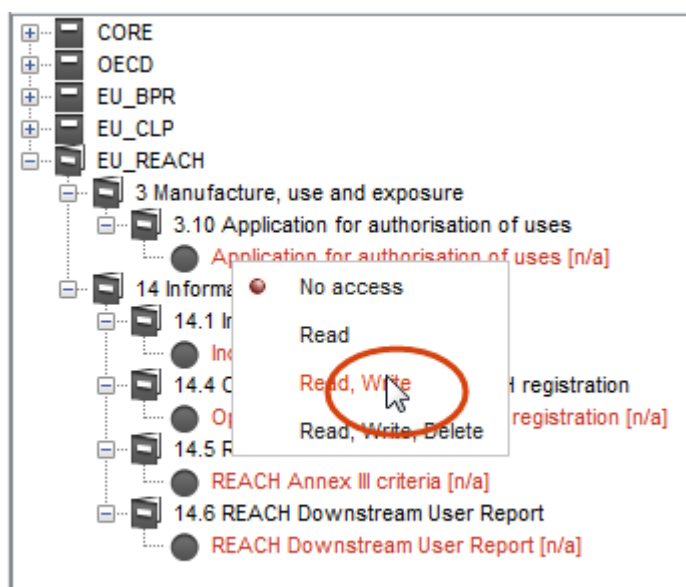
Here, access to data in *Substances* can be controlled at the level of section. The sections are shown in the default tree structure. Access rights can be set to one of the following values: *no access*, *read*, *read/write*, or *read/write/delete*. For a newly created Role, by default, the access is 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 103: 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 104: 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 8: Indication of access rights for documents

Access	Colour	Code
no access	■	[n/a]
read	■	[r/]
read/write	■	[r/w]
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 that can be granted from within the functionality of *Role*.

Note that this does not include permission to use the function *Inventory management*. Only the built-in *User* named SuperUser can do that, as described in section 18 Inventory management.

15.2.4.2. *Full access*

Grants read, write and delete access to all data such as *Substances* and *Dossiers*, but not to 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 data object *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 more than one *User* access to a document 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.

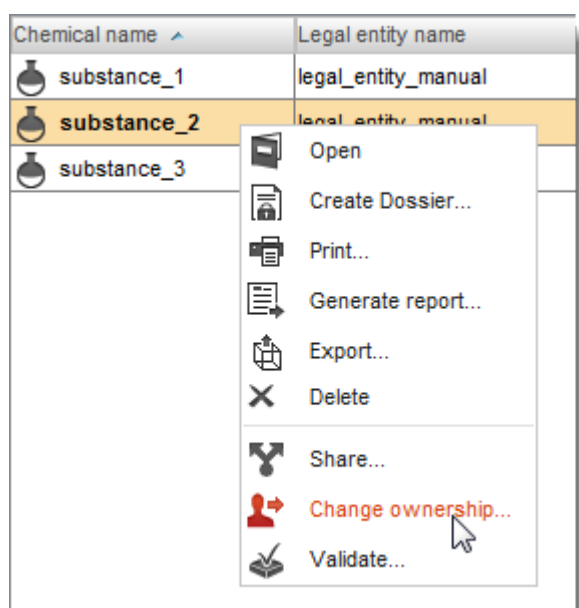
15.3.2.1. Change ownership

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.

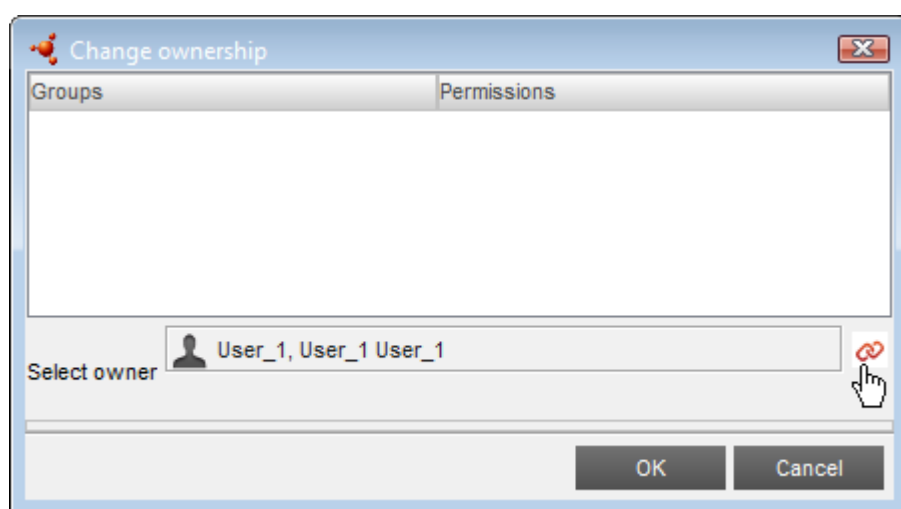
Table 9: Rights of a group manager

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 105: 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 106: 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

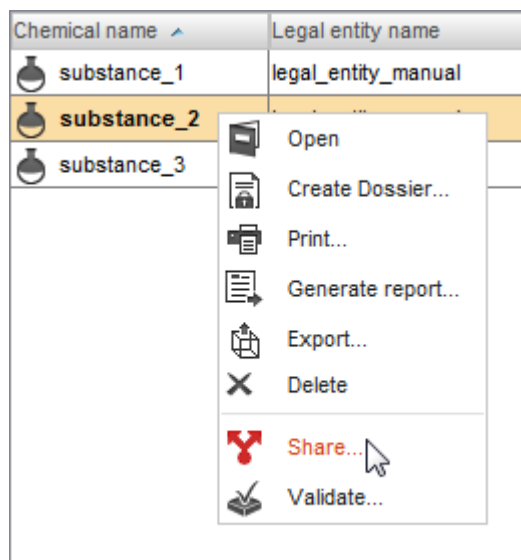
Share is an action in which access is granted manually to a document for the *Users* in a *Group* or *Groups*. This over-rides any access defined at the time of creation or importation of the document. The function share allows one of the following four states to be applied to a document per *Group*:

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.

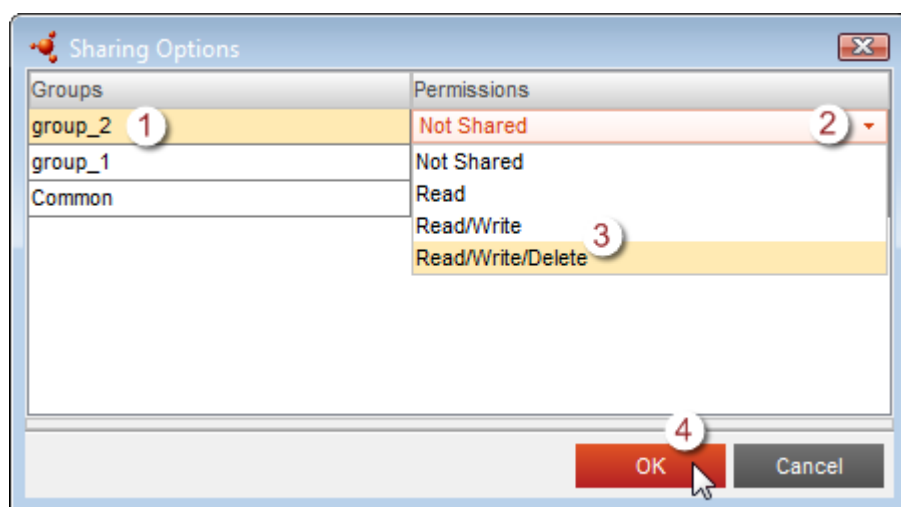
The option to share a document is accessed by right-clicking on the record of the document in the search results, as shown in the figure below. Sharing via the right-click method can be done for a multiple selection of documents.

Figure 107: 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 108: 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 10: 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 11: 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 <i>Resources \ Substance</i> for userA mean that when userA creates a <i>Substance</i> , all members of group1 are automatically given rwd rights to it. No rights are given for <i>Dossiers</i> .

User	Substance1	Dossier1	Comment
userC			There are no settings under <i>Resources</i> for userA that automatically confer access rights to userC for <i>Substances</i> or <i>Dossiers</i> .
userD			There are no settings under <i>Resources</i> for userA that automatically confer access rights to userD for <i>Substances</i> or <i>Dossiers</i> .

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

result 2: The following access has been granted.

Table 12: IBS exercise - result 2

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

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 13: 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 <i>share</i> the document. The permissions are rwd because the settings under <i>Resources \ Substance</i> for userA mean that when userA creates a <i>Substance</i> , 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 <i>share</i> the document. There are no permissions because the settings under <i>Resources \ Substance</i> for userA mean that when userA creates a <i>Substance</i> , not all <i>Users</i> 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 14: 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. Being able to change these permissions confers the ability to <i>share</i> the document. The permissions are rwd because the settings under <i>Resources \ Substance</i> for userA mean that when userB creates a <i>Substance</i> , 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 <i>share</i> the document. The permissions are rwd because the settings under <i>Resources \ Substance</i> for userB mean that when

Substance	Groups under sharing	Permissions under sharing	Comment
			userB creates a <i>Substance</i> , all <i>Users</i> 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 15: 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 <i>Users</i> 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 <i>Users</i> 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

The *Import* function of IUCLID 6 allows the import of *Dossiers, Substances, Mixtures, Templates, Categories, Legal entities, Legal entity sites, Reference substances, Annotations, Contacts, Literature references, Attachments, Inventories, and Test materials*. The *Import* function, along with *Export*, is designed primarily for the exchange of data between IUCLID installations.

16.1. Important information on importing

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

1. The import function works only for files with the filename extensions **i6z** or **i5z** that have been exported either from IUCLID 6, or the latest version of IUCLID 5 (version 5.6). *Inventories* cannot be exported from IUCLID 6, but they can be imported from a file with extension **i6I**.
2. In a single import process, the imported files must all have the same filename extension.
3. When importing an i5z file, the whole content of the file is imported. When importing an i6z file, it is possible to import a manual selection of its content.
4. In IUCLID 6 v2.0.0, compared to previous versions, there are some differences in the way that data is organised across the various fields. When data is imported in to IUCLID 6 v2.0.0 that was exported from a previous version of IUCLID 6, the import process applies a set of migration rules to the data to try to import as much data as possible in the most logically consistent manner. The migration rules are documented on the IUCLID website under the section [IUCLID format](#). An example is given in section *17.4.4 Export to previous major version*.

16.2. How to Import

To start the import process, click on **Import** in the **Administration** task panel on the IUCLID 6 home page, which launches 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 contains information about the selected file(s). The headings are:

1. *Pathname* (the pathway to the location of your file in 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.

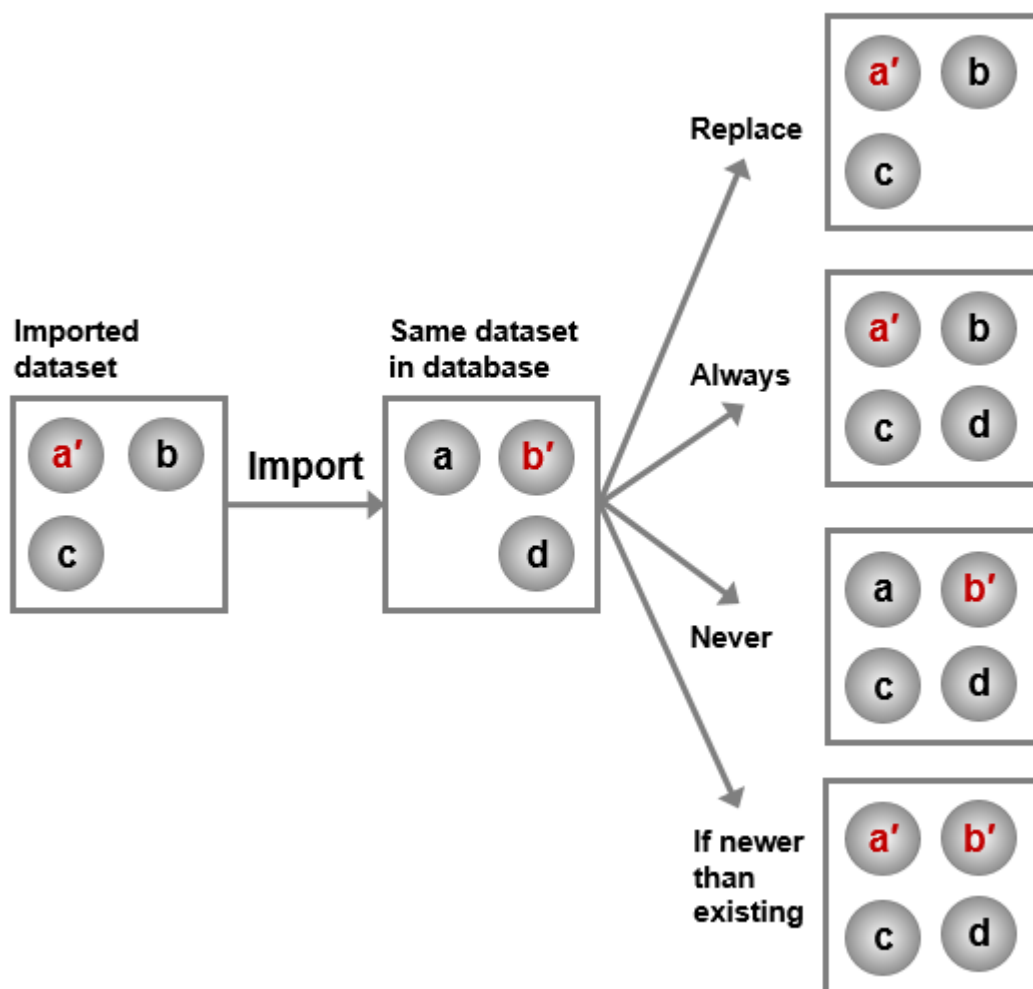
You can then select specific criteria which tell IUCLID how to treat the file(s) you wish to import, if the same Universal Unique Identifier (UUID) for the file already exists in your IUCLID system.

There are four options:

1. *Replace*: All entities and documents are imported. On overwriting an entity, it and any entities or documents it contains are first completely deleted. For example, if an import overwrites a dataset, after the import, only the imported documents or entities are present in the dataset. This option is useful if you and someone else work on the same dataset in parallel in different instances of IUCLID 6, and a new definitive version becomes available that you want to import without previous documents in your IUCLID 6 getting in the way. Such previous documents may be difficult to delete due to links in the database, but the *Replace* option solves that by removing the links.
The option *Replace* is not available if the import contains one or more IUCLID 6 Dossiers.
2. *Always*: All entities and documents are imported. If a dataset is imported so that it writes over a dataset in the database, any documents that are already in the database, but not in the import, are still in the dataset after the import.
3. *Never*: An entity or document is not imported if one with the same UUID exists within the IUCLID database.
4. *If newer than existing*: An entity or document is imported if it has the same UUID as one within the IUCLID database, but only if the modification date is more recent than that in the IUCLID database.

The behaviour for options above are expressed graphically in the figure below.

Figure 109: Import in to IUCLID 6 where datasets and/or documents already exist in the database



Key for Figure 109

a' is a newer version of **a**

b' is a newer version of **b**

A box represents a dataset. A circle represents a document in a dataset. Each letter represents a particular UUID.

The box on the left represents the dataset being imported. The box in the middle represents a dataset in the database that has the same UUID as the dataset being imported. The boxes on the right represent the outcomes after using the various different settings for import.

If Instance Based Security (IBS) is enabled in IUCLID 6, a field is shown called *Default group access*. For more information about IBS, see section 15.3 Instance based security (IBS). Where data is written over during an import, the feature *Default group access* does not change any access that has previously been defined using IBS.

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, in the second step of the Import assistant, you will be able to define specific records within the file you would like to import. This option is not available when importing two or more files.

16.4. Step 2 of Import

In *Step 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.

5. 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**.
6. 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.
7. 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.
8. 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 option from the menu.

Bulk export can be launched from the main menu *File*; from the home page; and by making a multiple selection from the search results, right-clicking, and then selecting the export option from the menu.

Bulk export contains options to export either a manual selection of data or, all of the following types of entity: *dossiers*, *substances*, *mixture/products*, *categories*, *templates*, *reference substances* or, all *test materials*. The manual selection allows the export of different types of entity in a single export process, for instance a combination of substance datasets, mixture/product datasets and reference substances. In addition, the manual selection option can be used to export single datasets and/or documents, as described in the sections below.

17.1. Important rules when exporting

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

1. Export requires the correct user rights. If you do not have these access rights, contact the user manager of your instance of IUCLID.
2. Referenced, or linked to, entities, datasets and/or documents are exported only if the reference is direct. For example, when a mixture/product is exported, the substances within it are exported, but a category is not exported solely because it refers to those substances.
3. In a dataset it is possible to create a dynamic reference to a document that is in the same IUCLID database. Such a link is created by *pasting as reference* from the clipboard. On export and dossier creation a dynamic reference is replaced by a static copy of the document. This is done for export because it is not known whether the destination document of the link will always be present in IUCLID database to which the dataset is exported. If it is missing, the link is broken. For a dossier, the dynamism of the link is removed because the content of a dossier cannot change.
4. When exporting a document that is part of a dataset, its parent entity, e.g. substance, mixture/product or template is also exported. However, when the document is exported, no sibling document, or template is exported.
5. Linked entities can be excluded from export because of access rights and/or confidentiality claims, regardless of whether or not the entity is linked via a mandatory field.
6. An Inventory entry cannot be exported on its own. It can be exported only along with an entity that refers to it.
7. In IUCLID 6 v2.0.0, compared to previous versions, there are some differences in the way that data is organised across the various fields. If data is being exported for import in to a previous version, use the option described in section *17.4.4 Export to previous major version*. The

differences between IUCLID 6 v2.0.0 and previous versions are documented on the IUCLID website under the section [IUCLID format](#).

17.2. Bulk export

The first step of the Bulk export wizard contains options of the following two types, which are described below in subsections:

1. Manually choose individual entities and/or document(s). The selection can be done across different types of entity. Multiple selections can be made, which are displayed in a list under *Document/Entity*. To edit the list, use the buttons + *Add* and *Remove*.
2. Export all entities of a specific type, e.g. dossiers, substances etc.. Select the type of entity, and then click *Next*;

17.2.1. Manual selection for bulk export

The window *Query for documents* is used to create search criteria that are applied either to all documents, or all of a particular type of entity, e.g. substance. To export different types of entity at once, use *Query for documents* more than once, to build up a list of items to export on the page *Document selection*.

17.2.1.1. Result type

Select either document, or a type of entity.

17.2.1.2. Query type

The type of query that can be selected depends on what is selected in *Result type*. For the entities, the search fields are properties of the entity, such as *name*. For documents, it is possible to search by universal unique identifier (UUID), and the containing dossier. For example, this allows individual endpoint study records to be selected.

If present, fields labelled “owner” and “group” are related to instance based security (IBS), which is described in section *15.3108 Instance based security (IBS)*.

To add search results to the list of data to be exported, click *Assign*.

17.3. Export of Datasets

Whenever a dataset has been selected to be exported, either in bulk or singly, a *submission type* must be selected. This allows the table of contents of the export to be tailored to different regulatory needs. The *submission types* presented for selection depend on the type of dataset. For example, for mixture/product they are only those that relate to the OECD harmonised templates, and the Biocides regulation of the EU (BPR). To not exclude data on regulatory grounds, select a submission type of *Complete table of contents*.

There is no option to select submission type when exporting a dossier because the selection was made when the dossier was created.

Whenever a dataset has been selected to be exported, either in bulk or singly, there is an option *Use advanced settings*. This option, as described below, allows fine control over what is exported from the within the selected entities and/or documents. To export all of the data in the selected entities and/or documents, leave this option unticked, and then click on *Next*.

17.3.1. Use advanced settings

This option allows fine control over what is exported from the within the selected entities and/or documents. Some parts of the data selection process are identical to that used during the creation of a dossier. Where that is the case, a link is provided to the relevant section of this document.

17.3.1.1. Detail level of document fields

See section 7.1.3.2 *Detail level of document fields*.

17.3.1.2. Confidentiality

See section 7.1.3.3 *Confidentiality and Use restricted to selected regulatory programmes*.

17.3.1.3. Use restricted to selected regulatory programmes

See section 7.1.3.3 *Confidentiality and Use restricted to selected regulatory programmes*.

17.3.1.4. Administrative data properties

This set of options is use to control which fields are exported from the *Administrative data* in a dataset. The fields are grouped as follows: *Robust study summary*, *Used for classification*, *Used for MSDS*, *Purpose flag*, *Data waiving*, *Study result type*, and *Reliability*. To open a grouping of fields, click on the black triangle to the left of the option *Yes*. By default, all fields are exported. To exclude a field, untick its box.

17.3.1.5. Included annotations

There are options to either include or exclude annotations. The option *Export main document's annotations only* is shown where a single entity is being exported. It allows the exclusion of annotations for referenced entities and/or documents.

17.3.1.6. Attachments

There are options to export either all or none of the attachments.

17.3.1.7. Verify selected documents

See section 7.1.3.6 *Document selection*.

17.4. Final step in Export

On the last page of the export wizard there are options that relate to the format of the output, and its compatibility with previous versions of IUCLID.

17.4.1. Export details / Specify destination folder

Click on *Browse*, then select the destination directory of the export.

17.4.1.1. Create new subfolder after ...

When the number of files in a directory grows beyond a certain limit, the filesystem can become unacceptably slow. This depends on the number of files, not their size. Therefore, an option is provided that allows an upper limit to be placed on the number of files in a directory. If the export includes more files than the limit, the files are divided up into batches with as many members as the limit, and each batch is written to a new directory created by the export process. Directories are created in the directory selected in the field above.

This feature is provided only for bulk export.

17.4.2. Export modification history

Select whether to export the history of modifications made to the data. This data is displayed in the *Information panel*.

17.4.3. Remarks

This is a free text field in which notes about the export may be recorded.

17.4.4. Export to previous major version

In IUCLID 6 v2.0.0, compared to previous versions, there are some differences in the way that data is organised across the various fields. For this reason, not all the data that can be entered in to IUCLID 6 v2.0.0, can be imported in to a previous version. By default, data files exported from IUCLID 6 v2.0.0 cannot be imported in to IUCLID 6 versions 1.0, 1.1, 1.2 and 1.3 (IUCLID 6 v1.x).

If you need to send data to a IUCLID user who is using IUCLID v1x, and you know that the data is not critically affected by the format changes in IUCLID v2.0.0, export the data with *Export to previous major version* enabled. This will allow the data to be imported in to IUCLID 6 v1.x.

Be aware that *Export to previous major version* does not reverse all the actions that can occur on migration from IUCLID 6 1.x, to IUCLID 6 v2.0.0.

The differences between IUCLID 6 v2.0.0 and previous versions are documented on the IUCLID website under the section [IUCLID format](#).

Example

In some cases, migration of data from IUCLID 6 1.x to IUCLID 6 v2.0.0 involves the merging of the text from two text fields in to a single text field. The migration process appends the text from the

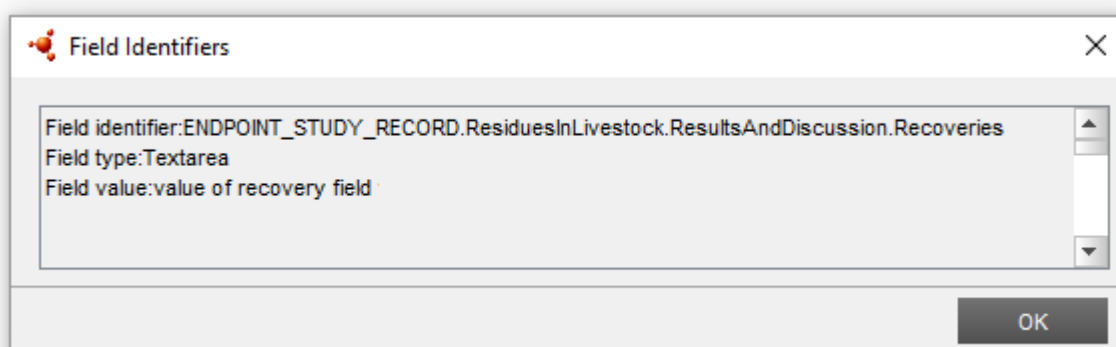
second field to the text from the first field, and then attempts to write all the text in to the destination field. If the text does not fit in to the destination field, only the text from the first field is written, and the text from the second field is saved as an attachment to the document. That way, at least no text is lost on migration. This process is not reversed on export from IUCLID 6 v2.0.0, even when *Export to a previous major version* is enabled. However, any text that was placed in an attachment is available in IUCLID 6 1.x, so if required, it can be pasted back in to the original field.

An attachment created during migration begins with the name and path of the field from which originated, followed by a brief statement of why the attachment was created. An example is shown below:

```
Not migrated field "Distribution of residues" (Path:
ENDPOINT_STUDY_RECORD.ResiduesInLivestock.ResultsAndDiscussion.Distrib
utionOfResidues) :
    value of distribution field ...
```

To see the path to a field, click on the field and then press the function key F12, as shown in the example below for a dossier.

Figure 110: View the path of a field using the function key F12



18. Inventory management

Inventory management is used to view, and change in bulk, references that point to *inventory entities* from other types of entity. The *inventory entities* are entities of type *Contact*, *Legal entity*, *Legal entity site*, *Literature reference*, *Reference substance*, and *Test materials*. The entities that can refer to these are *Substance*, *Mixture/Product*, *Template* and *Category*. These are all types of dataset.

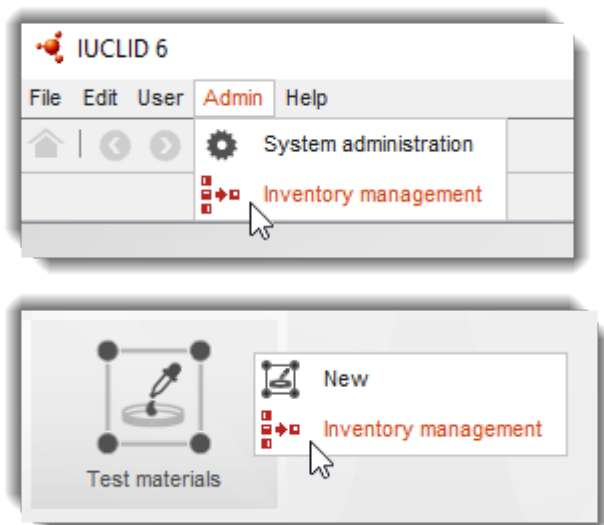
Inventory management replaces all the references from a particular set of entities, with references to a single inventory entity. After the replacement, the inventory manager deletes the inventory entities for which it replaced links. The copies of inventory entities in a Dossier are not affected.

Inventory management can be accessed by only the built-in *User SuperUser* or, where IBS is enabled, a *User* that has the right *Access all*, as described in section 15.1.2.4.1 *General*.

For example, all references to a User-defined set of Contacts from Substances, Templates Mixture/Products and Categories can be a replaced by references to a single, different Contact; after which all the Contacts in the User-defined set are deleted. The deletion is possible because there are no longer any references to the Contacts in the User-defined set. *Inventory management*

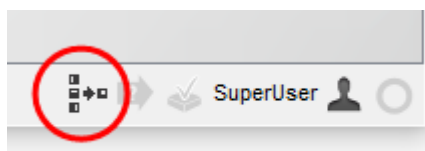
is launched from the administration section of the home page, or by right-clicking within the home page on an icon for inventory entity. An example is shown below:

Figure 111: Starting the inventory management wizard



Whilst the inventory management wizard is running, its icon in the lower menu bar is active, as shown below.

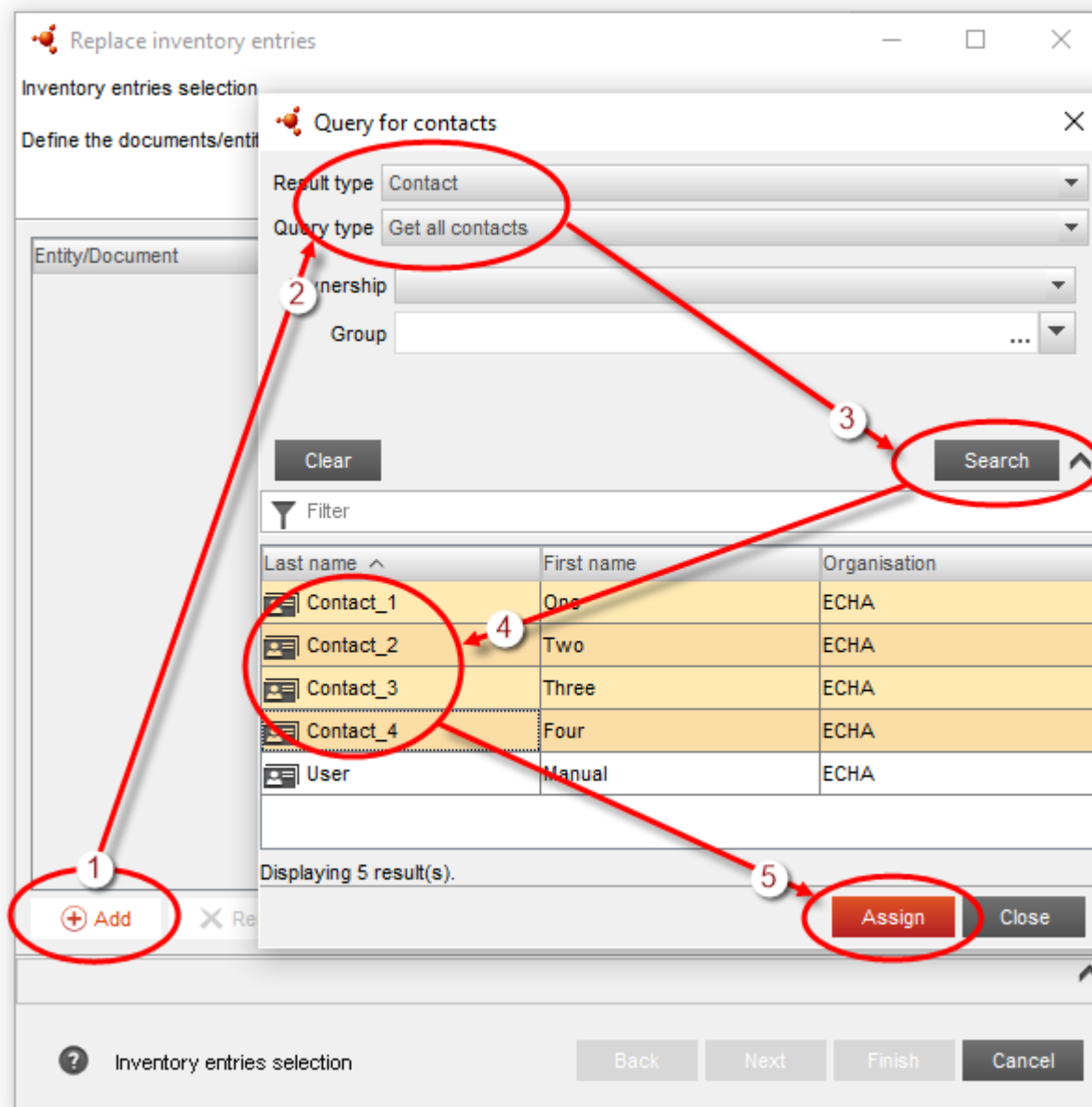
Figure 112: Bring the inventory management wizard to the front



Clicking on this icon brings the wizard to the front of the currently open windows. This is useful if the wizard is not visible because it is behind some other window, or it has been minimised.

The first page of the wizard allows for the selection of the inventory entities that will be replaced. An example is shown below for Contacts.

Figure 113: Selecting entities to replace in Inventory management



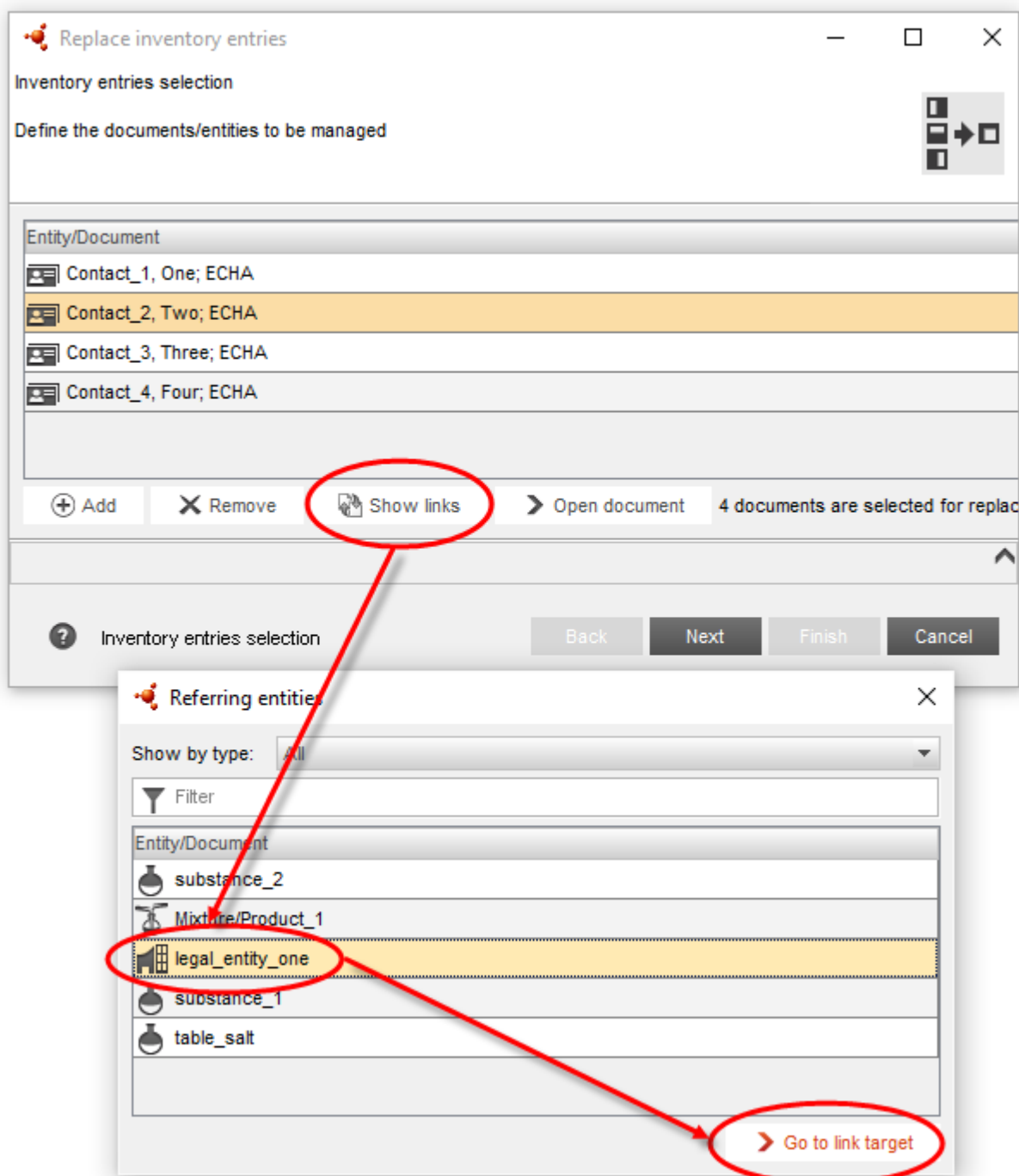
Key for Figure 97:

1. To select an entity for replacement, first click on the button *Add* button. When the wizard is first opened, there are no entities on the list, as shown above;
2. If the wizard were started from the Admin menu, use the field *Result type*, to select the type of entity to replace. This field is not shown if the wizard is started from a specific type of entity, in which case, the search can find only that type of entity. Select the type of search in the field *Query type*. If there is already one or more entities on the list, only the same type can be selected;
3. Search for the entities to be replaced, applying the criteria entered in *Query type*;

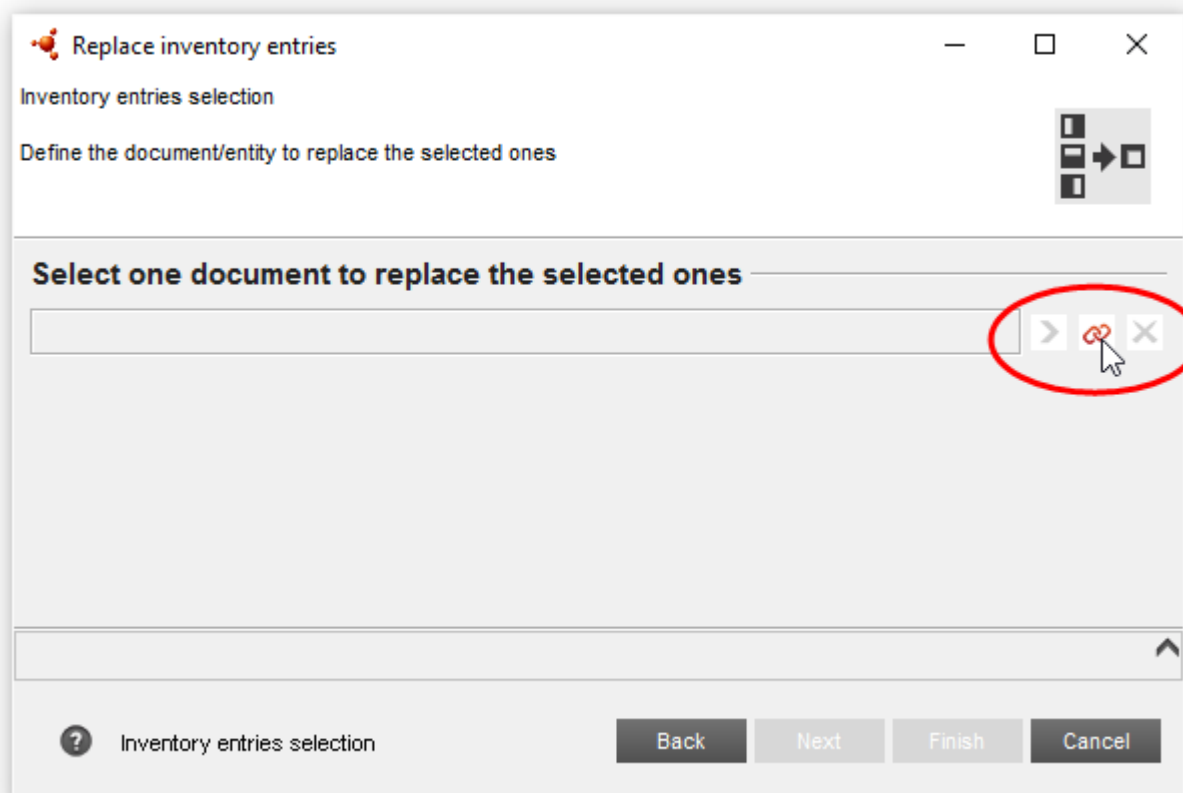
4. Select the entities to be replaced;
5. Click on the button *Assign* to add the selected entities to the list of those that will be replaced. For the example shown above, the list is shown in the figure below.

At the foot of the list of entities to be replaced there are buttons that provide a range of functions that allow the members of the list to be changed, and to check the relationships between entities. It is recommended to use these functions to ensure that the replacements of inventory entities are really what is required. Check the list carefully because the replacements cannot be undone. *Add* and *Remove* are used to determine which entities are on the list. *Open document* displays the selected document in the data window of IUCLID. *Show links*, opens a pop-up window that lists the entities that refer to the selected inventory entity. In the example shown below, the inventory entity `Contact_2` is referenced by several Substances, a Legal entity and a Mixture/Product.

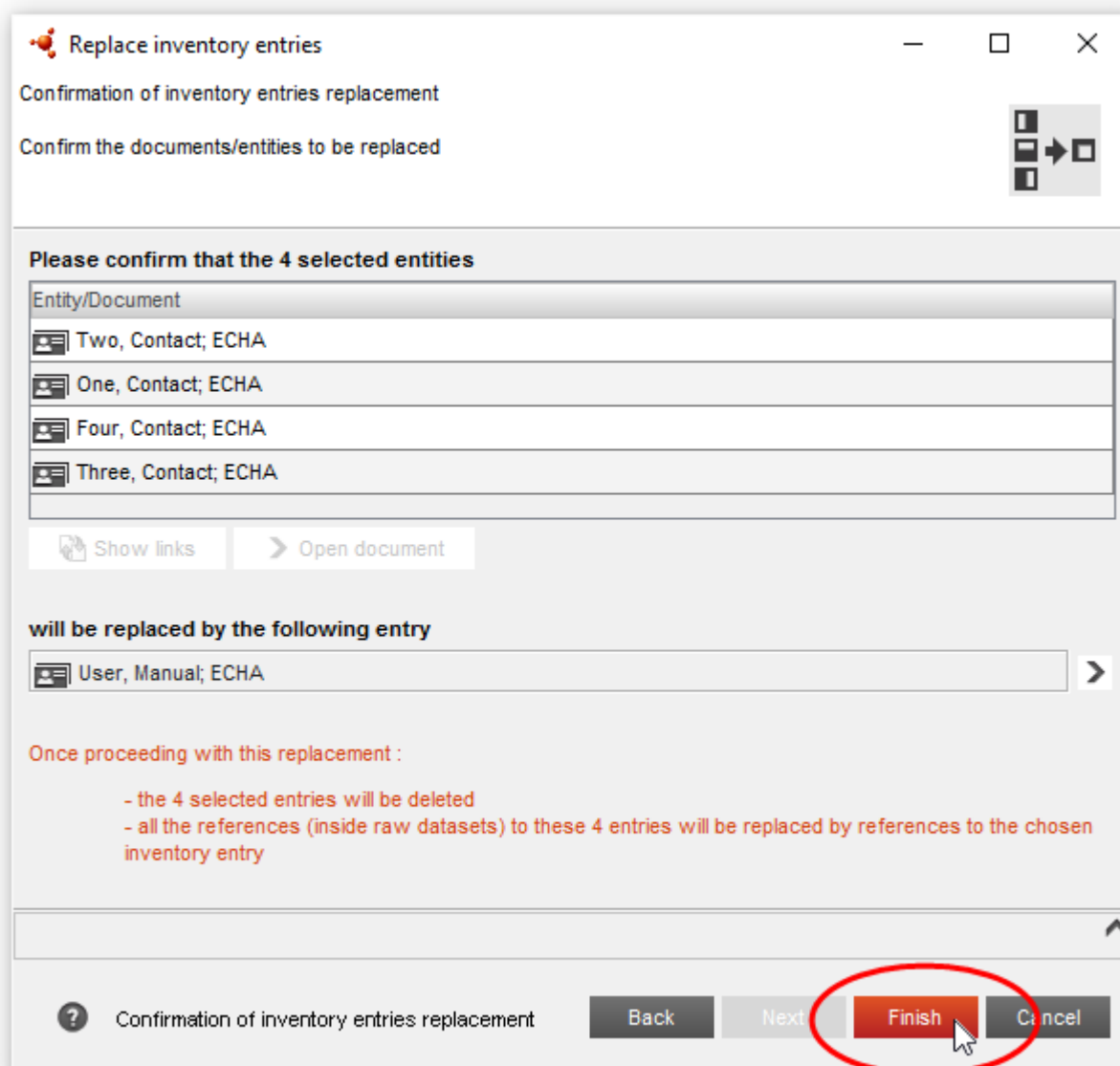
Go to link target displays the selected document in the data window of IUCLID.

Figure 114: In inventory management, show which entities refer to an inventory entity

When you are sure that the selection of inventory entities to be replaced is correct, click the button *Next* to open the second page of the wizard, and then select the inventory entity that will replace those on the list. The selection window is opened via the chain link icon highlighted below. Use the standard search feature to select an inventory entity.

Figure 115: Selecting the inventory entity that will replace those selected on the first page of the wizard

When the inventory entity has been selected, click on the button *Finish*. The confirmation window opens, as shown in the example below. This window contains a list of the inventory entities which will be replaced, and by what. The window contains the same features *Show links* and *Open Document* as described for the first page of the wizard. There is a warning that the inventory entities for which references are being replaced, will be deleted. If you have not already done so, it is recommended that you back up your database before proceeding, as described in section 24 *Backup/Restore*.

Figure 116: Confirmation of which inventory entities will be replaced, and by what

To carry out the replacement, click on the button *Finish*. When the replacement is finished, a report is shown like the one in the example below.

Figure 117: The report given by the inventory manager when it has finished making replacements

Replaced documents

Entity/Document	Document type	Document UUID
Two, Contact; ECHA	Contact	40285234-fc3e-423a-88d2-82fa85779bdd
Four, Contact; ECHA	Contact	9ff634ed-8c12-43b9-ba78-742b06630d70
Three, Contact; ECHA	Contact	f5f25c14-e734-455b-9def-47d13bdaf0e6
One, Contact; ECHA	Contact	0ab3367b-1a73-4f7f-8004-2ab762280b2f

Document that replaced the above list

Entity/Document	Document type	Document UUID
User, Manual; ECHA	Contact	7dfa1fdf-2084-454e-87e7-4c36336ab2c8

Replacement report

Export report Close

To export the report in CSV format, click on the button *Export report*, and then enter a filename and path for the file.

19. 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.

19.1. Print assistant


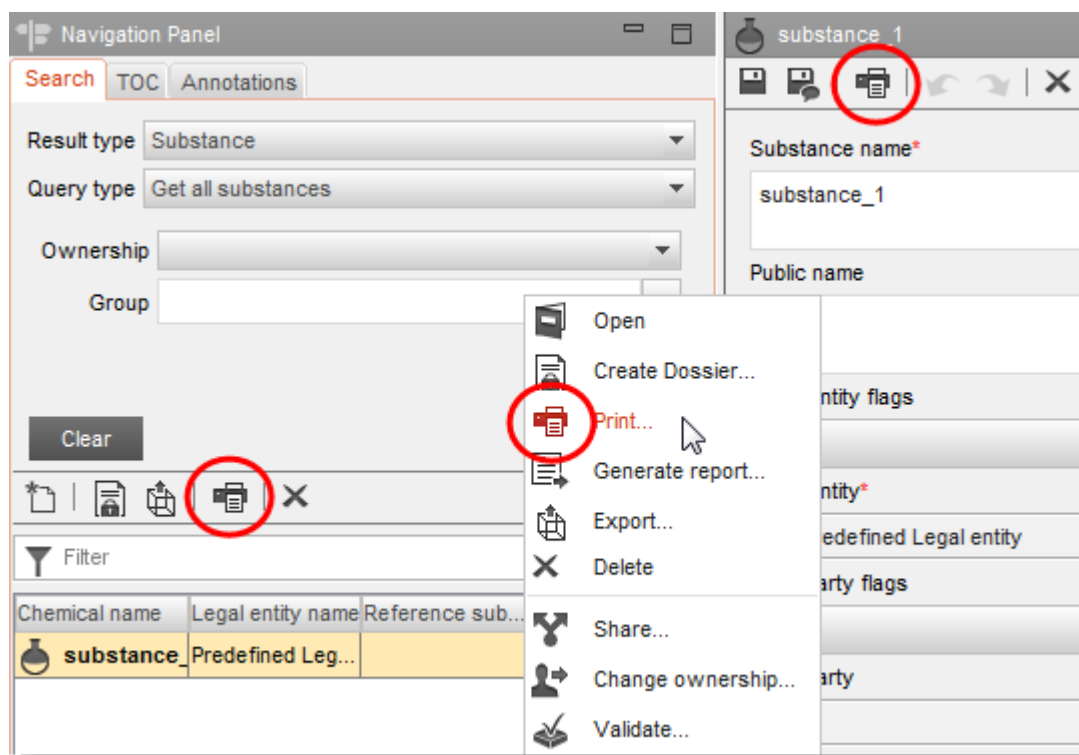
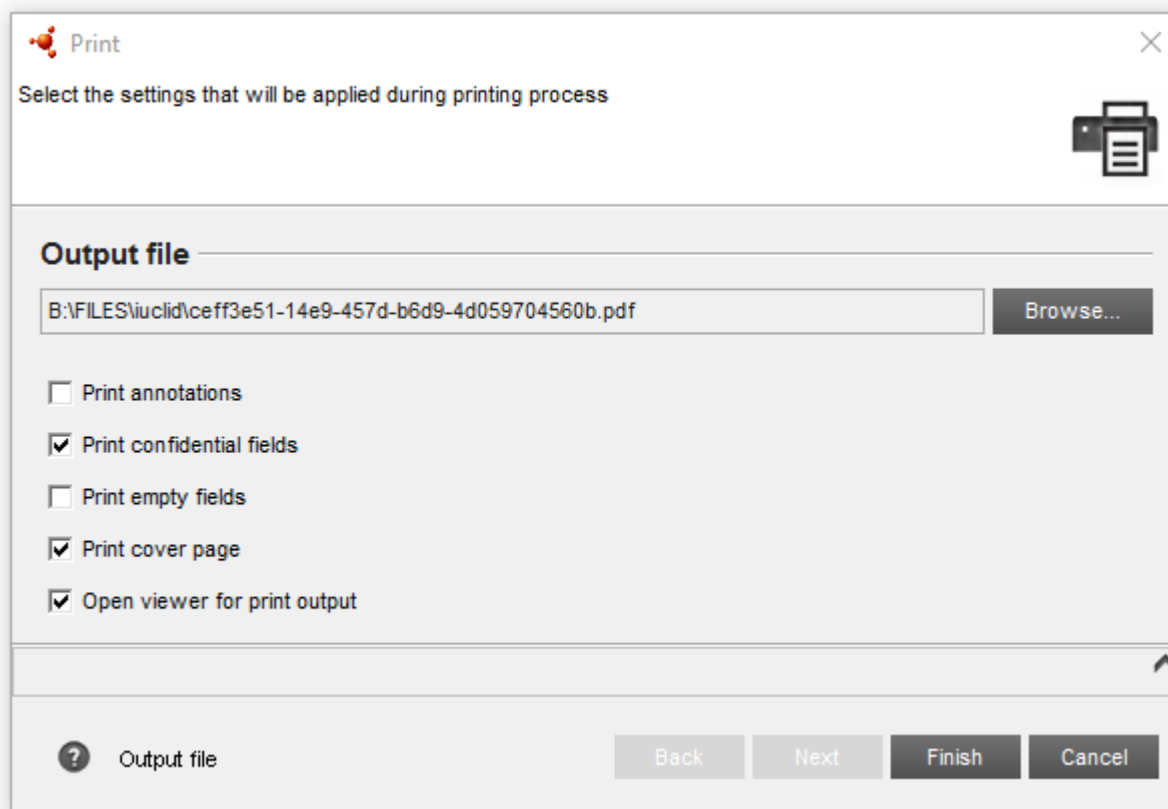
To launch the printing function, click on the print icon, , located as shown in the figure below. The menu is opened from within the *Navigation pane* by right-clicking on the search record of what is to be printed.

Figure 118: Launching the print function



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

Figure 119: 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 five 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 confidential fields* (by default unchecked)
If you check this option, all the fields that are marked (confidential) in the dataset, document or entity will be included in the generated PDF. These fields are nothing to do with flagged fields.
3. *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.
4. *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

5. *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 1.7.4 *Background jobs*.

19.2. 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.

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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

20. PNEC calculator

Under the REACH Regulation, manufacturers, importers, and downstream users must ensure that they manufacture, place on the market or use substances, in such a way that they do not adversely affect the environment.

A Predicted No-Effect Concentration (PNEC) defines the level of exposure to a substance below which adverse effects in the environmental sphere of concern are not expected to occur. In the Risk Characterisation (RC), the exposure of each environmental sphere known to be or likely to be exposed, is compared with the appropriate Predicted No-Effect Concentrations. The risk to the

environmental sphere can be considered to be controlled if the exposure levels do not exceed the related PNECs.

The aim of the PNEC calculator is to support the derivation of Predicted No-Effect Concentrations for the aquatic, sediment and terrestrial environmental protection targets based on [ECHA Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.10](#).

Note: The current version of the PNEC calculator supports the derivation of PNECs only for aquatic, sediments and terrestrial environmental protection targets. It does not support the calculation of PNECs for microorganisms in sewage treatment plants and the PNEC_{coral} used for the assessment of secondary poisoning.

The workflow followed by the PNEC calculator is the following:

1. The assessor selects (or creates) and endpoint summary in IUCLID section 6 - Ecotoxicological information in a substance dataset (or in a template) and launch the PNEC calculator in the menu that appears by right-clicking on it. The endpoint summary of section 6 enables the reporting of the hazard assessment conclusions for the environmental protection targets.
2. The PNEC calculator performs the following for deriving PNECs
 - a. Retrieves all the effect concentrations reported in the endpoint summaries in IUCLID sections 6.1.1 to 6.1.6 for the aquatic protection target, section 6.2 for the sediment protection target and sections 6.3.1 to 6.3.4 for the terrestrial protection target and selects the lowest short-term descriptor and the lowest long-term descriptor if available.
 - b. For aquatic and sediment protection target, data for freshwater are used as surrogate data in case the same type of data is not available for the marine and vice versa.
 - c. For sediment and soil protection target, the equilibrium partitioning method (EPM) may be used as an extrapolation method to calculate the PNEC and thus data for K_{oc} is retrieved from the endpoint summary in IUCLID section 5.4.1.
 - d. Selects the relevant effect concentrations and the corresponding assessment factor (AF) to calculate the PNEC, or when relevant, using the EPM for the PNECs for sediments and /or soil, according to the rules in [ECHA Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.10](#).
3. The PNEC calculator reports all the results in a screen available to the assessor.
4. The assessor can *finish* the actions keeping the calculations as proposed by the tool or modify some assumptions by *editing* the calculations (see section 20.4).
5. The PNEC calculator reports the outcome of the calculations, and related explanations when relevant, in the IUCLID endpoint summary section 6.

20.1. Input data

The input data for the PNEC calculator is the information available in the endpoint summaries in IUCLID sections 5.4.1 (Adsorption / desorption), 6.1.1 to 6.1.6 (Aquatic toxicity), 6.2 (Sediment toxicity) and 6.3.1 to 6.3.4 (Terrestrial toxicity).

The IUCLID endpoint summary is the document that summarises the information available in all the endpoint study records of a given Endpoint section. Therefore, it is expected that before running the PNEC calculator, the assessor should have already carried out the assessment of the available studies (reported in the form of endpoint study records in IUCLID) for the relevant endpoints by environmental protection target. Thus, the key effect concentrations should have been selected and reported in the endpoint summaries of sections 5.4.1, 6.1.1 to 6.1.6, 6.2 and 6.3.1 to 6.3.4.

20.1.1. Endpoint summary 5.4.1 (adsorption/desorption- Koc)

For sediment and terrestrial protection target, PNECs can be calculated using EPM depending on the experimental data that is available for those environmental protection targets. In that case, the adsorption coefficient (Koc) for the substance is necessary for the calculation and it is retrieved from the corresponding endpoint summary in IUCLID section 5.4.1.

If the adsorption coefficient is provided in its logarithmic form, the tool will calculate the Koc value using the conversion formula: $Koc = 10^{\log Koc}$

20.1.2. Endpoint summaries 6.1.1 to 6.1.6 (aquatic toxicity)

The following information is used by the PNEC calculator from each available endpoint summary of section 6.1:

1. Effect concentration type: either "EC50/LC50" or "EC10, LC10 or NOEC"
2. Aquatic environmental protection target: freshwater or marine
3. Value and unit: both value and unit should be reported. The PNEC tool considers negative or equal to zero values as invalid.

20.1.3. Endpoint summary 6.2 (sediment toxicity)

The following information is used by the PNEC calculator for the calculation of the PNEC sediment from the endpoint summary of section 6.2 if available:

1. Effect concentration type: either "EC50/LC50" or "EC10, LC10 or NOEC"
2. Sediment protection target: freshwater or marine
3. Value and unit: both value and unit should be reported. The PNEC tool considers negative or equal to zero values as invalid.

Data for freshwater is used as surrogate data in case the same type of data is not available for the marine and vice versa.

20.1.4. Endpoint summaries 6.3.1 to 6.3.4 (soil toxicity)

The following information is used by the PNEC calculator for the calculation of the PNEC soil from the endpoint summarise of section 6.3 if available:

1. Effect concentration type: either "EC50/LC50" or "EC10, LC10 or NOEC"

2. Value and unit: both value and unit should be reported. The PNEC tool considers negative or equal to zero values as invalid.

20.2. How the calculations are made

20.2.1. Aquatic environmental protection target

A precondition to calculate PNECs for the aquatic environmental protection target is that there should be experimental data for three aquatic species: fish, aquatic invertebrates and algae or aquatic plants.

The calculations required to establish the PNECs consist in dividing an initial effect concentration by an assessment factor.

The initial effect concentration is the lowest "EC50/LC50" or the lowest "EC10, LC10 or NOEC" depending on the availability or not of long-term data, for which species long-term data is available and whether the most sensitive species in the short-term studies and long-term studies is the same. It is to be noted that data for freshwater are used as surrogate data in case the same type of data is not available for the marine and vice versa.

The assessment factor depends on the number of species for which there is long-term data and the aquatic environmental protection target the PNEC is calculated for.

The current version of the PNEC calculator assumes that no further experimental information on other marine species like echinoderms or molluscs have been provided when setting the assessment factor (AF) for the default calculation of the PNECaqua,marine, since the current endpoint summary is not able to provide this information to the PNEC calculator. In case that experimental information on echinoderms and/or molluscs are available and provided, the assessor will need to modify the relevant parameters in the Edit mode (section 20.4).

More specifically, the calculations are done as it follows:

1. If an "EC10, LC10 or NOEC" is not available or is only available for algae and/or aquatic plants:

$$\text{PNECaqua,freshwater} = \text{Lowest "EC50/LC50"} / 1000$$

$$\text{PNECaqua,marine} = \text{Lowest "EC50/LC50"} / 10000$$

2. If an "EC10, LC10 or NOEC" is available for species other than algae and/or aquatic plants:

- a. If the most sensitive species in short-term and long-term studies are the same

$$\text{PNECaqua,freshwater} = \text{Effect concentration} / \text{AF for freshwater}$$

$$\text{PNECaqua,marine} = \text{Effect concentration} / \text{AF for marine water}$$

Data available	Effect concentration	AF for freshwater	AF for marine water
"EC10, LC10 or NOEC" available for three	Lowest "EC10, LC10 or NOEC"	10	100

species: fish AND aquatic invertebrates AND algae or aquatic plants			
“EC10, LC10 or NOEC” available for two species: fish AND/OR aquatic invertebrates AND/OR algae or aquatic plants	Lowest “EC10, LC10 or NOEC”	50	500
“EC10, LC10 or NOEC” available for one species: fish OR aquatic invertebrates	Lowest “EC10, LC10 or NOEC”	100	1000

b. If the most sensitive species in short-term and long-term studies are not the same

$PNECa_{\text{aquatic, freshwater}} = \text{Effect concentration} / \text{AF for freshwater}$

$PNECa_{\text{aquatic, marine}} = \text{Effect concentration} / \text{AF for marine water}$

Data available	Effect concentration	AF for freshwater	AF for marine water
“EC10, LC10 or NOEC” available for three species: fish AND aquatic invertebrates AND algae or aquatic plants	Lowest “EC10, LC10 or NOEC”	10	100
“EC10, LC10 or NOEC” available for two species: fish AND/OR aquatic invertebrates AND/OR algae or aquatic plants and no “EC10, LC10 or NOEC” available for the species having the lowest “EC50/LC50”	Lowest of “EC50/LC50” and “EC10, LC10 or NOEC”	100	1000
“EC10, LC10 or NOEC” available for two species: fish AND/OR aquatic invertebrates AND/OR algae or aquatic plants and “EC10, LC10 or NOEC” is available for the species	Lowest “EC10, LC10 or NOEC”	50	500

having the lowest "EC50/LC50"			
"EC10, LC10 or NOEC" available for one species: fish OR aquatic invertebrates	Lowest "EC50/LC50" if it is lower than (lowest "EC10, LC10 or NOEC") / 10	1000	10000
	Lowest "EC10, LC10 or NOEC" if condition above is not met	100	1000

The selection of the initial effect concentration and the appropriate assessment factor is done according to [ECHA Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.10](#).

20.2.2. Aquatic environmental protection target, intermittent release

A precondition to calculate PNECs for intermittent releases to the aquatic environmental protection target is that there should be short-term experimental data, i.e. "EC50/LC50" for three aquatic species: fish, aquatic invertebrates and algae or aquatic plants. It is to be noted that data for freshwater are used as surrogate data in case the same type of data is not available for the marine and vice versa.

The default value for the PNEC aquatic for intermittent releases for freshwater or marine water aquatic organisms is obtained by dividing the lowest "EC50/LC50" value by an assessment factor of 100 for freshwater and 1000 for marine water.

20.2.3. Sediment environmental protection target

A precondition to calculate PNECs for the sediment environmental protection target is that there is long-term data available for sediment organisms or, in the absence of such data, a value for Koc is available in IUCLID section 5.4.1 and the corresponding PNEC for the aquatic environmental protection target is available to calculate PNECs with the EPM.

It is to be noted that data for freshwater are used as surrogate data in case the same type of data is not available for the marine and vice versa. Also, EPM might be used to calculate the PNECs in the assumption that it is a valid method for the substance. If this assumption is not correct, the assessor should edit the calculated PNECs using the Edit mode (section 20.4).

The current version of the PNEC calculator assumes that only one species has been tested for the sediment protection target, when setting the assessment factor (AF) for the default calculation of the PNEC sediment, since the current endpoint summary is not able to provide this information to the PNEC calculator. In case that more than one species representing different living and feeding conditions have been tested, the assessor will need to modify the relevant parameters in the Edit mode (section 20.4).

For freshwater sediments, if there is long-term data the "EC10, LC10 or NOEC" is divided by an assessment factor of 100. If there is only short-term data the PNEC is calculated as the lowest of two values: i) the "EC50/LC50" divided by an assessment factor equal to 1000, and ii) a value resulting from applying EPM. If no experimental data is available for sediment environmental protection target, the PNEC is calculated by EPM:

$$\text{PNEC}_{\text{sediment,freshwater}} = \text{PNEC}_{\text{aqua,freshwater}} * (3.6 + 0.1 * \text{Koc})$$

For marine water sediments, if there is long-term data the "EC10, LC10 or NOEC" is divided by an assessment factor of 100 or 1000 depending on whether or not long-term data is available for both freshwater and marine water. If there is short-term data the PNEC is calculated as the lowest of two values: i) a value result of dividing the "EC50/LC50" by an assessment factor equal to 1000 or 10000 depending on whether or not short-term data is available for both freshwater and marine water, and ii) a value result of applying EPM. If no experimental data is available for sediment environmental protection target, the PNEC is calculated by EPM:

$$\text{PNEC}_{\text{sediment,marine}} = \text{PNEC}_{\text{aqua,marine}} * (3.6 + 0.1 * \text{Koc})$$

20.2.4. Terrestrial environmental protection target

A precondition to calculate PNECs for the terrestrial environmental protection target is that there is experimental data available for soil organisms or, in the absence of such data or only one effect concentration is available, a value for Koc is available in IUCLID section 5.4.1 and the $\text{PNEC}_{\text{aqua,freshwater}}$ for the aquatic environmental protection target is available. As in the case of the sediment protection target, EPM might be used to calculate the PNEC for soil in the assumption that it is a valid method for the substance. If this assumption is not correct, the assessor should edit the calculated PNECs using the Edit mode (section 20.4).

If there is no experimental data the $\text{PNEC}_{\text{soil}}$ is calculated with EPM:

$$\text{PNEC}_{\text{soil}} = \text{PNEC}_{\text{aqua,freshwater}} * (0.133 + 0.02 * \text{Koc})$$

If there is only one effect concentration available the $\text{PNEC}_{\text{soil}}$ is calculated as the lowest of two values: i) a value result of dividing the "EC50/LC50" by an assessment factor of 1000 or the "EC10, LC10 or NOEC" by an assessment factor of 100, and ii) a value result of applying EPM.

If there are more than one effect concentration but only short-term data, $\text{PNEC}_{\text{soil}}$ is calculated dividing the lowest "EC50/LC50" by an assessment factor of 1000.

If there are more than one effect concentration and only one "EC10, LC10 or NOEC", $\text{PNEC}_{\text{soil}}$ is calculated as the lowest of two values: i) a value result of dividing the "EC50/LC50" by an assessment factor of 1000, and ii) a value result of dividing the "EC10, LC10 or NOEC" by an assessment factor of 100.

If there are more than one "EC10, LC10 or NOEC", $\text{PNEC}_{\text{soil}}$ is calculated by dividing the lowest "EC10, LC10 or NOEC" by an assessment factor that depends on the number of terrestrial species for which an "EC10, LC10 or NOEC" is available according to [ECHA Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.10](#).

20.3. Output information

Once the PNECs are calculated, then the PNEC calculator shows them in a pop-up window.

This pop-up window is composed of two main sections. In the section at the top it displays a table with all the PNECs that have been calculated grouped by environmental protection target. The section below contains three tabs that show in a read-only mode the starting effect concentration and the assessment factor used for calculating the PNECs. For the sediment and terrestrial protection targets, the extrapolation method used to calculate the PNECs is also shown.

This pop-up window also contains four buttons: *Edit*, *Print*, *Finish* and *Cancel*.

The *Edit* button opens an edit window in which the starting effect concentration, assessment factor and/or extrapolation method can be modified providing a justification. See more information in section 20.4.

The *Print* button generates a report in RTF format documenting the information related to the PNEC calculation (input and output data). This report has the same format used by the CSR generator for section 7.5 of the CSR.

The *Finish* button closes the PNEC calculator and the relevant data is transferred automatically to the relevant fields in the summary of section 6 *Ecotoxicological information* from which the PNEC calculator was launched. Be aware that if the endpoint summary already has values, the tool will overwrite all the available values for the PNECs calculated. All other fields will not be affected and the values already indicated will neither be overwritten nor erased.

The *Cancel* button simply closes the PNEC calculator without any further action.

20.4. Edit mode

The assessor has the possibility to modify the starting effect concentration and the assessment factor which have been set by default by the PNEC calculator. For the sediment and terrestrial protection targets the assessor can also modify the default extrapolation method used for the PNEC calculation. This is done using the *Edit* button.

The *Edit* button opens a new pop-up window that shows all the inputs that the assessor is allowed to modify in the PNEC calculator for the selected environmental protection target.

1. Starting effect concentration: the PNEC calculator selects as default the lowest "EC50" or the lowest "EC10, LC10 or NOEC" considering the data available for an environmental protection target. If the assessor disagrees, another effect concentration can be selected from the picklist containing all the available effect concentrations in the relevant endpoint summaries for the environmental protection target. However, if a new starting effect concentration is selected the assessor needs to provide also the relevant assessment factor for the calculation and a detailed justification explaining why the new starting effect concentration is actually more relevant.
2. Assessment factor: the PNEC calculator applies the default assessment factors according to [ECHA Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.10](#) considering the information available in the relevant endpoint summaries for each environmental protection target. If the assessor has more information that can justify the use of values other than the default, the assessment factor can be modified after clicking on *Overwrite*. However, in that case, the assessor needs to provide a detailed justification explaining why the new assessment factor is actually more relevant.

3. Extrapolation method: for sediment and terrestrial protection target there are two extrapolation methods that can be used for calculating the PNECs depending on the availability of experimental data relevant for those protection targets. Thus, if there is enough experimental data the "assessment factor" method, consisting in applying an assessment factor to a effect concentration, will be used. However, if there is not enough data or no data at all, the "equilibrium partitioning method" (EPM) will be used by default to calculate the relevant PNECs from the PNECs for the aquatic environmental protection target. If the assessor disagrees with the extrapolation method chosen by the PNEC tool (e.g. the tool has used EPM but EPM is not applicable for the substance), the other extrapolation method can be selected instead. However, if a new extrapolation method is selected the assessor needs to provide a detailed justification explaining why the new extrapolation method is actually more relevant. In addition, if the new extrapolation method is "assessment factor" the assessor will be required as well to select a effect concentration from the picklist containing all relevant effect concentrations and an assessment factor.

If after having modified any of the input above the assessor wants to go back and use the default values as input, this can be done by clicking on *default*.

This pop-up window also contains two buttons: *Save* and *Cancel*.

The *Save* button closes the *Edit* pop-up window and the PNEC calculator will re-calculate the relevant PNECs using the new inputs from the assessor. The new results will be shown in the initial display window.

The *Cancel* button simply closes the *Edit* pop-up window without any further action and goes back to the initial display window.

20.5. Disclaimer

ECHA recommends using the optional PNEC calculator in IUCLID. Note that nevertheless the registrant remains responsible for the PNECs calculated.

21. DNEL calculator

Under the REACH Regulation, with regard to substances; manufacturers, importers, and downstream users must ensure that they manufacture them, place them on the market, or use them, in such a way that they do not adversely affect human health.

A Derived No-Effect Level (DNEL) defines the level of exposure above which humans must not be exposed. In the Risk Characterisation (RC), the exposure of each human population known to be or likely to be exposed is compared with the appropriate Derived No-Effect Level. The risk to humans can be considered to be controlled, if the exposure levels estimated do not exceed the appropriate DNELs.

The aim of the DNEL calculator is to support the derivation of Workers and General Population Derived No-Effect Levels for long-term systemic effects for oral, dermal and inhalation routes based on [ECHA Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.8](#).

Note: The current version of the DNEL calculator supports the derivation of DNELs only for long-term systemic effects from repeated dose toxicity or reproductive toxicity. It does not support the calculation of DNELs for acute toxicity or local effects, nor the use of human data and the derivation of DNEL for threshold carcinogens. Finally, the DNEL calculator does not support the calculation of Derived Minimal Effect Levels (DMELs) for non-threshold hazards.

The workflow followed by the DNEL calculator is the following:

1. The assessor selects (or creates) an endpoint summary in IUCLID section 7 *Toxicological information* in a substance dataset (or in a template) and launch the DNEL calculator by right-clicking on it. The endpoint summary of section 7 enables the reporting of the hazard assessment conclusions for human health (workers and general population).
2. The DNEL calculator performs the following for deriving DNELs for workers and the general population for a route of exposure.
 - a. Retrieves all the dose descriptors reported in the IUCLID endpoint summaries section 7.5 (Repeated dose toxicity) and section 7.8 (Toxicity to reproduction: effect on fertility and effect on developmental toxicity) and selects one or more *initial dose descriptor* to calculate a DNEL for each route of exposure (according to the rules described in section 21.2.1).
 - b. Retrieves the information in the IUCLID endpoint summary in sections 7.1 (Toxicokinetics, metabolism and distribution) if available and calculates a *default DNEL* for the general population and workers as described in section 21.2.2 and 21.2.3, for each selected *initial dose descriptor*.
 - c. Selects the initial dose descriptor leading to the lowest DNEL.
3. The DNEL calculator repeats the operations above for the two other routes of exposure and reports all the results in a screen available to the assessor.
4. The assessor can *finish* the actions keeping the calculations as proposed by the tool (corresponding to the default calculations as explained in [ECHA Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.8](#)) or modify some assumptions by *editing* the calculations (see section 21.4).
5. The DNEL calculator reports the outcome of the calculation and related explanations when relevant in the IUCLID endpoint summary section 7.

21.1. Input data

The input data for the DNEL calculator is the information available in the IUCLID endpoint summaries in IUCLID sections 7.1 (Toxicokinetics, metabolism and distribution), 7.5 (Repeated dose toxicity) and 7.8 (Toxicity to reproduction).

The IUCLID endpoint summary is the document that summarises the information available in all the endpoint study records of a given Endpoint section. Therefore, it is expected that before running the DNEL calculator, the assessor should have already carried out the assessment of the available studies (reported in the form of endpoint study records in IUCLID) for the relevant endpoints by route of exposure. Thus, the key dose descriptors should have been selected and reported them in the endpoint summaries of sections 7.1, 7.5 and 7.8.

To launch the DNEL calculator, the assessor needs to right-click on an existing endpoint summary section 7 *Toxicological information* in a *Substance* dataset, or in a *Template*. This endpoint summary enables the reporting of the hazard assessment conclusions for human health (workers and general population).

21.1.1. Endpoint summary 7.1 toxicokinetics, metabolism and distribution

The DNEL calculator considers the following information (if available): absorption rate oral (%), dermal (%) and inhalation (%).

If no information is present in one or more fields or if the endpoint summary is not available, the DNEL calculator will use default values as indicated in [ECHA Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.8](#), which is:

1. Oral default absorption rate: 100% (50% if oral-to-inhalation extrapolation)
2. Inhalation default absorption rate: 100%
3. Dermal default absorption rate: 100%

Note: in case a dermal-to-inhalation or dermal-to-oral extrapolation is made, if there is no information about dermal absorption, the DNEL calculator will use a dermal absorption of 10% as a reasonable worst-case scenario.

21.1.2. Endpoint summary 7.5 Repeated dose toxicity

The following information is used by the DNEL calculator for each route of exposure with available data:

1. Dose descriptor type, value and unit. The current version of the DNEL calculator can use NOAEL, LOAEL or BMDL05 for oral and dermal routes and NOAEC, LOAEC or BMCL05 for inhalation route. The benchmark dose/concentration calculated as the lower confident limit of the dose that produces a response of 5%, i.e. BMD(C)L05, are considered to be equivalent to NOAEL(C) for DNEL derivation. BMD(C)L10 dose descriptors cannot be used as input to the DNEL calculator.
2. Study duration: sub-acute, sub-chronic or chronic.
3. Species. The current version of the DNEL calculator can only derive DNELs if the experimental studies are carried out with the species mentioned in [ECHA Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.8](#), i.e. rat, mouse, hamster strains, Guinea pig, rabbit, monkey or dog.
4. Toxic effect type: dose-dependent or concentration-driven.

21.1.3. Endpoint summary 7.8 Toxicity for reproduction

The DNEL calculator uses the same type of information mentioned above for the endpoint summary 7.5 for both the effect on fertility and the effect on developmental toxicity for each route of exposure.

21.2. How the calculations are made

The DNEL derivation process follows a 3-step procedure as proposed by [ECHA Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.8](#):

Step 1. Selection of relevant dose descriptors: based on all dose descriptors available in the endpoint summaries for repeated dose toxicity and for reproduction toxicity the assessor will have selected key dose descriptors per route of exposure and reported them in the relevant endpoint summaries. The DNEL calculator will select relevant dose descriptors for each route;

Step 2. Modification of relevant dose descriptors: the DNEL calculator will apply appropriate correction factors to convert the relevant dose descriptors into a correct starting point depending on the DNEL calculated;

Step 3. Application of assessment factors: the DNEL calculator will apply appropriate assessment factor to the modified dose descriptors to address the differences between experimental data and the human situation to obtain the DNEL values.

Each of the steps are further explained below.

21.2.1. Step 1: selection of relevant dose descriptors

The DNEL calculator retrieves all dose descriptors provided in the endpoint summaries in IUCLID sections 7.5 and 7.8, and applies the following selection criteria for each route of exposure:

1. The DNEL calculator selects the dose descriptors from experimental studies carried out on the same route of exposure the DNEL is to be derived. If there are no dose descriptors for the route the DNEL is to be derived, the oral dose descriptors will be prioritised for derivation of DNELs for inhalation and dermal routes. For the derivation of DNEL for oral route both inhalation or dermal dose descriptors are used.
2. BMD(C)L05 dose descriptors are considered equivalent to NOAEL(C) and these are used if available. However, if an available LOAEL(C) is lower than the BMD(C)L05 and NOAEL(C), then the LOAEL(C) will be used for the derivation of the DNEL.

If more than one dose descriptor remains after applying the above selection criteria, the DNEL calculator derives all the corresponding DNELs following step 2 and 3 explained in sections 21.2.2 and 21.2.3 and selects the lowest DNEL.

21.2.2. Step 2: modification of relevant dose descriptors

The initial dose descriptors need to be modified with appropriate correction factors to convert them into more correct starting points considering the human population exposure conditions.

As a consequence, four correction factors are applied to the initial dose descriptors as explain in the sections below.

21.2.2.1. Correction factor for differences in bioavailability (ABS)

When the initial dose descriptor used for the calculation of the DNEL is from a study on the same route as the route for which the DNEL is to be derived, then the correction factor for difference in

bioavailability is set to 1 assuming the same bioavailability for experimental animals and humans in the absence of further information.

When a route-to-route extrapolation is made (if the experimental study is not carried out for the same route as the DNEL derived) then a correction should be made for the difference of bioavailability by route. In case of a route1-to-route2 extrapolation is made the following correction factor is applied: $\text{Absorption}(\text{route1-animal})/\text{Absorption}(\text{route2-animal})$. This is assuming the same bioavailability for experimental animals and humans in the absence of further information.

The correction factor for differences in bioavailability is calculated according to the rules described in the following table and using information provided in IUCLID endpoint summary of section 7.1 when available. Note that if no (or partial) information is provided in the endpoint summary of IUCLID section 7.1, the DNEL calculator uses default values as explained in [ECHA Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.8](#). In addition, in the event of using dermal-to-inhalation or dermal-to-oral extrapolation, if there is no information about dermal absorption the DNEL calculator will use a dermal absorption of 10% as a reasonable worst-case scenario.

Table 16: Values for ABS according to the route of initial dose descriptor and the route of DNEL being derived as well as whether data is provided in endpoint summary of section 7.1 or not

Route for dose descriptor	DNEL inhalation	DNEL dermal	DNEL oral
Inhalation	1	Inhalation absorption / dermal absorption If partial or no data, default values are: Dermal absorption = 1 Inhalation absorption = 1	Inhalation absorption / oral absorption If partial or no data, default values are: Oral absorption = 1 Inhalation absorption = 1
Dermal	Dermal absorption / inhalation absorption If partial or no data, default values are: Dermal absorption = 0.1 Inhalation absorption = 1	1	Dermal absorption / oral absorption If partial or no data, default values are: Dermal absorption = 0.1 Oral absorption = 1
Oral	Oral absorption / inhalation absorption If partial or no data, default values are: Oral absorption = 0.5 Inhalation absorption = 1	Oral absorption / dermal absorption If partial or no data, default values are: Dermal absorption = 1 Oral absorption = 1	1

21.2.2.2. Correction factor for differences in respiratory volume (SRV)

In case the inhalation route is involved in the DNEL calculation using route-to-route extrapolation, the dose descriptor used as starting point needs to be corrected considering the differences between metabolic rate of experimental animals and humans (allometric scaling) and human body weight scaling.

The use of the standard respiratory volume (sRV) for the experimental animal is the preferred way to correct the point of departure using the route-to-route extrapolation. The sRV for the

experimental animal is calculated from the standard respiratory volume for humans (per kg bw) and applying the corresponding allometric scaling factor.

Example:

$$sRV(\text{human } 70 \text{ kg, } 8\text{h}) = 6.7 \text{ m}^3/\text{person}/8\text{h}$$

If the respiratory volume is transformed per kg of body weight, it will depend on the average weight for each of the human populations. Thus:

$$RV(\text{human } 70 \text{ kg, } 8\text{h}) = 6.7 / 70 \text{ kg} = 0.0957 \text{ m}^3/\text{kg bw}/8\text{h}$$

If the experimental animal is rat (allometric scaling factor is 4), then:

$$sRV(\text{rat, } 8\text{h}) = sRV(\text{human, } 8\text{h}) \times \text{allometric scaling factor} = 0.0957 \times 4 = 0.38 \text{ m}^3/\text{kg bw}/8\text{h}$$

Since the relevant exposure time for the general population is 24 hours instead of 8, then:

$$sRV(\text{rat, } 24\text{h}) = sRV(\text{rat, } 8\text{h}) \times 24/8 = 1.35 \text{ m}^3/\text{kg bw}/24\text{h} \text{ for general population}$$

The DNEL calculator uses the default values as explained in [ECHA Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.8](#), as provided in the table below:

Table 17: Values for SRV according to the route of initial dose descriptor and experimental animal as well as route of DNEL being derived and population for that DNEL

Route for dose descriptor	Species	DNEL inhalation		DNEL dermal		DNEL oral
		Workers	General Population	Workers	General Population	General Population
Inhalation	Rat	n/a	n/a	0.38	1.15	1.15
	Mouse	n/a	n/a	0.67	2.01	2.01
	Hamster	n/a	n/a	0.48	1.44	1.44
	Guinea pig	n/a	n/a	0.29	0.86	0.86
	Rabbit	n/a	n/a	0.23	0.69	0.69
	Monkey	n/a	n/a	0.19	0.57	0.57
	Dog	n/a	n/a	0.13	0.40	0.40
Dermal	Rat	0.38	1.15	n/a	n/a	n/a
	Mouse	0.67	2.01	n/a	n/a	n/a
	Hamster	0.48	1.44	n/a	n/a	n/a
	Guinea pig	0.29	0.86	n/a	n/a	n/a
	Rabbit	0.23	0.69	n/a	n/a	n/a
	Monkey	0.19	0.57	n/a	n/a	n/a
	Dog	0.13	0.40	n/a	n/a	n/a
Oral	Rat	0.38	1.15	n/a	n/a	n/a
	Mouse	0.67	2.01	n/a	n/a	n/a
	Hamster	0.48	1.44	n/a	n/a	n/a
	Guinea pig	0.29	0.86	n/a	n/a	n/a
	Rabbit	0.23	0.69	n/a	n/a	n/a
	Monkey	0.19	0.57	n/a	n/a	n/a
	Dog	0.13	0.40	n/a	n/a	n/a

21.2.2.3. Correction factor for light activity at work (WORKER)

There is a difference in respiratory volumes between humans at rest (standard human respiratory volume: 6.7 m³/kg bw/8h) and humans performing a light activity (worker respiratory volume for light activity: 10 m³/kg bw/8h). Therefore for the derivation of worker-DNEL for inhalation route a correction factor of 0.67 (result from the ratio of the values above) needs to be applied.

21.2.2.4. Correction for differences between human and experimental exposure conditions (EXPCOND)

This correction factor is used to account for differences in the exposure conditions of experimental animals in a test study that may differ from the ones of the worker (or the general population). For example, in a repeated-dose inhalation study, the exposure is usually 6 hours per day (see OECD TG 413), which differs from that for workers which is usually assumed to be 8 hours per day. Thus, a correction factor is applied to the initial dose descriptor to calculate the DNEL, i.e. EXPCOND. EXPCOND is calculated in the following way depending on the route of the initial dose descriptor and the route for which the DNEL is derived:

1. For oral dose descriptor: days per week(experimental)/days per week(human population)
2. For inhalation or dermal dose descriptor: [hours per day(experimental) / hours per day(human population)] * [days per week(experimental) / days per week(human population)]

The DNEL calculator uses the following default experimental exposure conditions:

1. For dermal and inhalation studies: 6 hours per day and 5 days per week.
2. For oral studies: 7 days a week.

Those default values for experimental exposure conditions are compared to the exposure conditions for human population only when the toxic effect type is dose-dependent. For the worker population:

1. Exposure via dermal and inhalation routes: 8 hours per day and 5 days per week.
2. Exposure via oral route: 5 days per week.

For the general population:

1. Exposure via dermal and inhalation routes: 24 hours per day and 7 days per week.
2. Exposure via oral route: 7 days per week.

The default values for EXPCOND are reported in the following table:

Table 18: Values for EXPCOND according to the route of initial dose descriptor as well as route of DNEL being derived and population for that DNEL (only valid for dose-dependent toxic effects).

Route for dose descriptor	DNEL inhalation		DNEL dermal		DNEL oral	
	Workers	General population	Workers	General population	Workers	General population
Inhalation	0.75	0.178571	0.75	0.178571	0.75	0.178571
Dermal	0.75	0.178571	0.75	0.178571	0.75	0.178571
Oral	1.4	1	1.4	1	1.4	1

For concentration-driven toxic effects the EXPCOND is always set to 1.

It is foreseen that the exposure conditions in the experimental studies could be different from the default values or that for a specific exposure scenario the general population could be exposed less than 24 hours per day. In those situations, the assessor can use a different correction factor using the *Edit* mode functionality. In this situation, it will be required a detailed justification explaining why the correction factor is modified.

21.2.3. Step 3: application of assessment factors

In order to derive a DNEL for human health variability and uncertainty of experimental data is to be taken into account. Assessment factors (AFs) are therefore applied to the corrected dose descriptor (as obtained in step 2) to calculate VDNEL values. The DNEL calculator uses the recommended assessment factors in [ECHA Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.8](#).

21.2.3.1. Assessment factor for interspecies variability - allometric scaling factor (AF1)

Interspecies differences result from variation in the sensitivity of species due to differences in toxicokinetics and toxicodynamics. Some of the toxicokinetic differences can be explained by differences in body size (and related differences in basal metabolic rate). Allometric scaling, further explained in ECHA's Guidance Chapter R.8 is a factor applied to account for those differences in body size. The default values for this factor available in [ECHA Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.8](#) are used by default.

Table 19: Values for AF1 according to the experimental animal of initial dose descriptor.

Species	AF1
Rat	4
Mouse	7
Hamster	5
Guinea pig	3
Rabbit	2.4
Monkey	2
Dog	1.4

21.2.3.2. Assessment factor for interspecies variability - remaining differences (AF2)

This assessment factor, with a default value of 2.5, deals with other interspecies differences, i.e. toxicokinetic differences not related to metabolic rate (small part) and toxicodynamic differences (larger part). In case substance-specific information shows specific susceptibility differences between species, which are not related to differences in basal metabolic rate, the additional factor of 2.5 for *remaining differences* can be modified accordingly.

21.2.3.3. *Assessment factor for intraspecies variability (AF3)*

Humans differ in terms of sensitivity to chemicals and this factor deals with this uncertainty. In order to estimate the intraspecies variability a common approach is to separate the workers from the general population, as the worker population will usually not include the very young, the very sick and the very old people, thus leading (potentially) to a lower susceptibility for the workers compared to the general population. The default values for this factor in [ECHA Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.8](#) are applied, i.e. AF3 = 5 for workers and AF3= 10 for the general population..

21.2.3.4. *Assessment factor for differences in exposure duration (AF4)*

Most animal testing experiments are performed only for a limited period of time (e.g. 28 days or 90 days) and not for the entire life of the experimental animal. Therefore, an extrapolation factor is applied to account for the effects that may arise during the entire lifetime of humans. The most relevant animal study is the chronic study, which accounts for the toxic effects of the entire life of the experimental animal.

Default values for the relevant study duration in [ECHA Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.8](#) are applied, i.e. AF4= 1 for chronic studies, AF4= 2 for sub-chronic studies and AF4=6 for sub-acute studies.

21.2.3.5. *Assessment factor for dose-response relationship (AF5)*

The uncertainty in the dose-response relationship quantified by a dose descriptor (e.g. NOAEL or LOAEL) accounts for the uncertainty of true surrogate of the *No-Adverse Effect Level* (NAEL). Following [ECHA Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.8](#), the DNEL calculator has set this assessment factor to a default value of 3 if dose descriptor is LOAEC(L). For other dose descriptor the value is 1.

21.2.3.6. *Quality of database (AF6)*

An additional assessment factor on the quality of the whole database may be applied to account for the remaining uncertainties in any of the factors discussed in the three steps procedure.

The default value is 1 according to [ECHA Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.8](#).

21.2.4. **Formulas for DNEL derivation**

The formulas applied for the derivation of DNEL depend on the route and the human population for which the DNEL is derived. It also depends on whether the route of the dose descriptor is the same as the route for which the DNEL is derived. The formulas use the correction factors explained in section 21.2.2 and the assessment factors explained in section 21.2.3.

It is important to note that if more than one dose descriptor remains after applying the prioritisation criteria described in section 21.2.1 above, the DNEL calculator derives the corresponding DNELs will all the dose descriptors as starting point but will select only the lowest DNEL.

21.2.4.1. Worker-DNEL for inhalation route

If the route of the initial dose descriptor is inhalation, the following formula is applied:

$$\text{DNEL} = (\text{dose descriptor} * \text{ABS} * \text{WORKER} * \text{EXPCOND}) / (\text{AF1} * \text{AF2} * \text{AF3} * \text{AF4} * \text{AF5} * \text{AF6})$$

Alternatively, if the route of the initial dose descriptor is oral or dermal the following formula applies:

$$\text{DNEL} = (\text{dose descriptor} * (1/\text{SRV}) * \text{ABS} * \text{WORKER} * \text{EXPCOND}) / (\text{AF1} * \text{AF2} * \text{AF3} * \text{AF4} * \text{AF5} * \text{AF6})$$

21.2.4.2. General population-DNEL for inhalation route

If the route of the initial dose descriptor is inhalation, the following formula is applied:

$$\text{DNEL} = (\text{dose descriptor} * \text{ABS} * \text{EXPCOND}) / (\text{AF1} * \text{AF2} * \text{AF3} * \text{AF4} * \text{AF5} * \text{AF6})$$

Alternatively, if the route of the initial dose descriptor is oral or dermal the following formula applies:

$$\text{DNEL} = (\text{dose descriptor} * (1/\text{SRV}) * \text{ABS} * \text{EXPCOND}) / (\text{AF1} * \text{AF2} * \text{AF3} * \text{AF4} * \text{AF5} * \text{AF6})$$

21.2.4.3. Worker-DNEL for dermal route

If the route of the initial dose descriptor is inhalation, the following formula is applied:

$$\text{DNEL} = (\text{dose descriptor} * \text{SRV} * \text{ABS} * \text{EXPCOND}) / (\text{AF1} * \text{AF2} * \text{AF3} * \text{AF4} * \text{AF5} * \text{AF6})$$

Alternatively, if the route of the initial dose descriptor is oral or dermal the following formula applies:

$$\text{DNEL} = (\text{dose descriptor} * \text{ABS} * \text{EXPCOND}) / (\text{AF1} * \text{AF2} * \text{AF3} * \text{AF4} * \text{AF5} * \text{AF6})$$

21.2.4.4. General population-DNEL for dermal route

If the route of the initial dose descriptor is dermal, the following formula is applied:

$$\text{DNEL} = (\text{dose descriptor} * \text{SRV} * \text{ABS} * \text{EXPCOND}) / (\text{AF1} * \text{AF2} * \text{AF3} * \text{AF4} * \text{AF5} * \text{AF6})$$

Alternatively, if the route of the initial dose descriptor is oral or dermal the following formula applies:

$$\text{DNEL} = (\text{dose descriptor} * \text{ABS} * \text{EXPCOND}) / (\text{AF1} * \text{AF2} * \text{AF3} * \text{AF4} * \text{AF5} * \text{AF6})$$

21.2.4.5. General population-DNEL for oral route

If the route of the initial dose descriptor is inhalation, the following formula is applied:

$$\text{DNEL} = (\text{dose descriptor} * \text{SRV} * \text{ABS} * \text{EXPCOND}) / (\text{AF1} * \text{AF2} * \text{AF3} * \text{AF4} * \text{AF5} * \text{AF6})$$

Alternatively, if the route of the initial dose descriptor is oral or dermal the following formula applies:

$$\text{DNEL} = (\text{dose descriptor} * \text{ABS} * \text{EXPCOND}) / (\text{AF1} * \text{AF2} * \text{AF3} * \text{AF4} * \text{AF5} * \text{AF6})$$

21.3. Output information

Once the DNELs are calculated, then the DNEL calculator selects the lowest for each DNEL scenario and shows them in a pop-up window.

This pop-up window is composed of two main sections. In the section at the top it displays a table with all the DNELs that have been derived grouped by route. The section below contains two tabs called *Dose descriptor* and *Assessment factors*. The *Dose descriptor* tab shows in a read-only mode the starting dose descriptor used for calculating the DNELs for that route and the correction factors (section 21.2.2 above) that have been used to modify the starting dose descriptor. The *Assessment factors* tab shows in a read-only mode the assessment factors (section 21.2.3 above) that have been used in the derivation of the DNELs.

This pop-up window also contains four buttons: *Edit*, *Print*, *Finish* and *Cancel*.

The *Edit* button opens an edit window in which the starting dose descriptor, some correction factors and/or some assessment factors can be modified providing a justification. See more information in section 21.4.

The *Print* button generates a report in RTF format documenting the information related to the DNEL derivation (input and output data). This report has the same format used by the CSR generator for section 5.11 of the CSR.

The *Finish* button closes the DNEL calculator and the relevant data is transferred automatically to the relevant fields in the summary of section 7 *toxicological information* from which the DNEL calculator was launched. Be aware that if the endpoint summary already has values, the tool will overwrite all the available values for the Worker/General population long term systemic hazard conclusions (oral dermal and inhalation routes). All other fields will not be affected and the values already indicated will neither be overwritten nor erased.

The *Cancel* button simply closes the DNEL calculator without any further action.

21.4. Edit mode: modifying defaults from the DNEL calculator

The assessor has the possibility to modify the starting dose descriptor, some correction factors and/or some assessment factors which have been set by default by the DNEL calculator. This is done using the *Edit*.

The *Edit* button opens a new pop-up window which shows all the inputs that the assessor is allowed to modify in the DNEL calculator:

1. Starting dose descriptor: the DNEL calculator selects as default the dose descriptor available in the endpoint summaries of section 7.5 or 7.8 giving rise to the highest concern, i.e. the one leading to the lowest DNELs for a given route after applying the prioritisation criteria described in section 21.2.1 above. If the assessor disagrees, another dose descriptor can be selected from the picklist containing all the available dose descriptors in the study summaries of section 7.5 and 7.8. However, if a new starting dose descriptor is selected the assessor needs to provide a detailed justification explaining why the new starting dose descriptor is actually more relevant. It is important to note is that if a new starting dose descriptor is selected, the DNEL calculator will re-calculate the DNELs and will display the new default inputs used.
2. Correction for differences between human and experimental exposure conditions: the DNEL calculator uses default values as explained in section 21.2.2.4 above. If the experimental exposure conditions have been different from the default values, the assessor can modified this correction factor by clicking on *Overwrite*. However, the assessor needs to provide a justification explaining why and how this correction factor is modified. Since this correction

factor is different for different human populations, the assessor would need to modify it for both workers and general population.

3. Assessment factors AF2 to AF6: the DNEL calculator applies the default values according to ECHA's Guidance, Chapter R.8. If the assessor has substance-specific information that can justify the use of values other than default, the assessment factors AF2 to AF6 can be modified after clicking on *Overwrite*. However, the assessor needs to provide a detailed justification explaining how the factors in Annex I, Section 1.4.1. of the REACH Regulation have been taking into account.

If after having modified any of the input above the assessor wants to go back and use the default values as input, this can be done by clicking on *default*.

This pop-up window also contains two buttons: *Save* and *Cancel*.

The *Save* button closes the *Edit* pop-up window and the DNEL tool will re-calculate the relevant DNELs using the new inputs from the assessor. The new results will be shown in the initial display window.

The *Cancel* button simply closes the *Edit* pop-up window without any further action and goes back to the initial display window.

21.5. Disclaimer

ECHA recommends to use the optional DNEL calculator in IUCLID. Note that nevertheless the registrant remains responsible for the calculated DNELs.

22. Validation assistant

22.1. 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.

22.2. 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.

22.3. 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 current version of the Validation assistant includes a subset of *quality checks* to support users in improving consistent reporting of information. Further quality checks are under development and will be added in future versions.

22.3.1. 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 (TCC) 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 by ECHA staff. The responsibility remains with the registrant to 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 the IUCLID format. Furthermore, we recommend that all registrants get familiar with the document *Information on manual verification at completeness check*. Both the manual and the document are available at: <http://echa.europa.eu/manuals>

22.3.2. Business rules

The Validation assistant also incorporates several of the business rules (BR) checked at ECHA. 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. The manuals are available at:

<http://echa.europa.eu/manuals>

22.3.3. Quality checks

The quality check feature enables users to check their IUCLID substance datasets and dossiers for common shortcomings and inconsistencies before submitting them to ECHA. The quality rule set is updated on a regular basis with experience from ECHA's different evaluation and assessment activities. The quality rules in the current version of the Validation assistant cover the following areas:

- Substance identity information in sections 1.1, 1.2 and 1.4
- Information on classification and labelling in section 2.1
- Information on estimated quantities in section 3.2
- Administrative data in endpoint study records in sections 4-7
- Reporting of results in sections 7.3.1, 7.3.2 and 7.4.1

Further quality checks will be developed in future versions of the Validation assistant.

The quality checks have been designed to assist the user in detecting inconsistencies in the information provided. The Validation assistant does not offer an exhaustive verification of the quality of the entire dossier or substance dataset, and there may be special circumstances in which some of the quality warnings can be ignored. The responsibility remains with the user of the tool to ensure that the information submitted is adequate under the relevant regulation.

22.4. 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.

22.4.1. Launching the Validation assistant

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

22.4.1.1. 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 either from the Plugins menu in the upper menu bar, or 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 22.4.2.2 for further information.

Figure 120: Launching the Validation assistant from the IUCLID home page



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

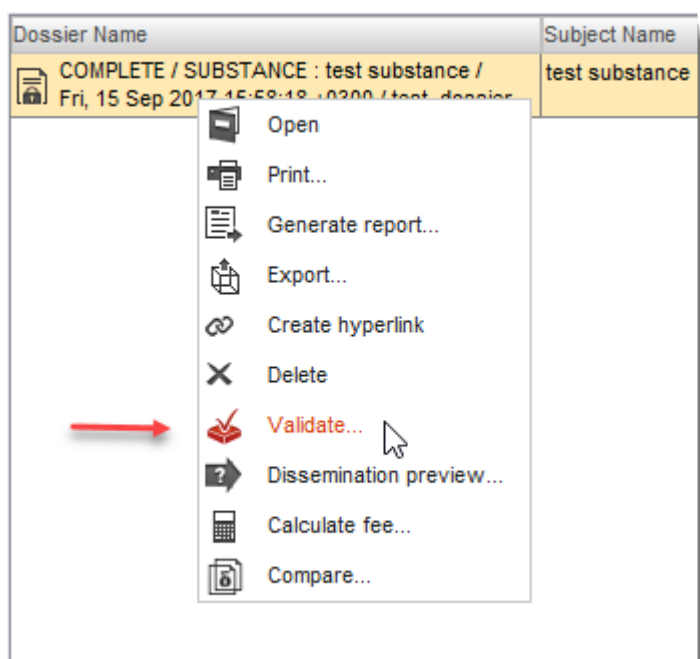
The following approach is most suitable in the case of working inside the Substance or Dossier menus of IUCLID, i.e. (i) you are working on a substance dataset and want to check interactively

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 22.4.2.2 for further information.

Figure 121: 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.

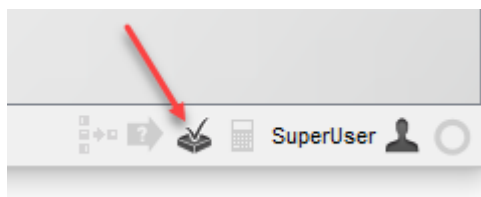


22.4.1.3. Hide/display the Validation assistant window

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.

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 cannot see the Validation assistant window because it has been minimised, clicking on this icon will bring it back up to the foreground where it can be seen.

Figure 122: The icon of the Validation assistant icon in the bottom right corner of the IUCLID interface.



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.

22.4.2. Checking dossiers and substance datasets

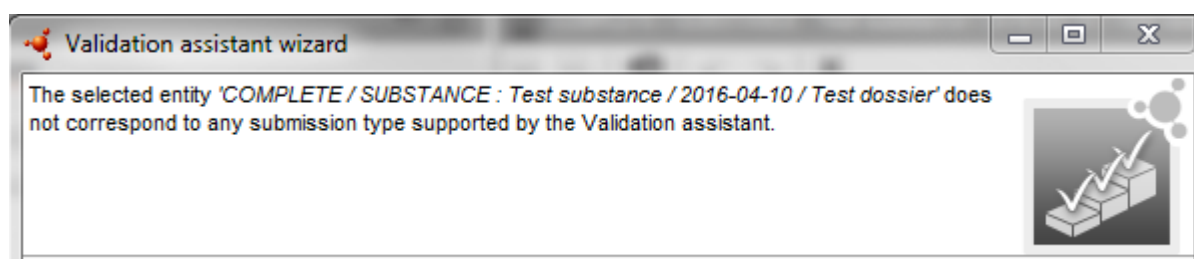
This section explains how to use the Validation assistant to check a dossier or a substance dataset.

22.4.2.1. 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 22.3), a business rules check is performed.
- The quality rule set is under continuous development; new rules are applied to all the dossier types they are relevant to.
- If you attempt to run the Validation assistant on a dossier type that it does not support, the report table will be empty and a message is displayed at the top of the Validation assistant results window, as shown in the figure below.

Figure 123: Running the validation on a dossier template that the Validation assistant does not support gives the message shown below.



22.4.2.2. 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 22.4.1.
- Step 2.** Select the type of dossier for which you want to validate the substance 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 substance dataset. The available fields depend on the type of dossier selected in step 2. For example, when validating the substance 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.
- Step 4.** Once the required information has been entered to identify the submission type, the validation will proceed as for dossiers.
- Step 5.** Unlike dossiers, substance datasets can be modified. When validating a substance dataset, you can keep the Validation assistant open and interactively correct the validation errors in the dataset; then saving and refreshing the validation result using the *Re-check* button to confirm that the correction was successful.

You should only activate the *Use advanced settings – select information to be checked based on confidentiality and regulatory programme flags* feature, mentioned in step 2, when the data to be validated has been flagged systematically with regulatory programme flags throughout the substance dataset, and when there is a need to distinguish between data to be submitted for different regulatory purposes in the same dataset. In all other cases, the default settings of the Validation assistant are appropriate for the validation, and the advanced settings should not be used.

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 are validated against the correct submission type (scenario) and that all the information provided in the dossier header has been considered.

22.4.3. Validation assistant results window

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

Figure 124: Validation assistant results display. The numbers shown for the different interface elements correspond with the numbering of the following subsections.

Validation assistant wizard

Validated entity: Test substance / Test
Time of validation: 2016/09/02 09:45:31
Validation scenario: SC0018 - Registration, individual 100-1000

Submission checks (4) Quality checks (6)

Business rules (0), Completeness check rules (4)

No business rule failures were detected by the Validation assistant. Please note that some of the business rules can only be checked at dossier level. Also note that as the Validation assistant only verifies information within the IUCLID dossier/dataset, it cannot perform all the business rules checks that apply when the dossier is submitted to ECHA.

Re-check Open document Open document Copy report Copy selected row(s) Filter: All Rule level: All

Rule	Section number	Section name	Document name	Message	Rule type	Rule level
TCC_050203_01	5.2.3	Biodegradation in soil, Half-life / dissipation time of parent compound, (1)	Biodegradation in soil.001	'Results and discussion' is not complete. For each endpoint study record marked as 'key study' or 'weight of evidence', at least one of the tables '% Degradation' or 'Half-life / dissipation time of parent compound' must be filled in. In the table '% Degradation' the fields '% Degr.', 'Parent time' must be filled in, with unit. In the table 'Half-life parent compound' the fields 'Half-life' and 'Temp.' must be filled in, with unit. If you add several rows in the table, then all of them must be filled in. If you select 'other:' in any of the picklists, then all of them must be filled in. If a quantitative result was not determined, an explanation must be provided in the field 'Remarks on result'. If none of the available picklist values apply, select 'other:' and provide the reason for not determining a quantitative result in the adjacent field.	Completeness check	Failure
TCC_070401_A01	7.4.1	Skin sensitisation		To fulfil the information requirement for section 7.4.1 at the selected tonnage band, at least one record indicated as a key study, weight of evidence or data waiving must contain one of the following 'Endpoint'	Completeness check	

Validation assistant - Report Back Next Finish Cancel

22.4.3.1. 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.

In the tab headers, numbers are displayed in brackets. They indicate the number of messages (validation errors) displayed for each tab. In the upper part of the active tab an information message is displayed, explaining the implication of the validation result to the user.

22.4.3.2. Validation assistant report toolbar

The Validation assistant report toolbar contains the following elements:

<https://iuclid6.echa.europa.eu>

 Re-check	<p>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.</p>
 Copy report	<p>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 <i>Copy report</i>, or by using the keyboard shortcuts CTRL+A and CTRL+C.</p>
 Copy selected row(s)	<p>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 <i>Copy selected row(s)</i>, or by using the keyboard shortcut CTRL+C.</p>
 Open document 	<p>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 <i>Open document</i>. Navigation to a document is not possible when the validation error is caused by a missing document.</p>
 Open document 	<p>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 <i>Open document</i>. Navigation to a document is not possible when the validation error is caused by a missing document.</p> <p>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.</p>

22.4.3.3. 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 cannot be successfully submitted. Messages reported in the *Quality checks* tab are of the level warning or reminder. If left uncorrected, the dossier can be successfully submitted to ECHA, but they may trigger follow-up actions later on when the dossier is under scrutiny by evaluators/assessors.

Note that unlike the other types of messages reported by the Validation assistant, messages of the level reminder cannot be removed by a certain corrective action by the user. Reminder messages may be disregarded once the user has followed the recommendation given.

22.4.3.4. 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 <i>Half-life / dissipation time of parent compound</i> 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 22.4.3.2), 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 <i>Submission checks</i> 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 <i>Submission checks</i> tab are of the level failure. Messages reported in the <i>Quality checks</i> tab are of the level warning or reminder.

By default, the validation report displays the outcome sorted by the column *Section number*, in ascending numerical order. By clicking on a column header of the validation report, you can sort

the report by that column in ascending or descending order. For example, you can sort the report by the column *Rule* if you wish to correct all failures reported by a certain rule regardless of the section they appear in.

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 registrant 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.

22.4.3.5. Information about the validation

In the top left corner of the Validation assistant report, you can see information about the validated entity (substance dataset or dossier), the time of validation, as well as the validation scenario (submission type). This information is included if you copy the report to the clipboard, to facilitate traceability of the validation result.

22.5. 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**.

22.6. 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.

23. Report generator

The *Report generator* offers the possibility to generate a readable and printable report of IUCLID information from a *Substance Dossier or Dataset*, or a *Mixture/product Dossier or Dataset*. The *Report generator* is most frequently used for generating a Chemical Safety Report (CSR). The *Report generator* can also be used to generate customised reports of IUCLID information using

user-defined report templates which allow a user to extract IUCLID information for other purposes, for instance, analysing the literature references or confidentiality claims contained in a dossier. For a short introduction on creating customised report templates, see the IUCLID website [here](#).

23.1. Report generator wizard

The *Report generator* wizard allows you to generate either a pre-defined and in-built report, such as the Chemical Safety Report, or a report which a user has customised and uploaded into IUCLID for their own purposes using the *Report generator* manager.

The *Report generator* wizard is launched from either the main menu of IUCLID under *Plugins*, the icon on the home page (by left-clicking on the icon and selecting 'Generate reports'), or by right-clicking on the record of a *Substance Dataset or Dossier*, *Mixture/product Dataset* or *Dossier* in the navigation panel and selecting 'Generate report'.

The first page of the *Report generator* wizard is used to select the source of the data from which the report is derived, and the type of report. If the *Report generator* is launched by right-clicking, the source is pre-selected. The types of pre-defined reports which are offered depend on the type of the source data and, if you have created your own report through the *Report generator* manager, then the reports you have assigned to be used with a *Substance* or a *Mixture/product* will also be available to select.

The second page of the *Report generator* wizard is used to select the format of the report, and the location to where it is saved. If you have opted to use a customised report which is created in the *Report generator* manager, you are also able to select which Stylesheet you wish to use with the report. The supported output formats for predefined templates are RTF, PDF and XML. If you have created a customised report in the *Report generator* manager, you have the possibility to create other output formats such as TXT format.

23.2. Report generator manager

The *Report generator* manager which allows a user to upload, store and manage their own customised IUCLID report is launched by left-clicking the *Report generator* icon on the home page of IUCLID and selecting to 'Manage reports'.

The first page of the *Report generator* manager is used to add a new report type, to edit an existing report type, or to delete an existing report type. To delete a report, select the report name so that it is highlighted and select 'Delete'. If you wish to add or edit an existing report, select 'Add' or 'Edit' respectively.

If you are adding or editing an existing report, the second page of the *Report generator* manager is used to define or change the criteria of the report. These criteria include the name of the report, the templates which are used for defining what is extracted from IUCLID, the output format of the report, the Stylesheet(s) you wish to use with the report and which govern its display, the entity type from which the report is generated (*Substance* or *Mixture/product*), and the submission types the report is relevant for.

When uploading your template(s) into the *Report generator* manager, which are used to define what IUCLID information is extracted, you cannot upload and overwrite a template which has the same filename as an existing template which you have stored for the report you are editing.

Therefore, it is recommended to delete the existing template you wish to replace before uploading a new template.

Once you have added or edited a report in the *Report generator* manager, select 'Save' and the report you have defined will appear as an option in the first page of the *Report generator* wizard as a report type to select. The report is only available to select if the *Report generator* is launched from an entity (*Substance* or *Mixture/product*) assigned to the report you have created. The Stylesheets and the output formats you have assigned to the report will all be available to select in the second page of the *Report generator* wizard.

23.3. Preparing the Chemical Safety Report (CSR)

The *Report generator* 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.

23.3.1. 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.

23.3.2. CSR part A

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

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

23.3.3. 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.

23.3.4. 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.

23.3.4.1. 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.

23.3.4.2. 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.

23.3.4.3. 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.

23.3.4.4. 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.

23.3.4.5. Assessment entities

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

23.3.5. 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.

23.3.5.1. 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.

23.3.5.2. 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".

23.3.5.3. 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*.

23.3.6. 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).

23.3.6.1. Overview tables for summarising the relevant studies

The following approach is applied for generating overview tables:

- An overview table 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."

23.3.6.2. 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 follows 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.

23.3.6.3. 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).

23.3.6.4. Elements included in overview tables

23.3.6.4.1. 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.

23.3.6.4.2. 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".

23.3.6.5. 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<<<.

23.3.6.6. 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).

23.3.7. 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.

23.3.8. 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

23.3.9. 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".

23.3.10. 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

23.3.11. 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).

23.4. Generating an XML file for use with the SPC Editor

The Report generator can create an XML file of type *Summary of product characteristics (SPC) report* from either a *Mixture/Product* dataset, or a *Dossier* that has been specifically designed for import into the [SPC Editor](#). The SPC templates that are currently available on the IUCLID website, and used to generate manually the SPC report, are built-in to the *Report generator* and used automatically when the output is set to *Summary of product characteristics (SPC) report*.

The *SPC Editor* is used to support companies in preparing their applications for authorisation of biocidal products. The *Report generator* facilitates this process by extracting information from the sections listed below of a *Mixture/Product* dataset or *Dossier*, and converts this information into an XML file which is compatible with the *SPC Editor*:

- 1.3 Biocidal product manufacturer
- 2.1 Trade name of proposed trade name
- 2.3 Representative biocidal product composition
- 6.1 Function and mode of control
- 7.1 Field(s) of use envisaged for representative biocidal products and treated articles
- 7.6 Method of application and a description of this method
- 11 Measures to protect humans, animals and the environment
- 12.1 GHS Record
- 12.3 Packaging (12.7 in Annex III of BPR)
- 13 Summary and evaluation

Importation of the XML file in to the *SPC Editor* populates the following sections: Administrative information, Product Information, Hazard and Precautionary Statements, Authorised Uses, and Other Information.

Currently, the extraction is compatible only with Single Products, but not Product Families, of a biocidal product submission. Moreover, not all fields of the *SPC Editor* are meant to be populated

by IUCLID 6 information, and the user will need to check the information in the *SPC Editor* to ensure it is complete and accurate.

There are two generic rules of note when using the *Report generator* to generate an XML file for the *SPC Editor*:

1. The *Report generator* will generate the file from a *Mixture/Product* dataset or *Dossier* only if there is a biocidal composition in section 2.3.
2. As a general rule, if a section such as 12.3 or 7.1 contains more than one composition, only the first composition is taken into consideration when extracting information.

24. Dissemination preview

24.1. 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 created 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 titled *Dissemination and Confidentiality under the REACH Regulation*, which is included in the IUCLID help system, and is available in PDF format on the ECHA website at:

<https://echa.europa.eu/manuals>.

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.

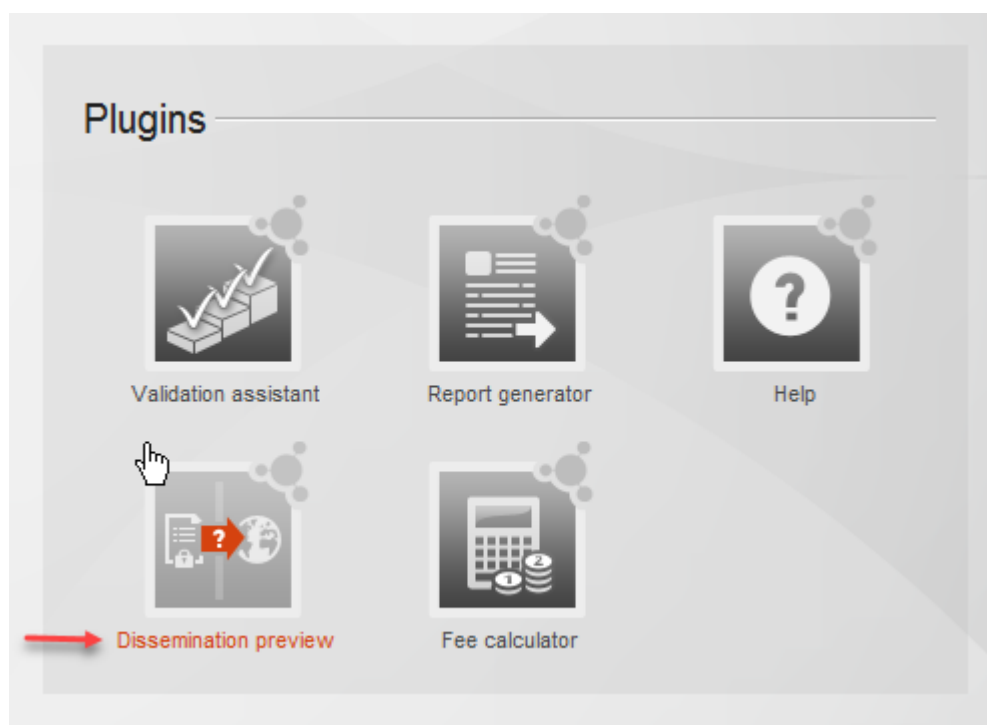
Note: It is recommended to always check that you have the latest version of the preview tool, to ensure you always have the same Filtering Rules as ECHA. Choose to be notified of when new versions of IUCLID or its components are available on the website, as described in section 15.1.2.5 Updates of the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

24.2. Starting the Dissemination preview

24.2.1. From the IUCLID home page

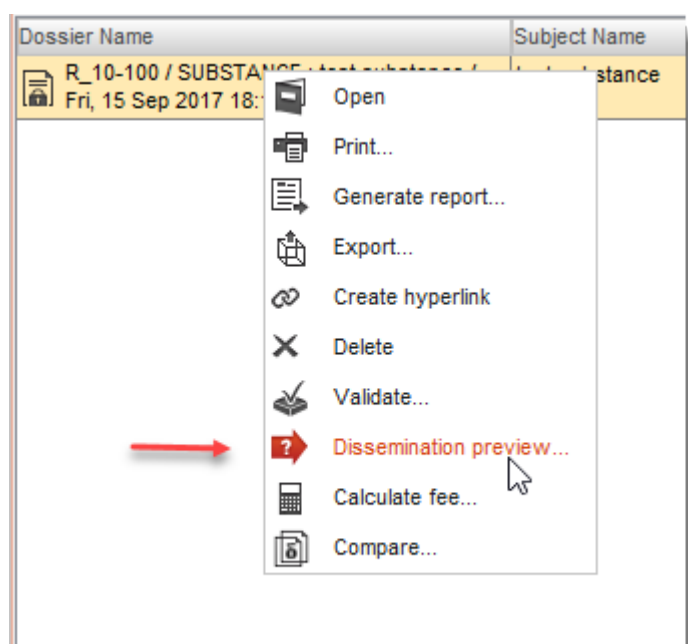
From the IUCLID home page the Dissemination preview can be started by clicking on the icon in the *Plugins* section as shown below. There is also a link in the upper menu under *Plugins*.

Figure 125: Starting the Dissemination preview from the IUCLID 6 home page



24.2.2. 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 126: Starting the Dissemination preview from the Dossier view

24.3. Using the Dissemination preview

24.3.1. 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*.


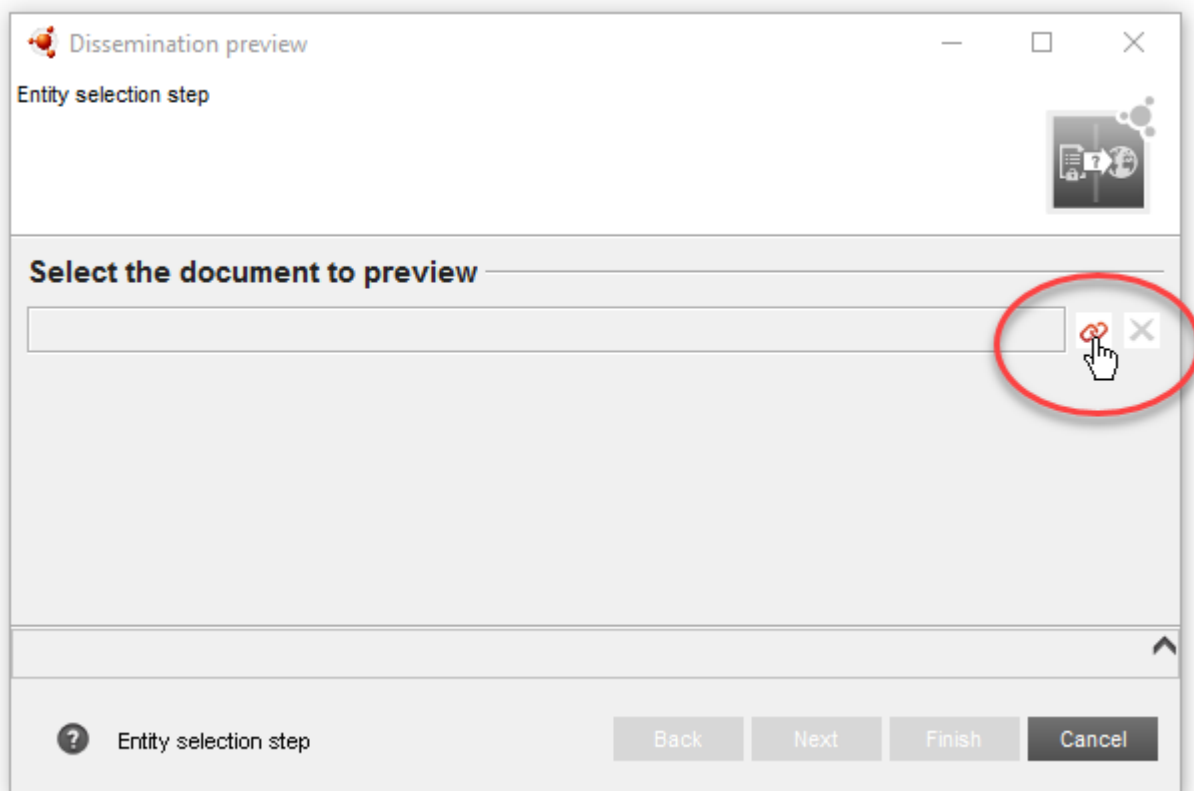
If you start the preview from the IUCLID Home view, you need to select the dossier to filter. Click on the  icon to bring up a standard IUCLID search dialog which you can use to locate the dossier you wish to preview in a disseminated form.

Figure 127: Dossier selection from the IUCLID home page

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

24.3.2. 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 128: Name and Comment for Filtered Dossier

Dissemination preview

Disclaimer:
This plug-in simulates which information from a registration dossier ECHA will make available to the public over the internet, according to Article 119 of Regulation(EC) No 1907/2006 ("the REACH Regulation"). Please note that the Dissemination preview plug-in by default removes information claimed confidential under Article 119(2). ECHA will however perform an assessment of each such confidentiality claim. Should ECHA reject any confidentiality claim(s), the information claimed confidential may be disclosed at a later stage, after consultation with the registrant.

Please also note that in case of a joint submission, all members of the joint submission will contribute to the information made available on the internet.

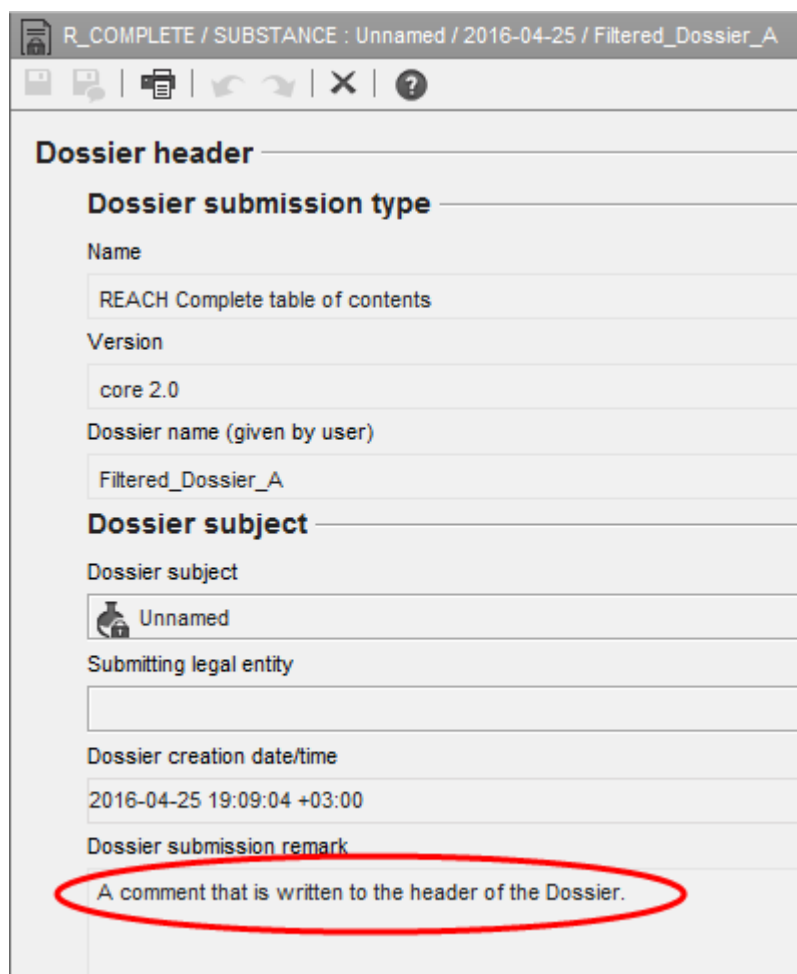
Enter a name for the filtered document you are creating and a comment if desired. Choose a name which will help you to identify and find the filtered dossier.

Name

Comment

Note: Names and comments will not be published on the ECHA website. They are used in the plug-in purely for informational purposes.

The comment, if any, will be saved in the *Dossier submission remark* in the *Dossier header*, as shown in the example below.

Figure 129: Comment for Filtered Dossier

R_COMPLETE / SUBSTANCE : Unnamed / 2016-04-25 / Filtered_Dossier_A

Dossier header

Dossier submission type

Name
REACH Complete table of contents

Version
core 2.0

Dossier name (given by user)
Filtered_Dossier_A

Dossier subject

Dossier subject
Unnamed

Submitting legal entity

Dossier creation date/time
2016-04-25 19:09:04 +03:00

Dossier submission remark
A comment that is written to the header of the 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.

24.4. 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.

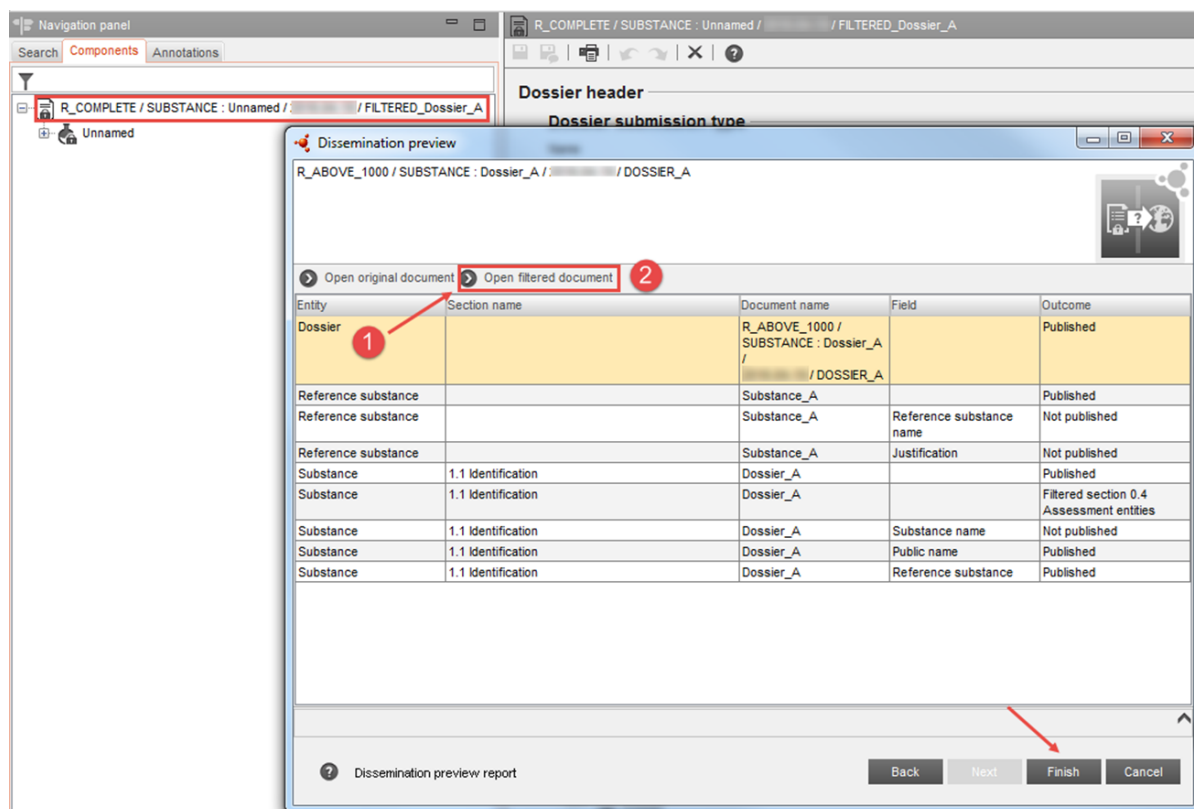
You can review more specific details on the filtering outcome from the report table.

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.

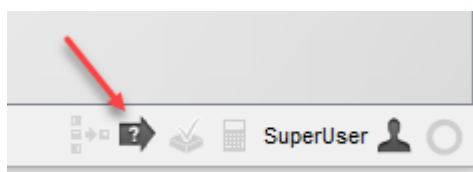
Figure 130: Dissemination preview report



The Dissemination preview window can be minimised by clicking on the bar icon located at the top right of the window, 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.

Whilst the Dissemination preview plugin is running, its icon in the bottom right corner of the IUCLID interface is dark grey. In that state, clicking on the icon displays the plugin window uppermost.

Figure 131: The icon for the Dissemination preview plugin in the bottom right corner of the IUCLID interface



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.

25. Fee calculator

25.1. Introduction

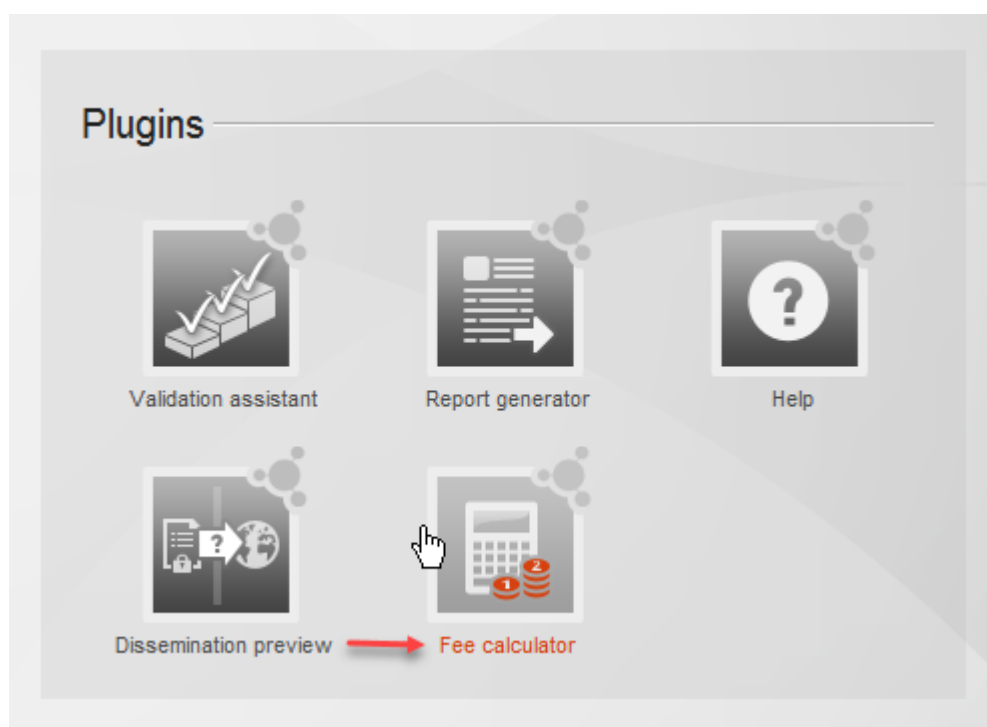
The aim of the Fee calculator is to assist users in calculating the fees for their IUCLID dossiers, according to the [REACH Fee Regulation](#) (No 340/2008 of 16 April 2008, and subsequent amendments). The Fee calculator supports the validation of all dossier types that industry users can submit to the European Chemicals Agency (ECHA) under the REACH regulation.

25.2. Launching the Fee calculator

The *Fee calculator* can be launched from various of locations, according to user preference, and way of working.

25.2.1. Launching the Fee calculator from the Plugins menus

Launch the *Fee calculator* either from the *Plugins* menu in the upper menu bar, or by clicking on the icon in the *Plugins* section of the home view, as shown in the figure below.

Figure 132: Starting the Fee calculator from the IUCLID 6 home page


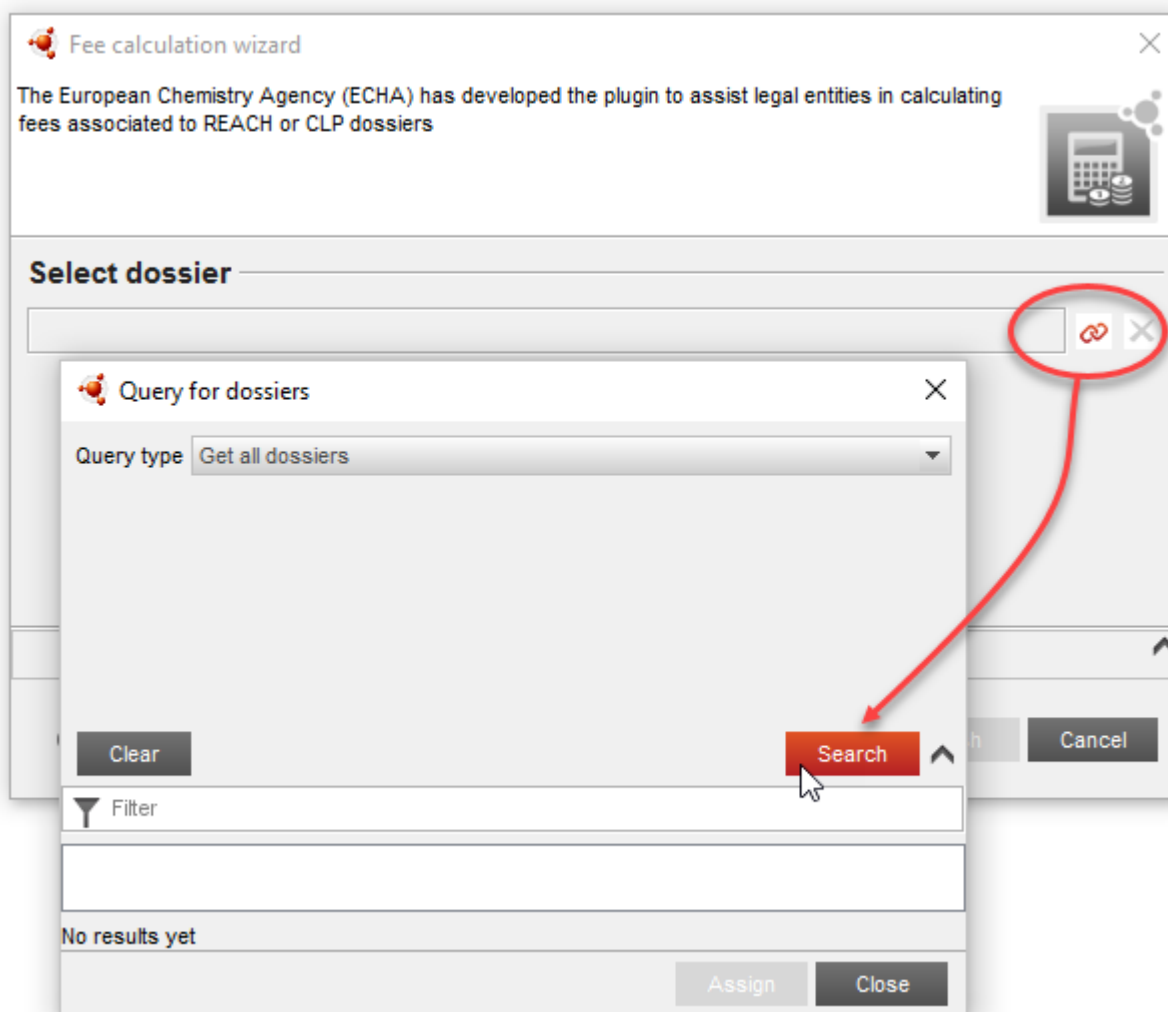
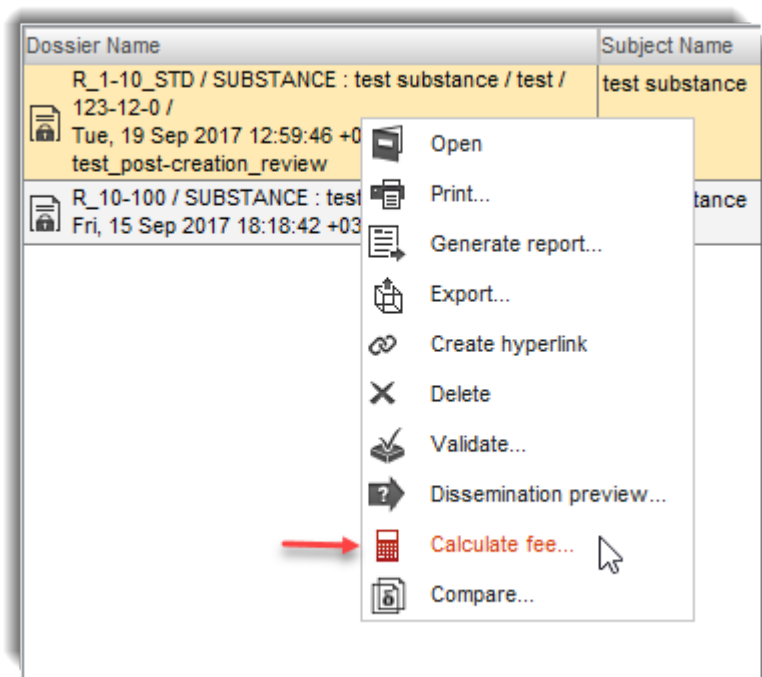
Click on the link icon  to select the dossier for which to calculate the fees. A query window opens from where you can search for the dossier, as shown below.

Figure 133: Search for and select a dossier for the calculation

Select the dossier from the search results list, and then click on *Assign* to load it in to the *Fee calculator*. Continue by clicking on *Next*.

25.2.2. Launching the Fee calculator from the Dossier view

This approach is most suitable when the dossier is visible as a search result in the Navigation pane. Right-click on the name of the Dossier, and then select *Fee calculator* as shown below.

Figure 134: Starting the Fee calculator from the Dossier view

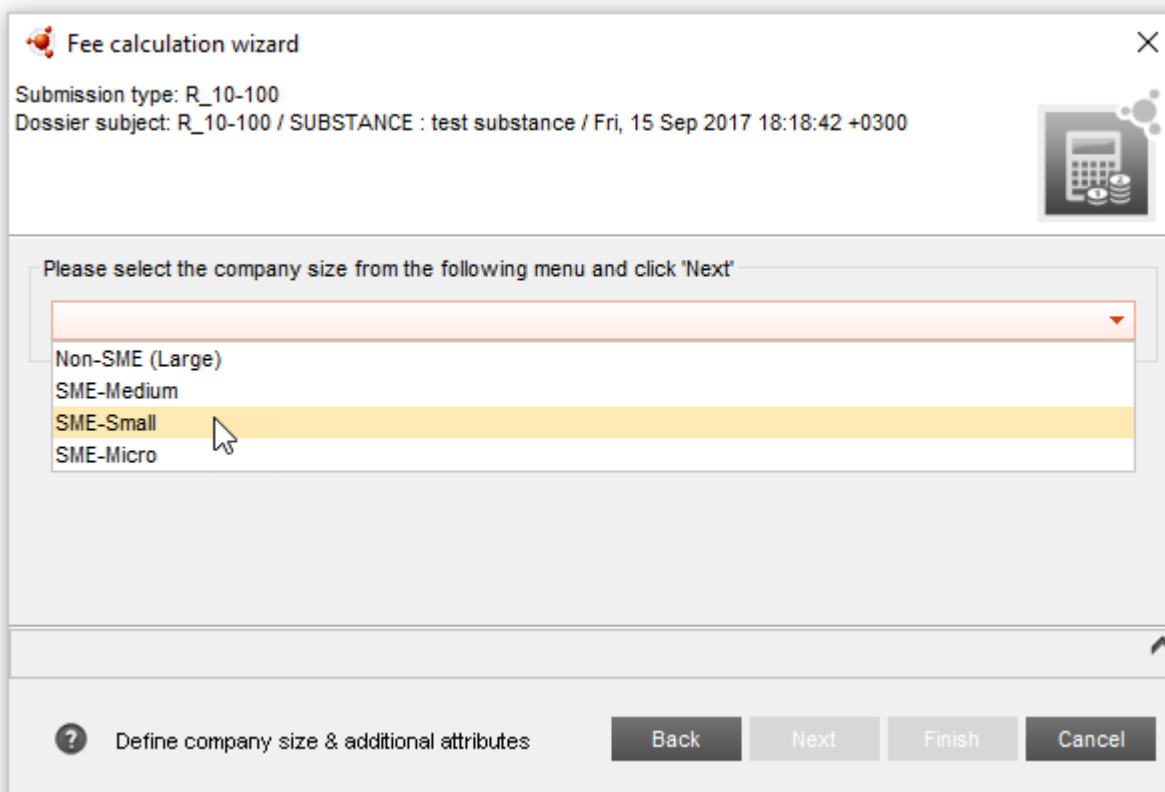
The selected dossier is loaded in to the *Fee calculator*. Continue by clicking on *Next*.

25.3. Calculating the fee for a dossier

Go through the steps in the *Fee calculator* wizard, entering the appropriate values for the dossier and its submission.

25.3.1. Selecting the company size

For all dossiers, you first need to specify the size of the company. To do so, make a selection from the appropriate drop-down list.

Figure 135: Selecting the company size

25.3.2. The Indicators needed for the fee calculation

Some indicators appear when there are confidentiality claims in the dossier OR when the fee waiver has been claimed.

For calculating the fees of some confidentiality claims, you will need to indicate whether:

1. the substance is hazardous as defined in the amended Articles 119(2) (f) or (g) and 14(4) of the REACH Regulation and if the substance is assessed to be PBT/vPvB;
2. a safety data sheet is required for the substance.

The indicators will appear only if they are relevant for calculating the fee AND if the required information is not included in the dossier. For example, if there are no confidentiality claim flags in the dossier, the indicators will not appear.

For calculating the fees of dossiers with tonnage band 1 – 10 tonnes/year where the fee waiver has been claimed, you will need to indicate whether the substance fulfils the Annex III criteria.

25.3.2.1. Hazardous Substance indicator

If the substance is classified as hazardous and is assessed to be PBT/vPvB according to Articles 119(2) (f) or (g) and 14(4) of REACH Regulation, tick the box next to the “Hazardous Substance indicator”.

This indicator is shown when the required information is not included in the dossier.

Figure 136: Hazardous substance indicator

Hazardous substance indicator

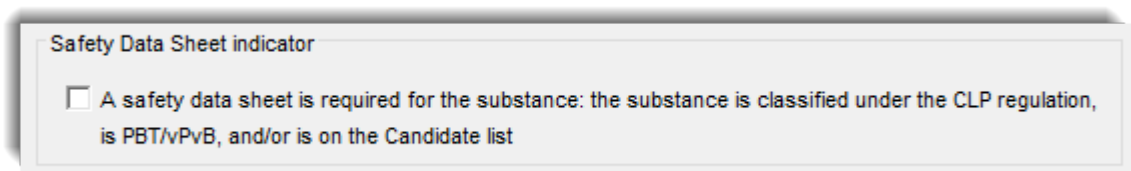
The substance is hazardous as defined in Articles 119(2) or (g) and 14 (4) of the REACH regulation

For more information, check the manual *Dissemination and confidentiality under the REACH Regulation*: <https://echa.europa.eu/manuals>.

25.3.2.2. Safety Data Sheet indicator

If the safety data sheet is required for the substance according to Article 31 of REACH Regulation, tick the box next to the *Safety Data Sheet indicator*. A safety data sheet is required when the substance is classified under the CLP regulation, is PBT/vPvB, and/or is on the Candidate list.

This indicator is shown when the required information is not included in the dossier.

Figure 137: Safety Data Sheet indicator

Safety Data Sheet indicator

A safety data sheet is required for the substance: the substance is classified under the CLP regulation, is PBT/vPvB, and/or is on the Candidate list

For more information, check the manual *Dissemination and confidentiality under the REACH Regulation*: <https://echa.europa.eu/manuals>.

25.3.2.3. Annex III criteria indicator

If the substance does not fulfil the Annex III criteria according to REACH Regulation, and the full Annex VII is voluntarily provided, tick the box next to the "Annex III criteria indicator".

The Annex III criteria is not fulfilled when:

1. there is no indication that the substance has carcinogenic, mutagenic or toxic to reproduction (CMR, category 1A or 1B), persistent, bioaccumulative and toxic (PBT) or very persistent, very bioaccumulative (vPvB) properties, OR
2. there is no indication that a substance with dispersive or diffuse uses would be classified as hazardous for human health or as an environmental hazard under the CLP Regulation.

This indicator is shown when the fee waiver is claimed in dossiers with standard tonnage band 1 - 10 tonnes/year.

Figure 138: Annex III criteria indicator

Check the following option if the Annex III criteria are not fulfilled

Annex III criteria indicator

Not fulfilling Annex III criteria and voluntarily providing Annex VII. This means that:

- there is no indication that the substance has CMR or PBT/vPvB properties, and
- there is no indication that this is a substance with dispersive or diffuse uses, classified as hazardous for human health or as an environmental hazard under the CLP Regulation, and
- the full Annex VIII is being provided

25.3.3. Select the tonnage range of the previous submission and payment information for intermediate use

If the dossier is an update, select the tonnage range of the previous submission and tick the appropriate box if the onsite or transported intermediate use has been previously paid.

Figure 139: Select the tonnage range of the previous submission and payment information for intermediate use

Fee calculation wizard

Submission type: R_100-1000
Dossier subject: R_100-1000 / SUBSTANCE : test substance / test / 123-12-0 / Tue, 19 Sep 2017 19:10:42 +0300 / update_1

Please select the company size from the following menu and click 'Next'

SME-Small

Please select the highest tonnage band for the standard registration fee that you have previously paid

Tonnage band

between 100 to 1000 tonnes/year

Please check the following options if you have previously paid for on-site or transported isolated intermediate use

Isolated intermediates

On-site isolated intermediates

Transported isolated intermediates

Hazardous substance indicator

The substance is hazardous as defined in Articles 119(2) or (g) and 14 (4) of the REACH regulation

Define company size & additional attributes


Back Next Finish Cancel

25.3.4. Fee calculator results window

The last window of the Fee calculator shows the fees calculated according to the dossier information and the information you inserted manually, in a table with the description and exact amount charged for each fee applied. At the bottom of the table, it is shown the total amount of all the fees.

Figure 140: Fee calculator results window

Fee calculation wizard ✕


Submission type: R_ABOVE_1000
 Dossier subject: R_ABOVE_1000 / SUBSTANCE : test substance / test / 123-12-0 / Tue, 19 Sep 2017
 19:15:55 +0300 / update_2 

Selected values

Company size: SME-Small
 Update info: between 10 to 100 tonnes/year
 Dangerous info: No

No ^	Fee description	Fee amount	Select
1	Fee for the update of registrations under article 22 from 10-100 tonnes range to over 1000 tonnes range	10159.0	<input checked="" type="checkbox"/>
2	Request of confidentiality for relevant tonnage band (dossier header)	571.0	<input checked="" type="checkbox"/>
3	Request of confidentiality for a study summary or a robust study summary: 7.1.1/Basic toxicokinetics.001	1712.0	<input checked="" type="checkbox"/>
4	Request of confidentiality for a study summary or a robust study summary: 5.1.2/Hydrolysis.001	1712.0	<input checked="" type="checkbox"/>

Total amount: € 14,154

 Fee amounts Back Next Finish Cancel

The Fee calculator gives you the possibility to remove any fee that is linked to a confidentiality claim by selecting/deselecting the checkbox on the right hand side of the table. After each change in the selected fees, the calculator re-calculates the total fee, and updates the total amount; as shown in the example below. Note how the total amount has gone down compared to the value shown above.

Figure 141: Calculate the cost reduction of removing a confidentiality claim

No ^	Fee description	Fee amount	Select
1	Fee for the update of registrations under article 22 from 10-100 tonnes range to over 1000 tonnes range	10159.0	<input checked="" type="checkbox"/>
2	Request of confidentiality for relevant tonnage band (dossier header)	571.0	<input checked="" type="checkbox"/>
3	Request of confidentiality for a study summary or a robust study summary: 7.1.1/Basic toxicokinetics.001	1712.0	<input checked="" type="checkbox"/>
4	Request of confidentiality for a study summary or a robust study summary: 5.1.2/Hydrolysis.001	1712.0	<input type="checkbox"/>

Total amount: € 12,442

Keep in mind that, by selecting/deselecting any of the confidentiality claim fees in this table the claim is **not** added/removed from the dossier.

The registration fees cannot be deselected. The respective checkbox is inactive and its value cannot be changed.

25.4. Hide/display the Fee calculator window


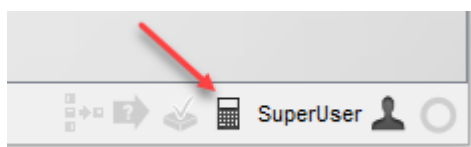
The Fee calculator window can be minimised by clicking on an icon located at the top right corner of the window (). This action will hide the Fee calculator window, but retain all the information about the ongoing calculation. To display the Fee calculator window again, click on the Fee calculator icon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

Figure 142: The Fee calculator icon in the bottom right corner of the IUCLID interface

You cannot launch multiple instances of the Fee calculator at the same time. You therefore need to close a running instance of the Fee calculator, before launching a new one.

25.5. Version update

It is important to use the latest version of the Fee calculator. 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*.

25.6. Disclaimer

The fees calculated by the Fee calculator are only estimates and do not replace the fees specified in the actual invoice you will receive in REACH-IT after the submission of your registration dossier. It is the responsibility of the submitter to ensure that the dossier fulfils the appropriate data requirements and to monitor the receipt of the invoice in REACH-IT.

26. 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.eu/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.

26.1. 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*.

27. 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.

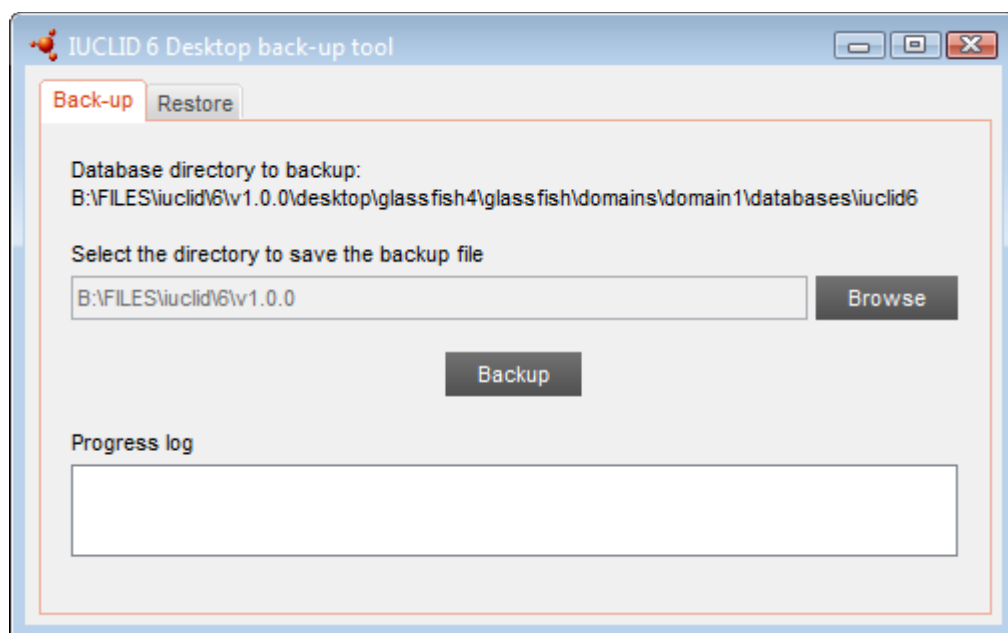
To run the backup/restore application double-click on the file `iuclid6-backup-restore.exe`. There is no need to shut IUCLID 6 down first. If IUCLID 6 Desktop is running, it is automatically shut down, and then restarted after the backup or restore process has finished.

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

27.1. Backup

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

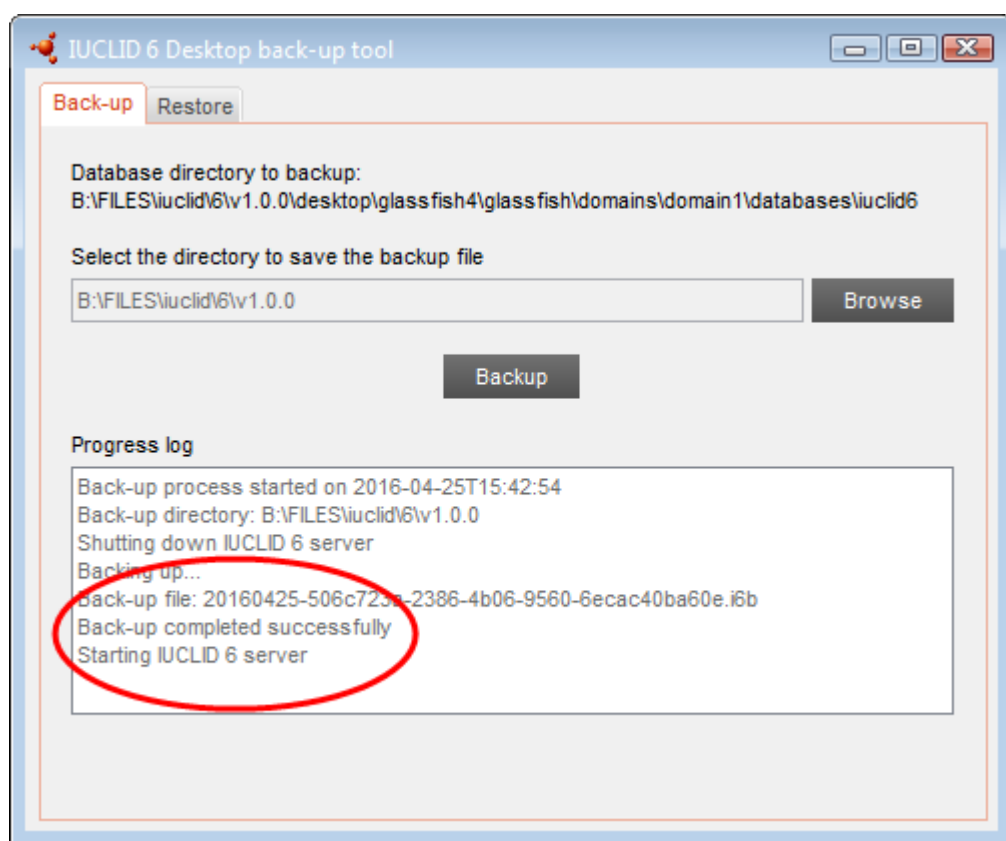
Figure 143: Backing up all the data in an installation of IUCLID 6 Desktop



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:

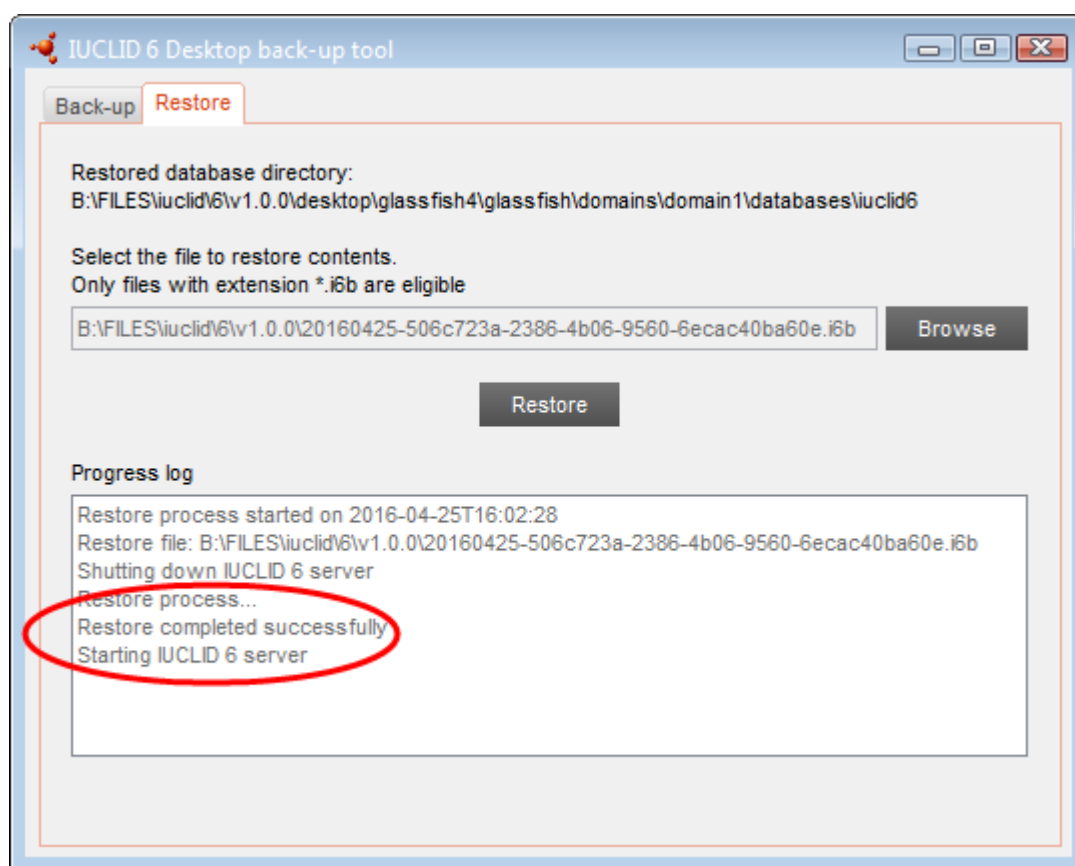
```
<installation  
folder>\glassfish4\glassfish\domains\domain1\databases\iuclid6
```

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

27.2. 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 145: A successfully completed restoration of data to an installation of IUCLID 6 Desktop

28. 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.