IUCLID User Manual

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Table of Contents

Table of Figures

Table of Tables

1. Overview of the user interface

The IUCLID graphical user interface is displayed in a web browser. The address is of the form:

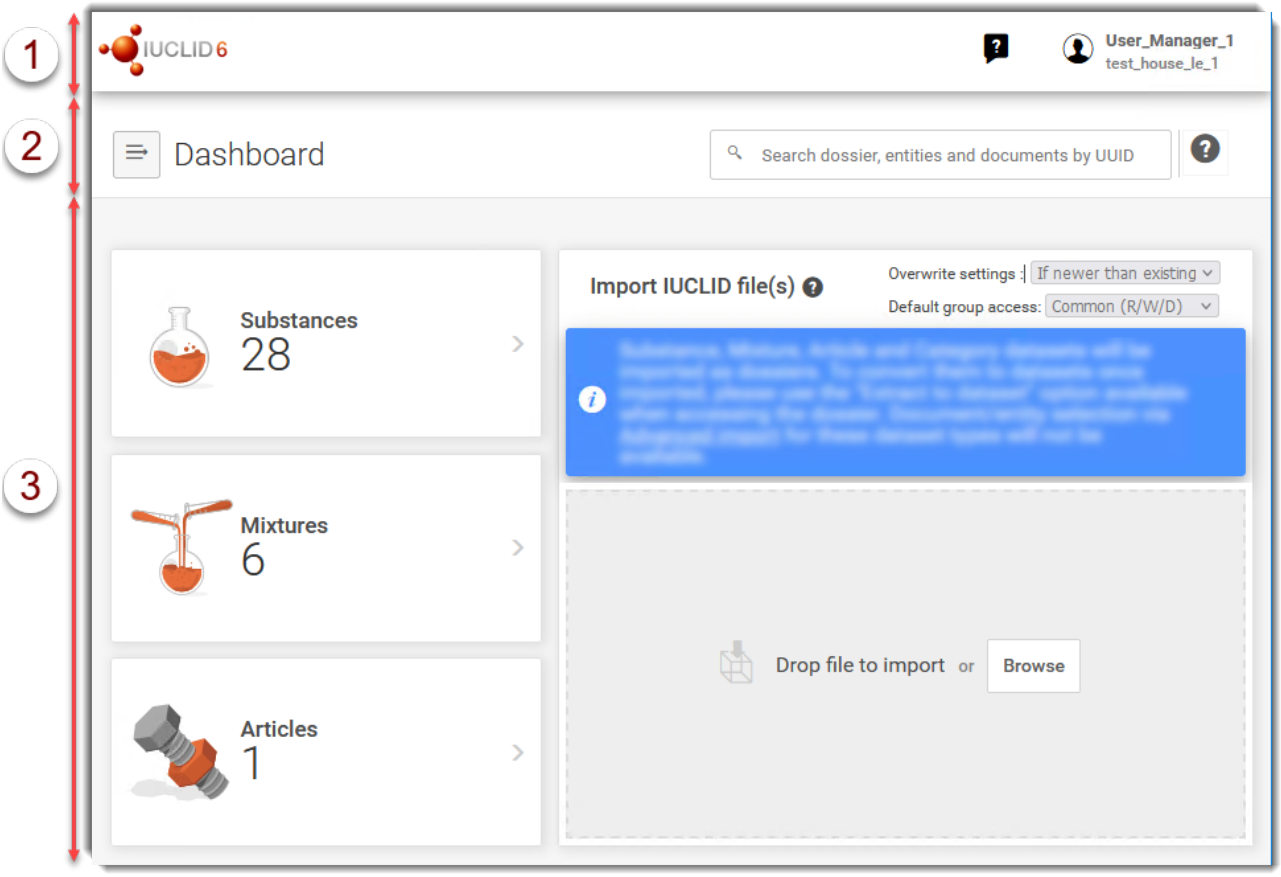
<protocol>://<server>:<port>/iuclid6-web

Example

http://localhost:8080/iuclid6-web

The page shown on starting the interface, or on logging in, is the *Dashboard*. The IUCLID icon at the top left of the screen links to the *Dashboard*. Across the top of the interface there are the *top bar* (1), and then the *application bar* (2). Under those there is a larger area for navigation and data entry (3), as shown below.

Figure 1: The structure of the user interface of IUCLID - Dashboard

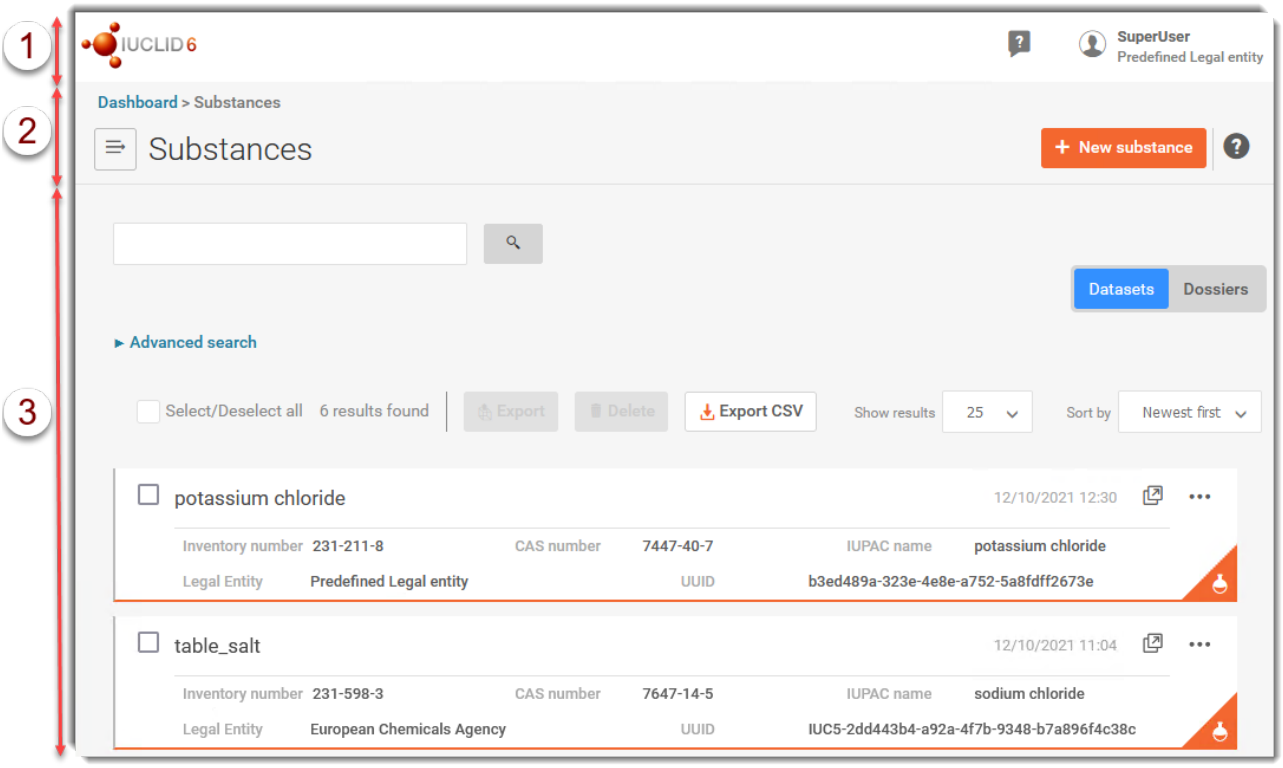


Legend for Figure 1:

1. The top bar: This bar always contains the same options, no matter what is shown in the rest of the interface. The IUCLID icon on the left brings the user back to the *Dashboard* shown in this figure. The dialogue icon leads to external sources of information. For IUCLID 6 Server, on the right there is the name of the IUCLID user, and its working *Legal entity*. Clicking on the name opens a menu that offers options to view the user settings, and to log out.

2. The application bar: The application bar gives access to various functionalities, dependent on whether the *Dashboard* is in view, and what is being viewed in the data area (3). An example is given in the next figure. On the *Dashboard*, the options are: a link to the *Main menu*, *Search entities and dossiers by UUID*, and a link to this manual.
3. The data area: On the *Dashboard* this area contains links to lists of entities, and the functions for importing data in to IUCLID.

Figure 2: The structure of the user interface of IUCLID - List of Substances



Legend for Figure 2:

1. The top bar.
2. The application bar. The application bar gives access to various functionalities, dependent on what is being viewed in the data area (3). In this example, because the data window contains a list of *Substances*, there is an option to create a *Substance*. The text *Dashboard* is a link back to the *Dashboard*.
3. The data area. This is where entities are listed, and data is edited. In this example, the data window contains a list of *Substances*.

1.1. Technical terms specific to IUCLID

The terms in the table below are used throughout the interface and documentation of IUCLID. Knowing what the terms mean will help you understand IUCLID, and how it can be used.

Table 1: Technical terms and their meaning within the context of IUCLID

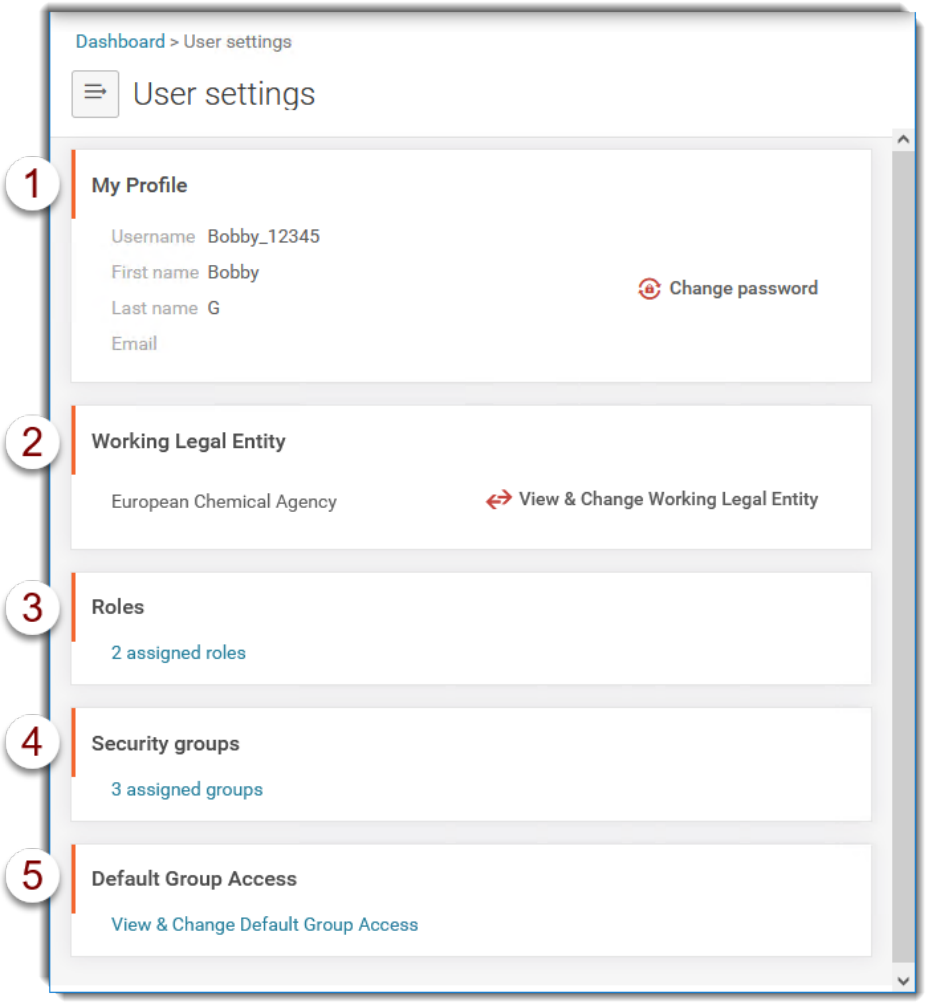
Term	Description
Entity	Entities in IUCLID are software objects that are used to store data that has a particular purpose, which depends on the type of entity. The types of entity are: *Dossier*, *Substance*, *Mixture/Product*, *Template*, *Annotation*, *Legal entity*, *Legal entity site*, *Reference substance*, *Test materials*, *Contact*, *Literature reference*. Entities can be viewed, printed, and deleted individually. They can also be exported and imported as individual files. With the exception of *Dossier*, 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 *Dossier*, which is a read-only snapshot of data.
Dataset	A *dataset* is a collection of documents that relate to a particular chemical substance, or grouping of chemical substances. It can be of the following types: *Substance*, *Mixture/Product*, *Template*. For clarity and where appropriate, the type of the dataset should be stated, for example *Substance dataset*.
Document	A *document* is a page that contains functionality for creating, viewing, or modifying an *entity*, a *record*, or a *summary*. The term *document* 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 *Acute toxicity: oral*, 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. For more information about types of documents, see section *1.7.12 Table of contents*.
Fixed	The term *fixed* means that a document is in a section that can contain only one document.
Field	A *field* 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 *IUPAC name*.

1.2. User Settings

If you are using IUCLID 6 Desktop, by default, this option is not shown because there is no log in process. In that case you are automatically logged in as SuperUser.

If you are using IUCLID 6 Server, you will have logged in as a *IUCLID User*, which is defined within the IUCLID application. To view the settings for the current *IUCLID User*, open *User Settings* from the menu at the top right of the interface, as shown below. The concepts mentioned in *User settings* are described in detail in section *24 User management*.

Figure 3: User settings with Instance based security (IBS) active



Legend for Figure 3

1. Open *User settings*;
2. My Profile: Details about the current User. The password can be changed;
3. Working Legal Entity: A User may have more than one *Legal entity* associated with it, but at any one time, only one is the *working Legal entity*. When a User creates certain types of entity, the *working Legal entity* is associated with the entity automatically. To view the details of the working *Legal entity*, or to select a different one, click on the link *View & Change Working Legal Entity*. If you cannot find the *Legal entity* you are looking for, contact your system administrator. If you have the *Legal entity* as an i6z file, import it and then try to find it again;
4. Roles: The *Roles* of the current user. A link is supplied and a count of the number of *Roles*. To see the names of the *Roles,* click on the link. To find out what these *Roles* mean, contact your system administrator.

5. Security groups: This is shown only if IBS is active. For a description of IBS, see section *24.4 Ownership and Sharing - Instance based security (IBS)*.
6. Default group access: This is shown only if IBS is active. These settings can also be changed by a user manager. For more information see section *24.2.7 Default group access for a User*.

1.3. What is a UUID and where can I find it?

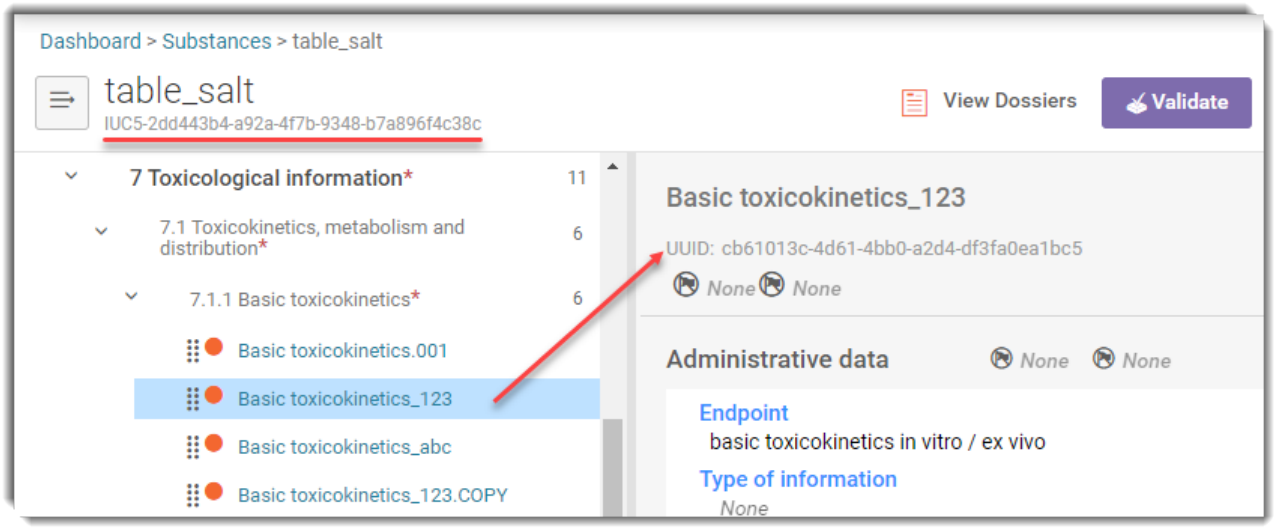
Every entity and document in IUCLID has a Universally Unique Identifier (UUID). When an entity or document is created in IUCLID, it is automatically given a new UUID. In the current version of IUCLID the format for a document contains 32 characters in blocks separated by hyphens, for example:

`4afac895-f978-4b74-9939-5a895ce72fc9`

The UUID of a top-level entity is displayed under its name. The UUID of an open document is displayed at the top of its record in the data window.

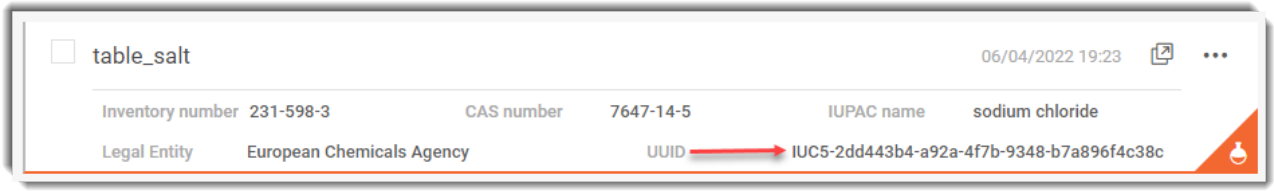
In the example below, the UUID of a Substance dataset is shown under its name. The UUID of an open document within the Substance is shown in the data window. Note that the UUIDs are different.

Figure 4: UUIDs of an entity and a document inside it



The UUID of an entity is shown on its record within a list page, as shown below.

Figure 5: UUID of an entity in a list of entities

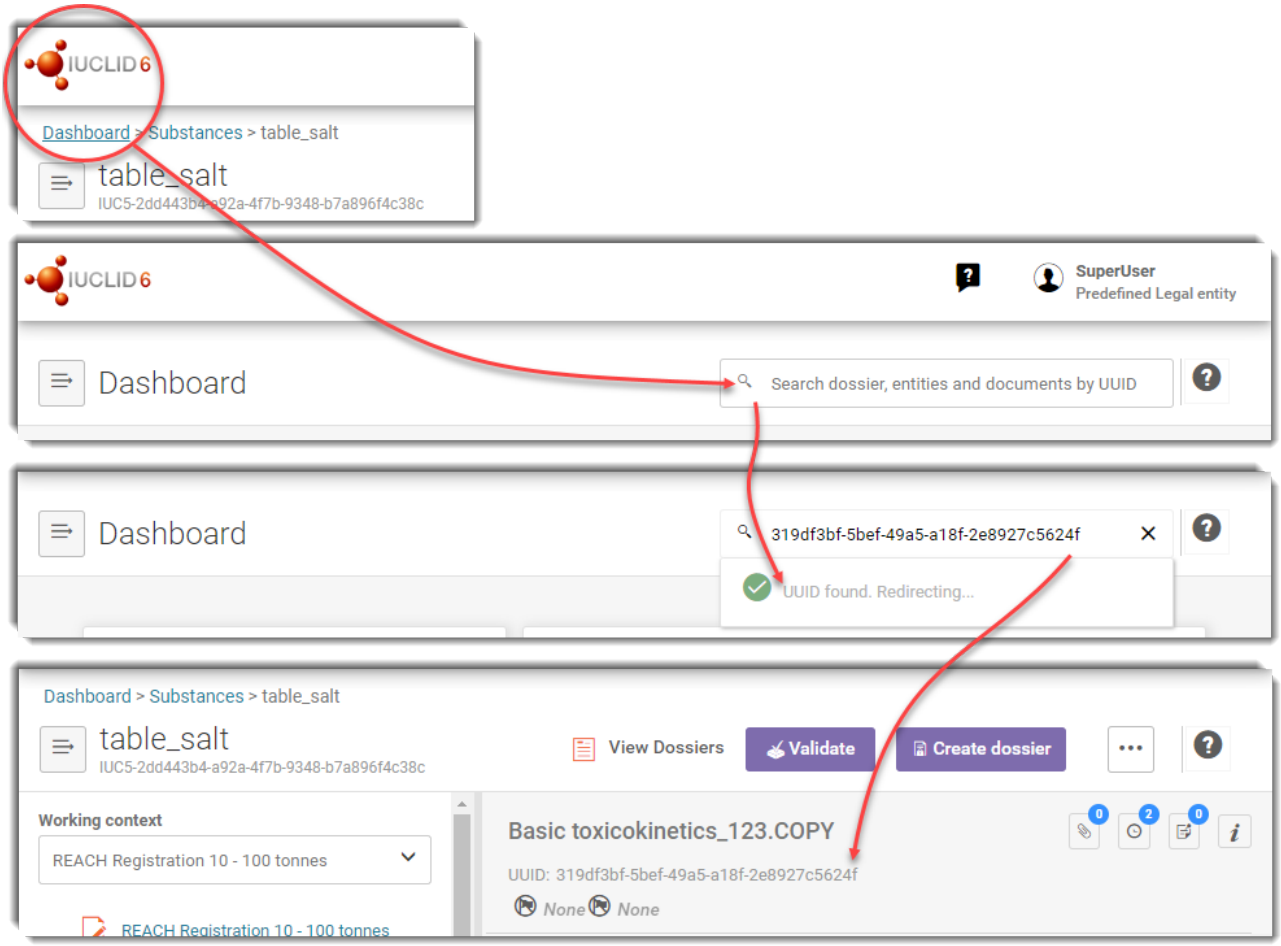


UUIDs are used to refer between entities and/or documents. They are also used in the names of files exported from IUCLID.

1.4. Search by UUID across all entities and documents

The function *Search dossier, entities and documents by UUID* finds and opens anything in the database that has a UUID that is visible in the interface. It is accessed from the *Dashboard*, which can be opened by clicking on either the IUCLID logo at the top left of the interface, or the text *Dashboard* in the breadcrumbs.

Figure 6: Search by UUID across all entities and documents

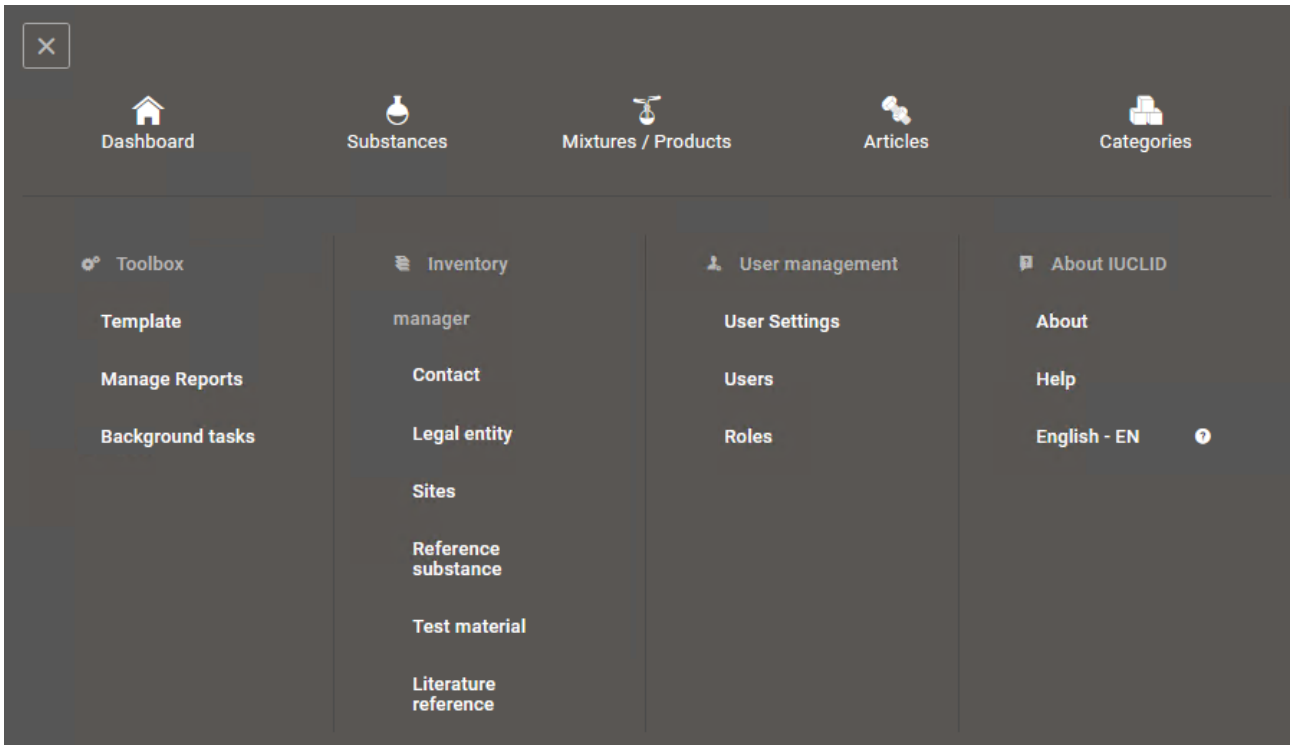


To search by UUID paste the UUID into the box. The search begins automatically. If a match is found for which there is only one instance in the database, the entity or document is opened automatically. If there is more than one match, a list is displayed from which an entity or document can be opened. If the document or entity is in a dossier, the UUID of the dossier is also shown on the list. The searching works for all types of entities and all documents, so long as a UUID is displayed in the interface. For example, it does not work for *Annotations*, and items associated with user management.

1.5. The main menu

The main menu is accessed via the icon at the left of the application bar ( ). It contains direct links to the list pages of the entities, and other items such as *About*. There is a link to this manual, and an *About* window for the instance of IUCLID.

Figure 7: The main menu



1.5.1. About

About displays the version of the instance of IUCLID, and its *Third-party licences*.

1.5.2. Help

Help contains a link to this manual.

1.5.3. Language (English – EN)

To change the language, click on the current language, and then select a different language from the menu. The default original language is English, from which other languages are translated. Translations are provided for use *only* in the working context of SPC for biocides. Not all the text has been translated.

1.6. Navigation using the keyboard

As an alternative to using a mouse to navigate within the user interface, there are various keyboard shortcuts.

1.6.1. Tab / Shift Tab

Tab moves the focus to the next selectable field, button, or tick-box. The movement is throughout all the interface, except the *Table of contents*. The opposite is *Shift Tab*.

Warning

Be aware that the *Tab* movement scrolls through all of the browser window, including its top bar and menus. For example, if you move the selection forwards beyond the *Save* button, it can take 25 *Tab* presses to scroll round to the top of the IUCLID interface. If you press *Tab* and nothing seems to be being selected, if possible, reset the selection position by clicking somewhere in the IUCLID interface, and then try *Tab* again.

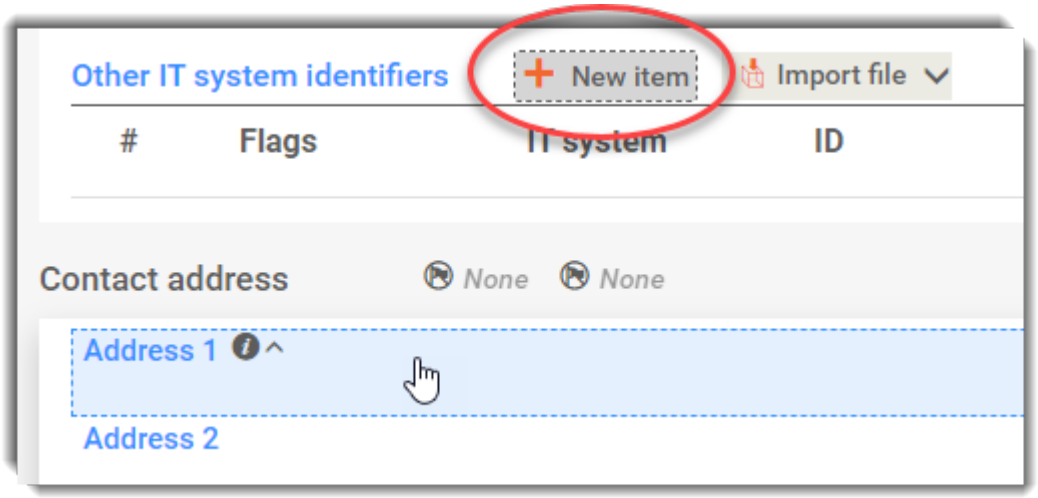
1.6.2. Enter

Enter is equivalent to a mouse click on an object that has been selected using *Tab*. Selection is indicated by a dashed border around the object. For example, the *Save* button can be selected using *Tab*, and then the data saved using *Enter*.

Figure 8: The Save button when selected, or 'brought in to focus', using Tab

Be careful not to confuse an object that is high-lighted by the mouse hovering over it, with a selection made using *Tab*. *Enter* acts on an object that has been selected using *Tab*, independently of the location of the mouse pointer. In the example below, the field *Address 1* is highlighted in blue and has a dotted border, but *Enter* would act on the button *New item*.

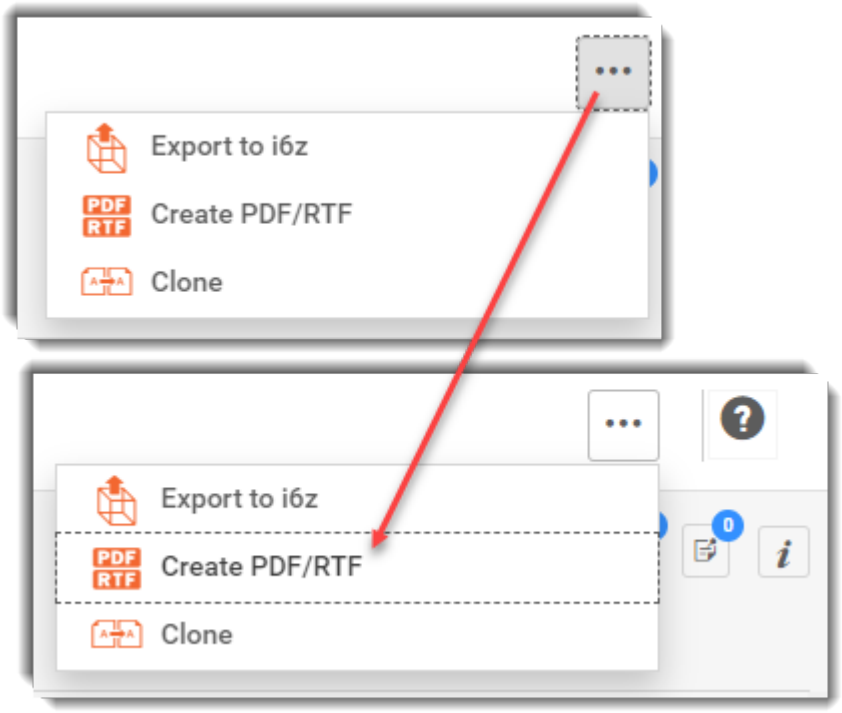
Figure 9: Enter acts on an object that has been selected using Tab, not the focus of the mouse



1.6.3. Shift Enter

To open or close a three-dot menu, *select* the icon with *Tab* and then press *Shift* and *Enter* at the same time. To move through the menu items, use *Tab*. Use *Enter* to open a selected item. In the example below, pressing *Enter* opens the sliding window for *Create PDF/RTF*.

Figure 10: Select an item from a three-dot menu without using the mouse:



1.6.4. Escape

Escape switches a field out of edit mode.

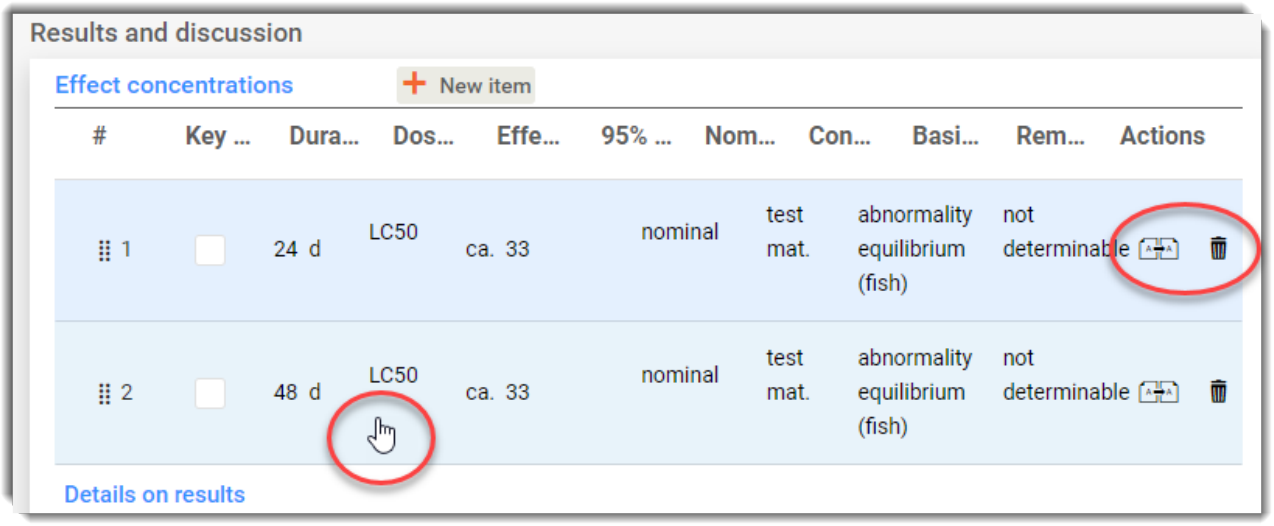
1.6.5. Up and down arrow keys ↑ / ↓

The up and down arrow keys, move up and down in pick lists. They also work where the browser has stored a history of values, such as previous searches.

1.6.6. Clone and Delete in repeatable tables using Ctrl C and Ctrl D

In repeatable tables, the functions clone and delete can be executed using *Ctrl C* and *Ctrl D* on the selected row. The selection must be done using *Tab*. In the example below the lower row is highlighted because the mouse is hovering over it, but the upper row will be acted upon because it has been selected using *Tab*. Note the slightly different colour.

Figure 11: Difference between highlighting by mouse hover, and selection using Tab



1.7. Functionalities available in the data area

The following functionalities are used throughout the data area.

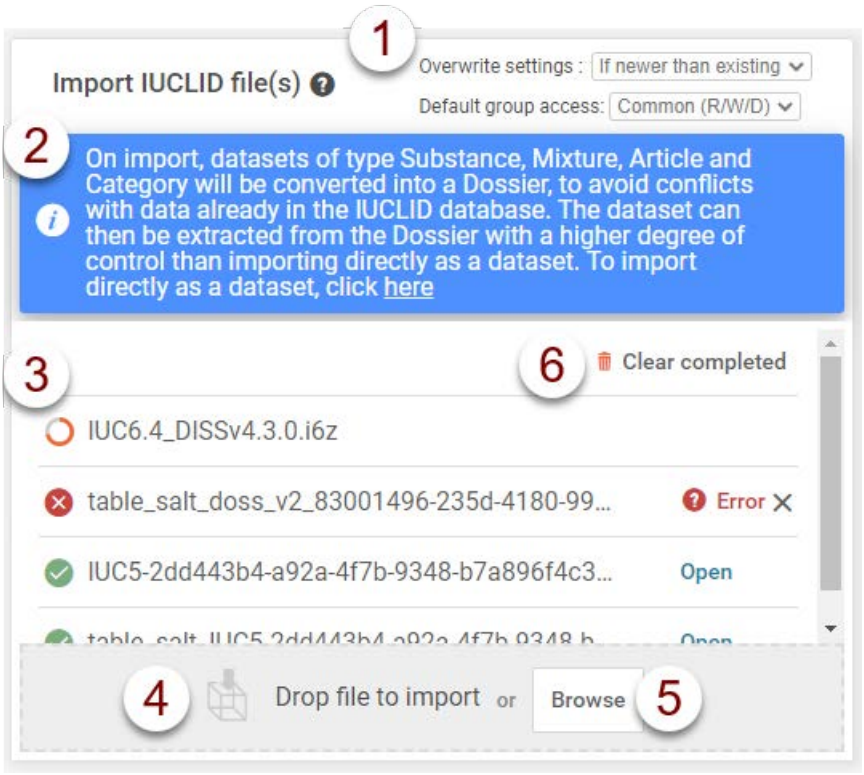
1.7.1. Import

Data is imported in to IUCLID from the home page. Only valid IUCLID data from versions 5.6 onwards can be imported. The file extension can be i5z, i6z, or XML. When data is imported 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.

By default, a dataset of type *Substance*, *Mixture*, *Article* or *Category* is imported as a *Dossier*. After import, it can be converted into a dataset as explained in section *6.4 Extract to Dataset*.

More than one file can be imported at once. Either browse to files, or drag and drop them in to the upload area, which is marked by a dashed boundary. Imports are listed per file, as shown in the example below. *Import* is run as a background task, as described in *23 Background tasks*.

Figure 12: Import data in to IUCLID



Legend for Figure 12

1. The *Overwrite settings* are described below in the next section.
2. By default, certain types of datasets are converted into a dossier on import. To import as a dataset instead, and have a choice of which entities and documents are imported, click here. See section *1.7.1.3 Import to* dataset;
3. The state of the import: A ring icon indicates the progress of an import. Do not shut down IUCLID whilst an import is in progress, because it will cancel the import of that file. A green tick means that the import was completed successfully, and the import is accessible via the link *Open*. A red cross means that the import failed. To see a brief error message, hover the cursor over the red question mark. If more detail is required, click on the word *Error* to download an error message in a text file. If that message states only “undefined”, check the file format;
4. Files to be imported can be dragged and dropped into the grey area;
5. To navigate to a file, click on *Browse*;
6. To remove jobs from the list that have finished, click on *Clear completed*;

1.7.1.1. Overwrite settings - Import

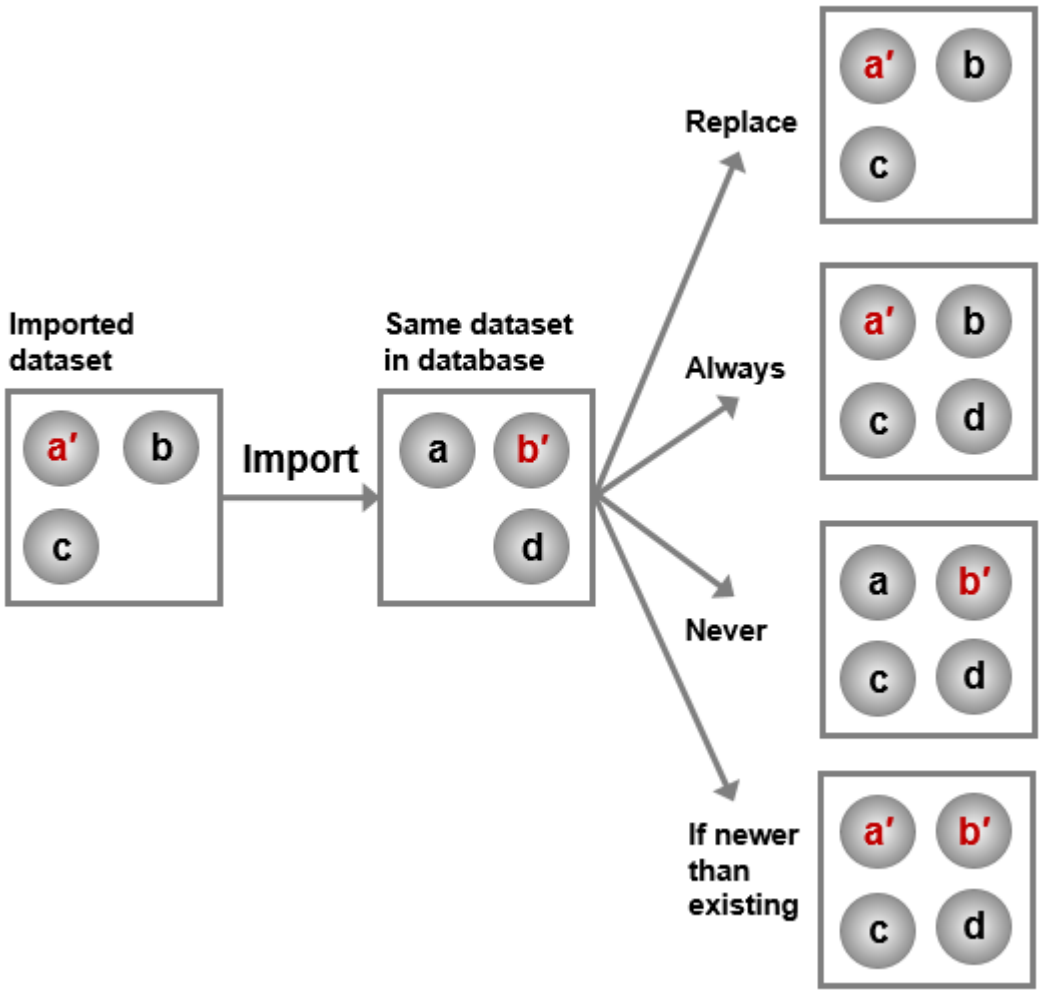
Whether an entity or document is already in the IUCLID database is determined from its *Universal Unique Identifier (UUID)* that is stored in the database. On import, UUIDs are read from the file being imported. The name of the file does not matter. The import compares the UUIDs to what is already in the database, and then acts according to one of the four options listed below.

Overwriting is not allowed for IUCLID 6 Dossiers. An attempt to overwrite a *Dossier*, results in an error message.

1. *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 *Last modification date* is more recent than that in the IUCLID database. The *Last modification date* can be viewed by hovering the cursor over the name of the entity or document that is shown in *Advanced import*. For an example, see section *1.7.1.3 Import to* dataset.
2. *Never*: An entity or document is not imported if one with the same UUID exists within the IUCLID database.
3. *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.
4. *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 behaviours for the options above are expressed graphically in the figure below.

Figure 13: Import in to IUCLID 6 where datasets and/or documents already exist in the database



Legend for Figure 13:

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.

1.7.1.2. Default group access - Import

If Instance Based Security (IBS) is enabled in IUCLID 6, a field is shown called *Default group access*. For more information see sections *24.2.7 Default group access for a User* and *24.4 Ownership and Sharing - 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.

1.7.1.3. Import to dataset – Advanced settings for import

This functionality is available on the *Dashboard* from a link within *Import*. It allows individual entities and documents to be excluded from an import.

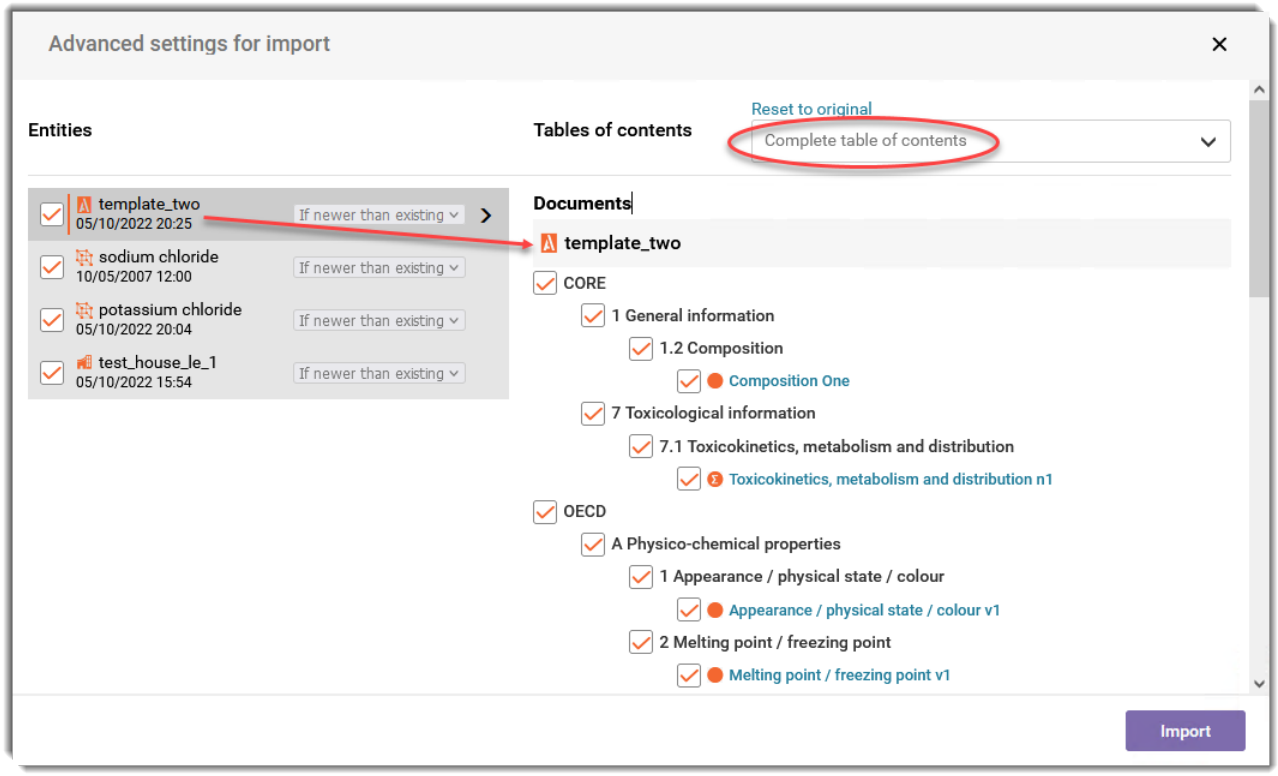
This does not apply to *Dossiers*, and datasets of type *Substance*, *Mixture*, *Article* and *Category*, for which document selection is not allowed. On import, by default, a dataset of one of those types is converted into a *Dossier*, which can then be converted into a dataset as explained in section *6.4 Extract to Dataset*.

Entities are listed on the left, documents on the right. Selecting an entity shows the documents it contains, organised according to the working context shown above the documents. On opening an archive, the working context is *Complete table of contents*.

In *Advanced import*, only one file can be imported at a time, so only one file can be selected for import, and it cannot be a zip archive.

See the example below for the import of a *Template* dataset named *template_two*.

Figure 14: Advanced import: View on opening an i6z file to import

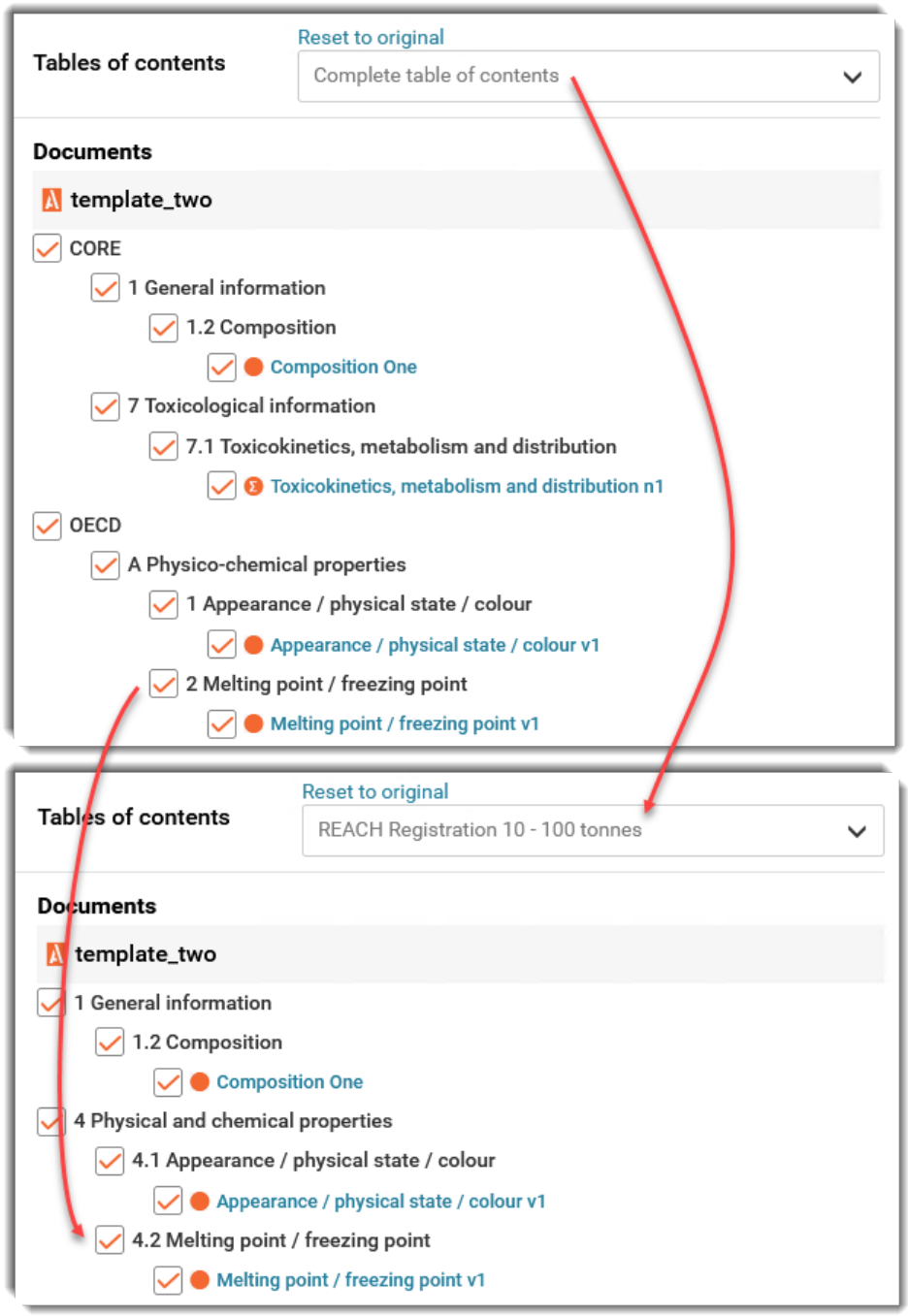


On opening an archive, the working context is set to *Complete table of contents*. This cannot be changed for datasets of type *Substance*, *Mixture*, *Article* and *Category* and *Dossier*.

Entities are listed on the left, documents on the right. Selecting an entity shows the documents it contains, organised according to the working context shown above the documents.

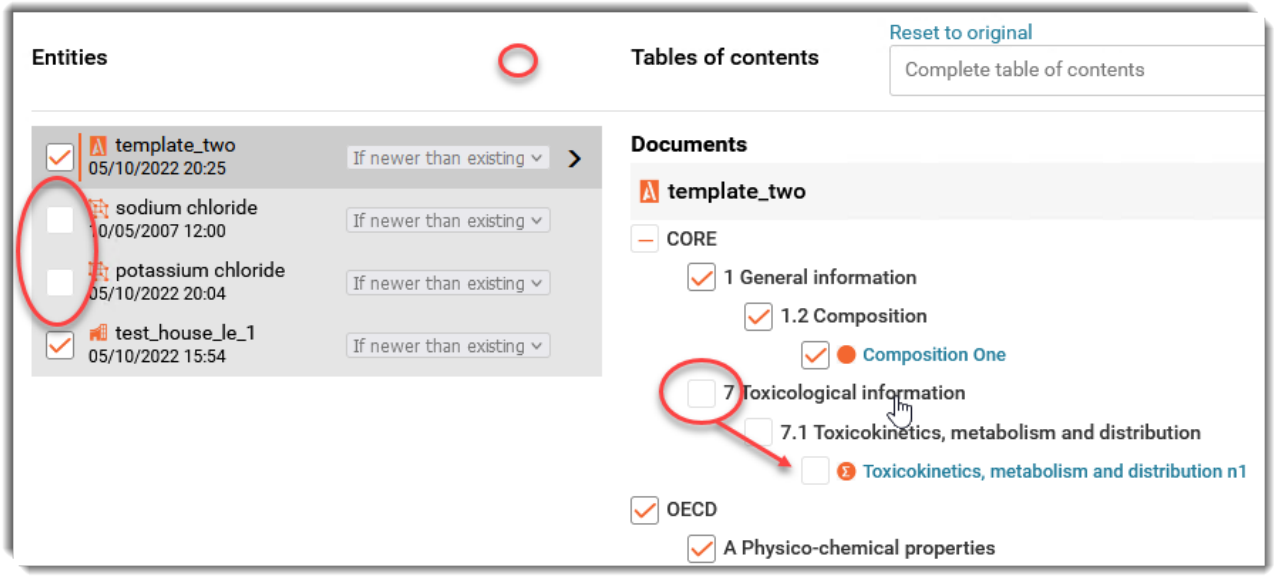
The effect of changing the working context is illustrated in an example below. Note the change in numbering and names of sections, but the name of the document does not change.

Figure 15: Advanced import: Change the working context



Unticking a box for an entity excludes the entity and its documents from the import. Individual entities, documents and sections of documents can be excluded by unticking their boxes.

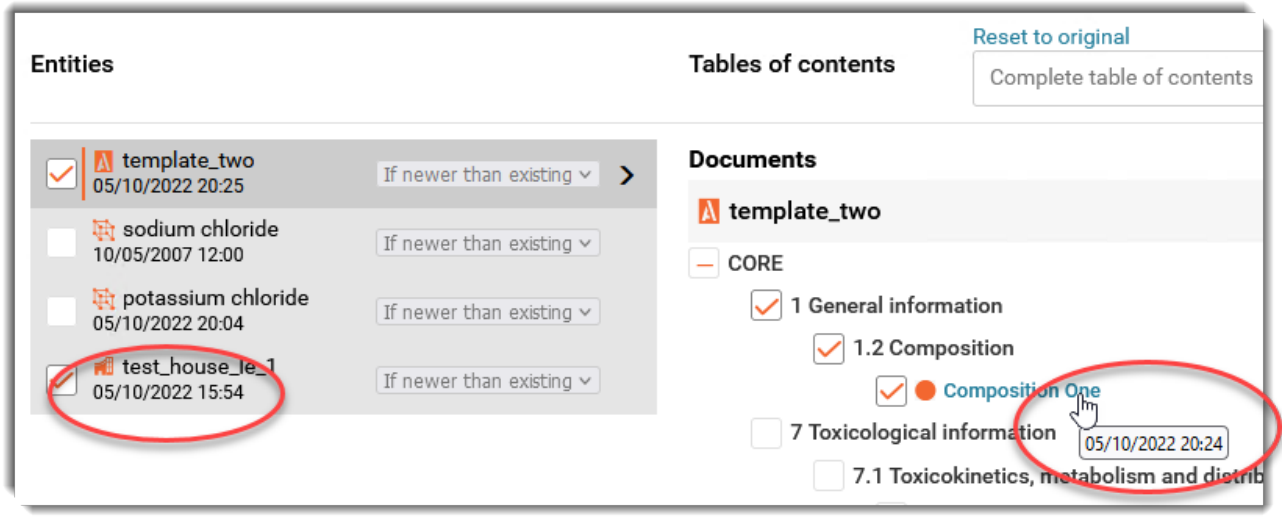
Figure 16: Advanced import: Deselect boxes to remove from the import



The overwrite mode can be set per entity, whereby it also applies to the documents in the entity. The modes are explained in section *1.7.1.1*

Overwrite settings - Import. The default value is *if newer than existing*. This compares the values of *Last modification date* in the file with those in the IUCLID database. The value of *Last modification date* for an entity is shown under its name. To see the value for a document, hover the cursor over its name. An example is given below.

Figure 17: View the Last modification date



1.7.1.4. Bulk import

To import more than one entity from i6z files at once, place the i6z files in a zip archive, and then import the archive. A zip archive created using the bulk export feature of IUCLID can be imported. The number of files that can be imported at once using this method may be limited by system performance. If you have difficulty importing large numbers of documents or entities, try doing the

import in smaller batches of a few hundred. If that is not practical, contact the IUCLID helpdesk for advice. Whilst a bulk import is running, do not logout of IUCLID 6 Server, because this stops the import.

1.7.2. Breadcrumbs

The term *Breadcrumbs* refers to the statement of the path to a page in the interface that is shown in the application bar. Each level in the page hierarchy is a link delimited by the greater than character >. The links provide a convenient way to navigate upwards in the hierarchy. In the example shown below, a link in the breadcrumbs is being clicked to jump from a *Substance dataset* to the list of all the *Substance datasets*.

Figure 18: Navigation using breadcrumbs

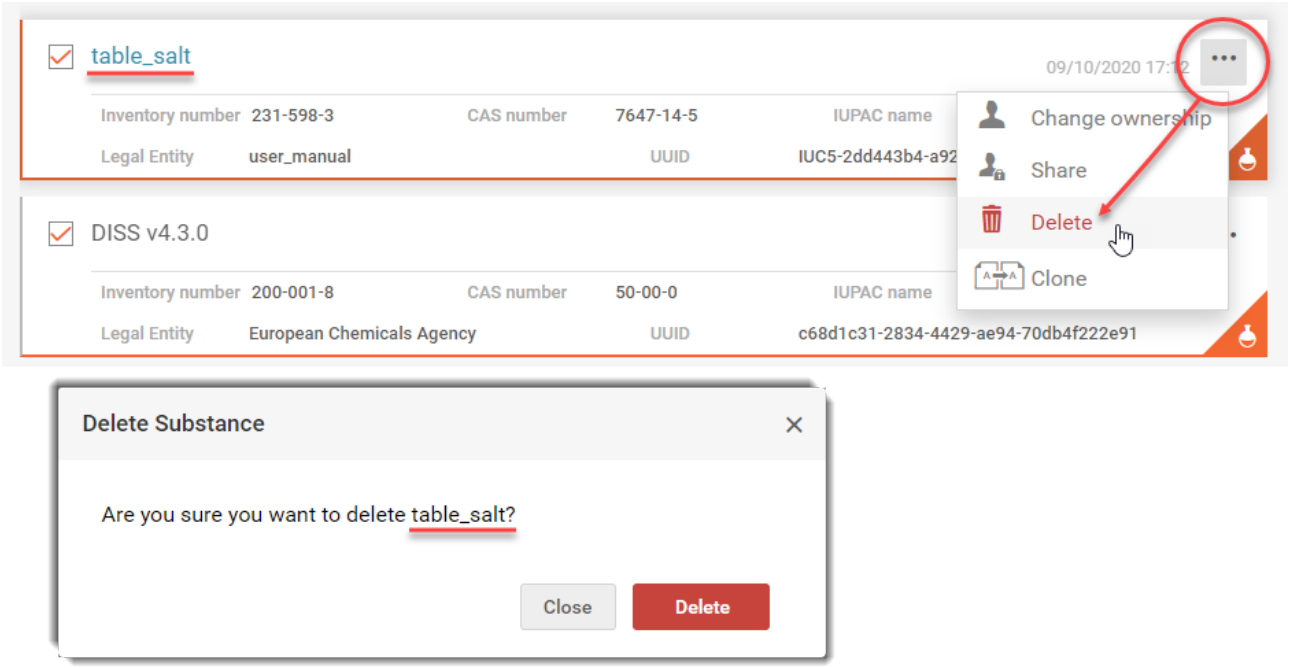
1.7.3. Individual versus bulk actions on entities

Each entry on a list page of entities has a tick box on the left, and a menu button ··· on the right. The tick box is used to include an entity in a bulk action. The menu is used to perform a task on only that entity. The bulk actions are *Export* and *Delete*, as described in later sections.

1.7.4. Deleting entities

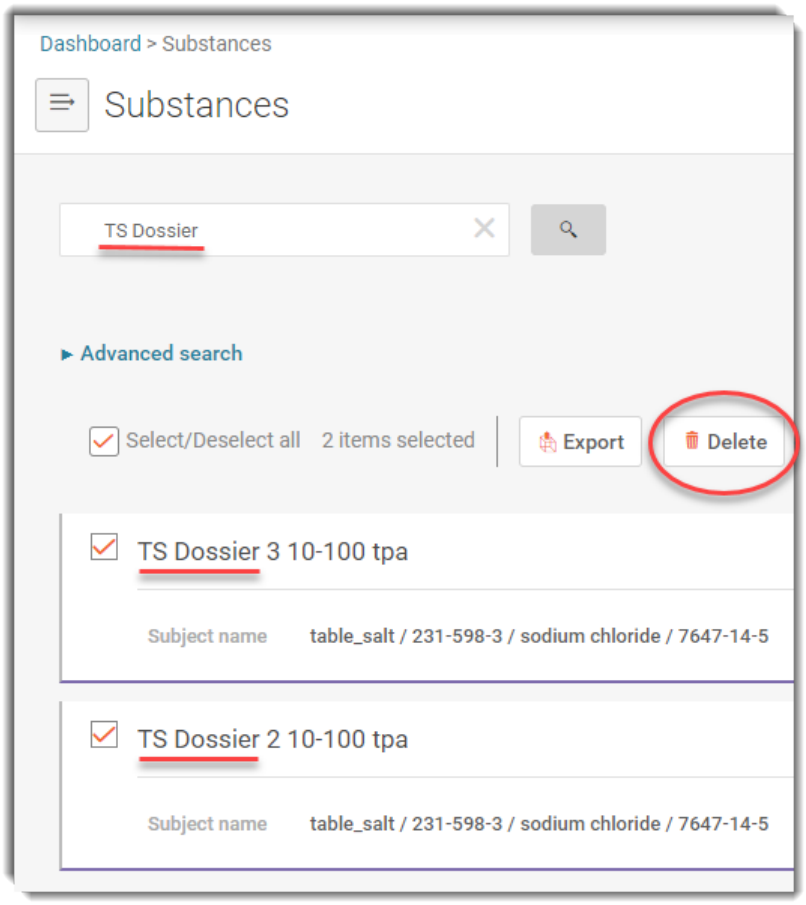
To delete a single entity from a list on entities, right-click on the menu button ··· at the upper right of its list entry, and then select *Delete*. An example is shown below.

Figure 19: Delete a single entity in a list of entities



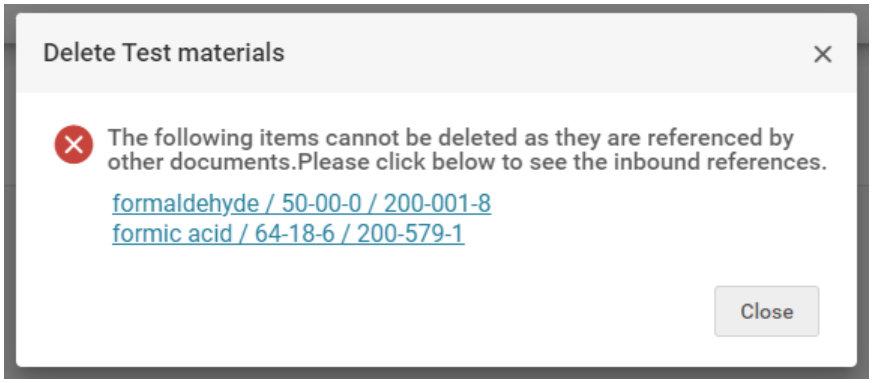
To delete more than one entity at once, select the entities by ticking their boxes on the left, and then click on the *Delete* button situated at the top of the listing. Entities can be selected individually, or using the feature *Select/Deselect all*, which selects all the records currently visible. If search criteria are applied, *Select/Deselect all* selects only the entities that match the search criteria. *Delete* works per page, thus the maximum number of entities that can be deleted in a single action is 100. An example is shown below.

Figure 20: Delete entities in bulk



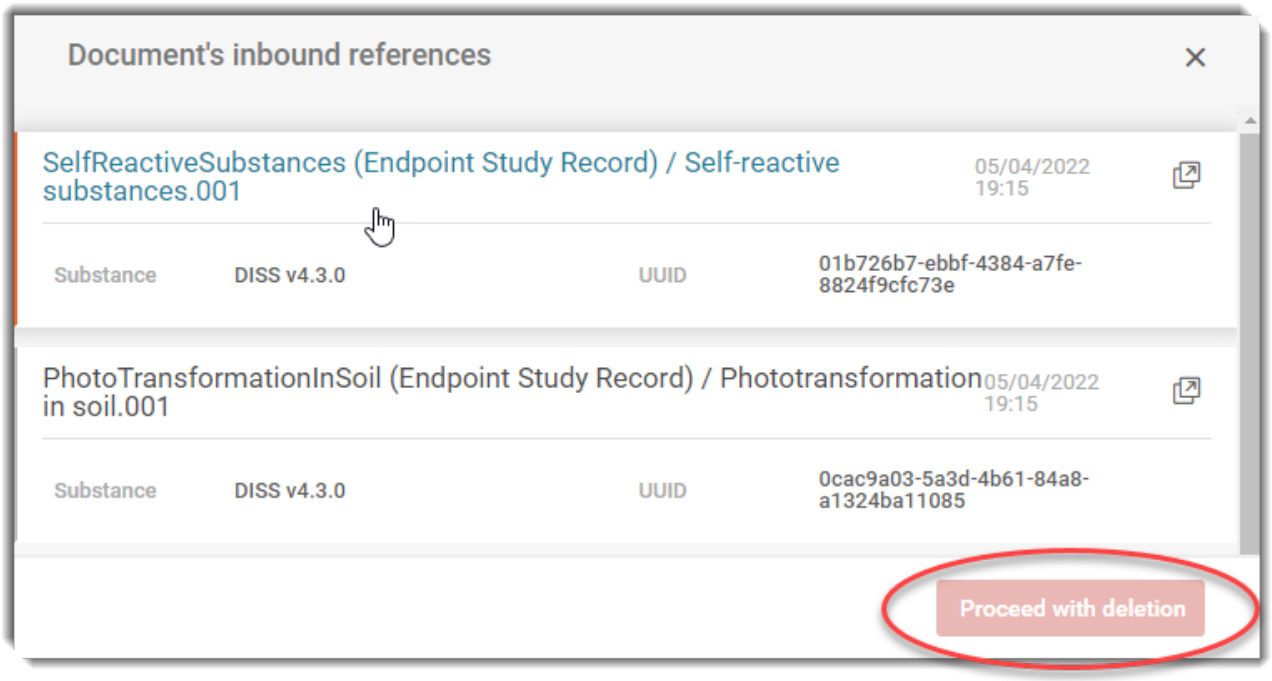
If an entity has an inbound reference, it cannot be deleted because the document or entity where the reference is defined would then have a link that points to nothing. The link would be broken. Such links can be analysed before deletion using the feature *Inbound references* described in section 1.8. However, if an attempt is made to delete an entity that has an inbound reference, the request to delete it invokes the *Inbound references* functionality. A link is provided for each entity being deleted, which opens a list of the referring documents for that entity, as shown below.

Figure 21: Delete multiple entities that have inbound references



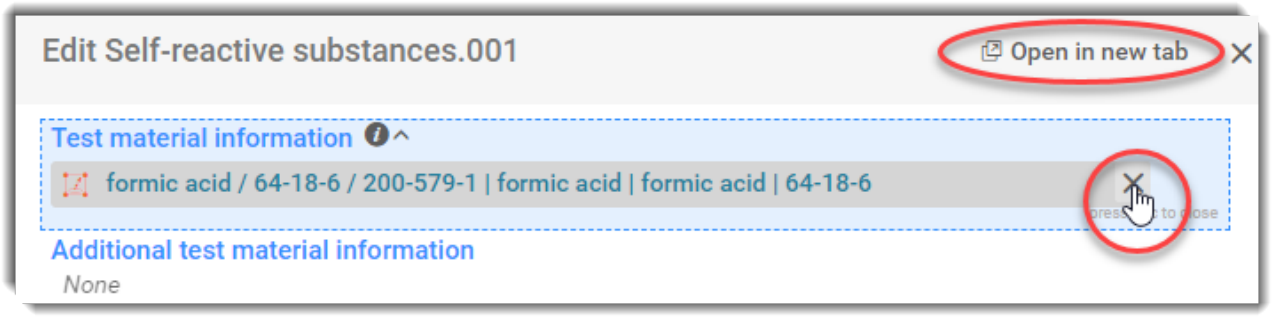
On clicking a link shown above, the inbound references are shown in a window with the delete button *Proceed with deletion* greyed out, as shown in the example below for the deletion of a *Test material* that is referred to by a *Substance*.

Figure 22: Inbound references preventing deletion



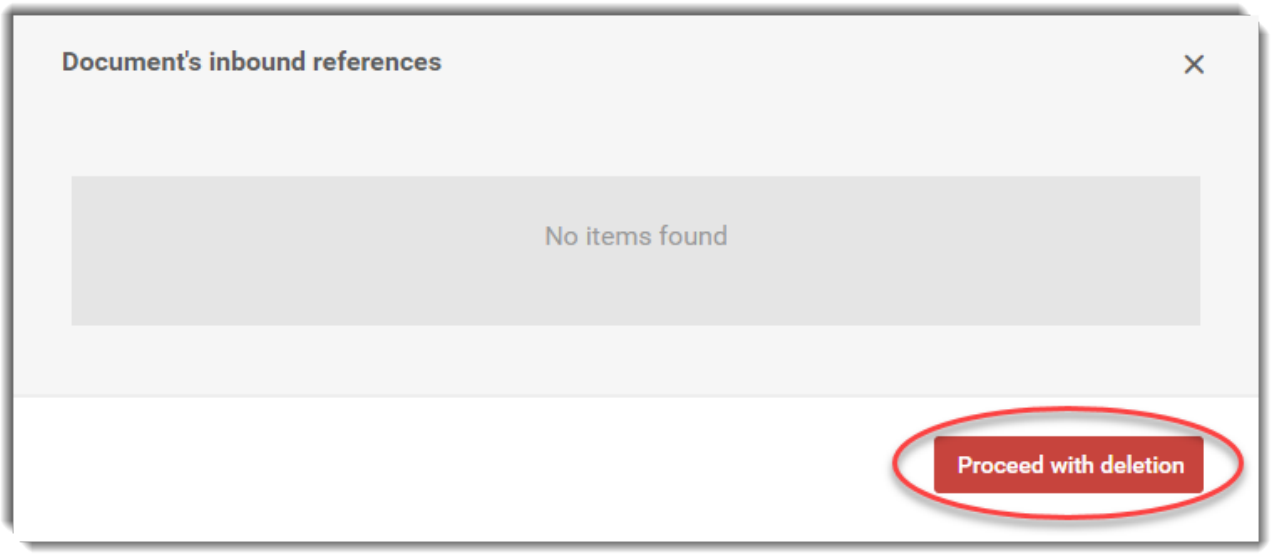
The referring entity or document can be opened for editing from the link provided. This can be done in a new tab, which can help to keep track of what you are doing if there are multiple references to remove. See below, in which a reference to the *Test material* is being deleted.

Figure 23: An inbound reference being deleted



When all the inbound references have been deleted, the button *Proceed with deletion* becomes active.

Figure 24: Proceed with deletion is active



1.7.5. Export CSV

Export CSV outputs a file that contains the information that is provided in the listing of entities. Data are output for all of the entities of that type. The tick boxes and pagination are ignored, but the order of the listing is preserved in the output. The format of the file is comma separated text. If a value contains a comma, the whole value is placed in double quotes, as shown in the example below. The file can be opened in Windows using Microsoft Excel. If the system delimiter is set to comma, the data are automatically arranged in columns, and any double quotes that were added to escape a comma are not shown.

Table 2: Export CSV – the columns and an example

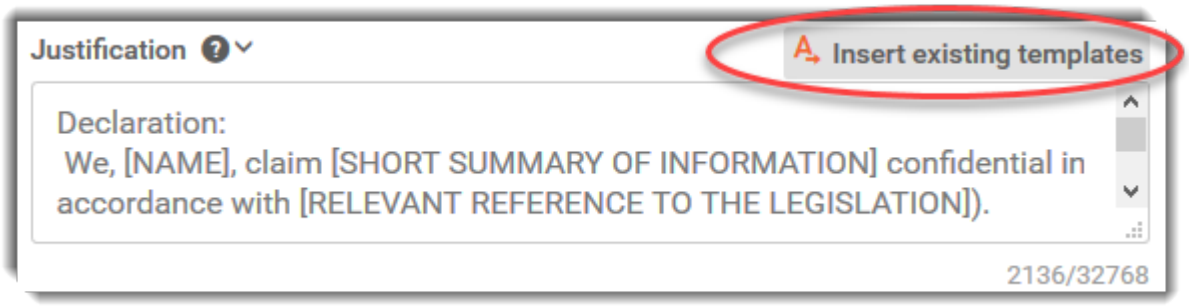
Header	Example value in the CSV file
Substance name	"1,2-dichloroethane"
Inventory number	203-458-1
CAS number	107-06-2
IUPAC name	
Legal Entity	Predefined Legal entity
UUID	3b8ab9b2-3b63-4fb0-8c70-f5cfaf021e51
Last modified date/time	2021-08-20T14:35:28.102Z
IUCLID entity URL	localhost:8080/iuclid6-web/?key=3b8ab9b2-3b63-4fb0-8c70-f5cfaf021e51/0

1.7.6. 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 text field. It provides a model text, which must then be edited to fit in with the circumstances of the user, in that context. Text that *must* be changed, is surrounded in square brackets [like this].

To open a free-text template, click on the icon that shows the letter A with an arrow at its lower right, . To copy the text from the template to the field, click on the button labelled *Insert…* . Next, edit the text in square brackets, as required. An example is shown below.

Figure 25: Free-text template



1.7.7. Flag

Some fields, items, and documents can be labelled with flags to indicate that the data they contain is confidential in some way, and/or that it relates to a particular regulatory programme. Flags allow the data to be excluded when creating a dossier, exporting data, or printing data. There are two types of flags, each with its own icon, as described in the table below:

Table 3: The icons for the states of a flag

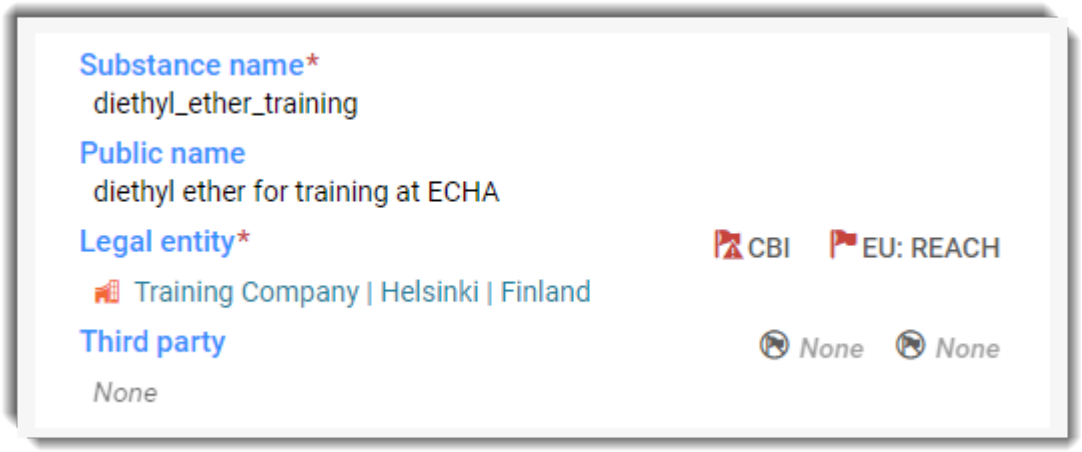
Icon	State
	The flag is not set.
	A flag is set that involves confidentiality.
	A flag is set for a regulatory programme.

Flags are shown as a pair, with the flag for confidentiality on the left, and the flag for regulatory programme on the right.

The flag for a regulatory programme is followed by a code for that programme, which consists of two abbreviations separated by a colon. The first abbreviation denotes the origin of the programme, whilst the second denotes the programme itself: for example, **EU: CLP**. More than one programme can be set per flag.

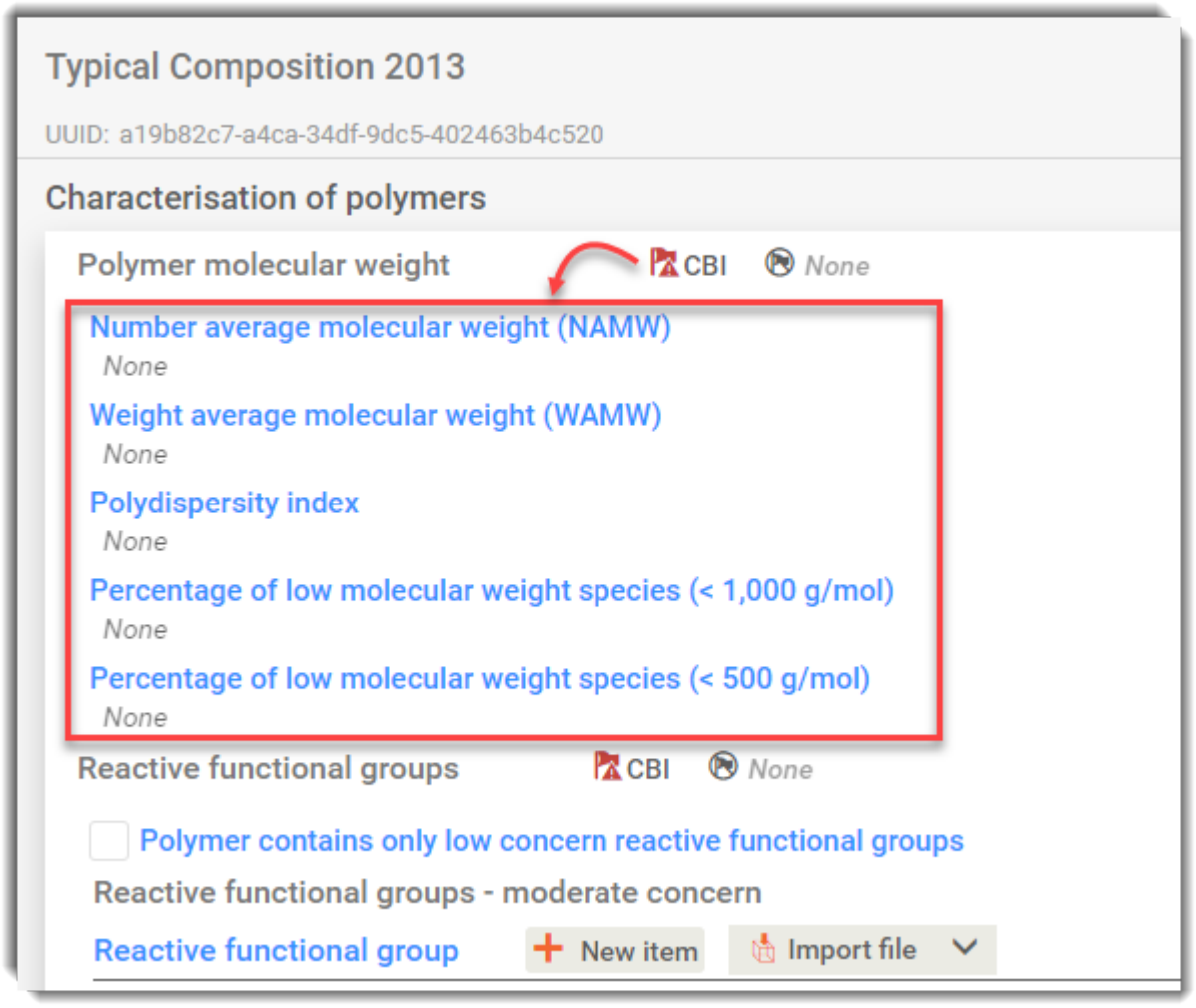
If a field can have a flag set, flag icons are shown to the right of the field label, as shown in the example below for *Legal entity*.

Figure 26: Flags applied individually to fields



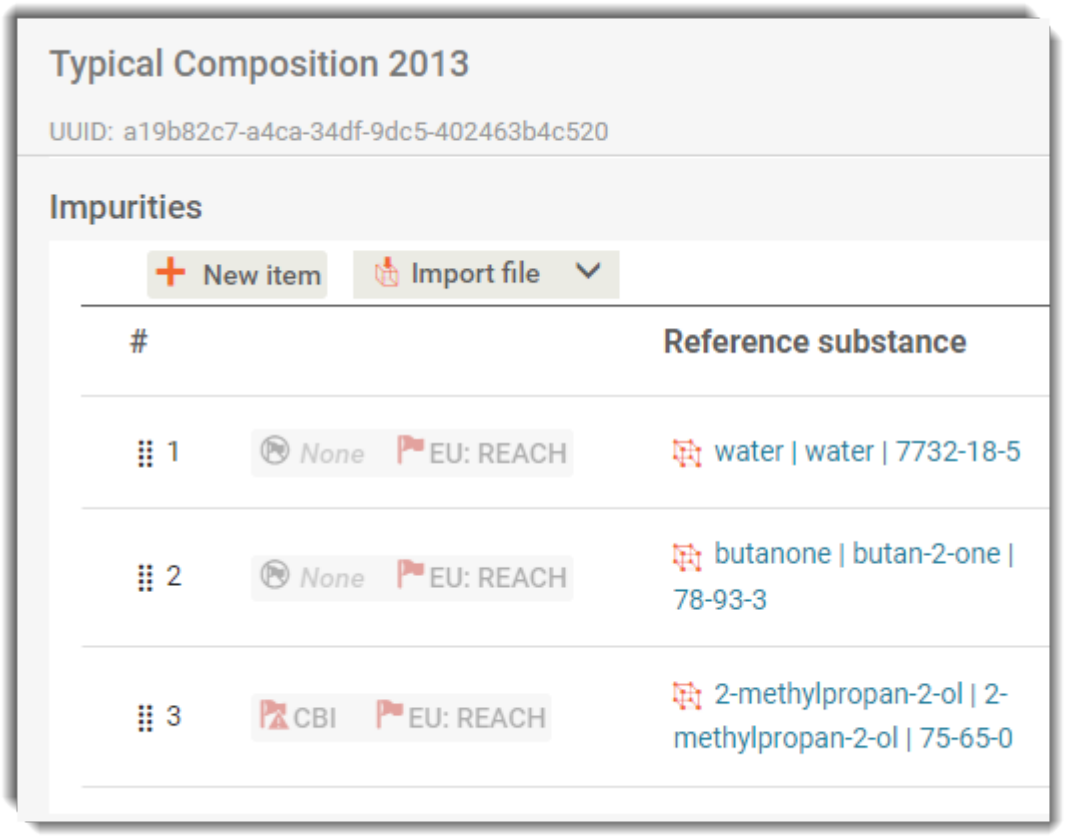
A flag can be applied to all the fields in a section at the same time, whereby the flag is to the right of the section header. as shown below for *Polymer molecular weight*.

Figure 27: Flags applied to all the fields in a section



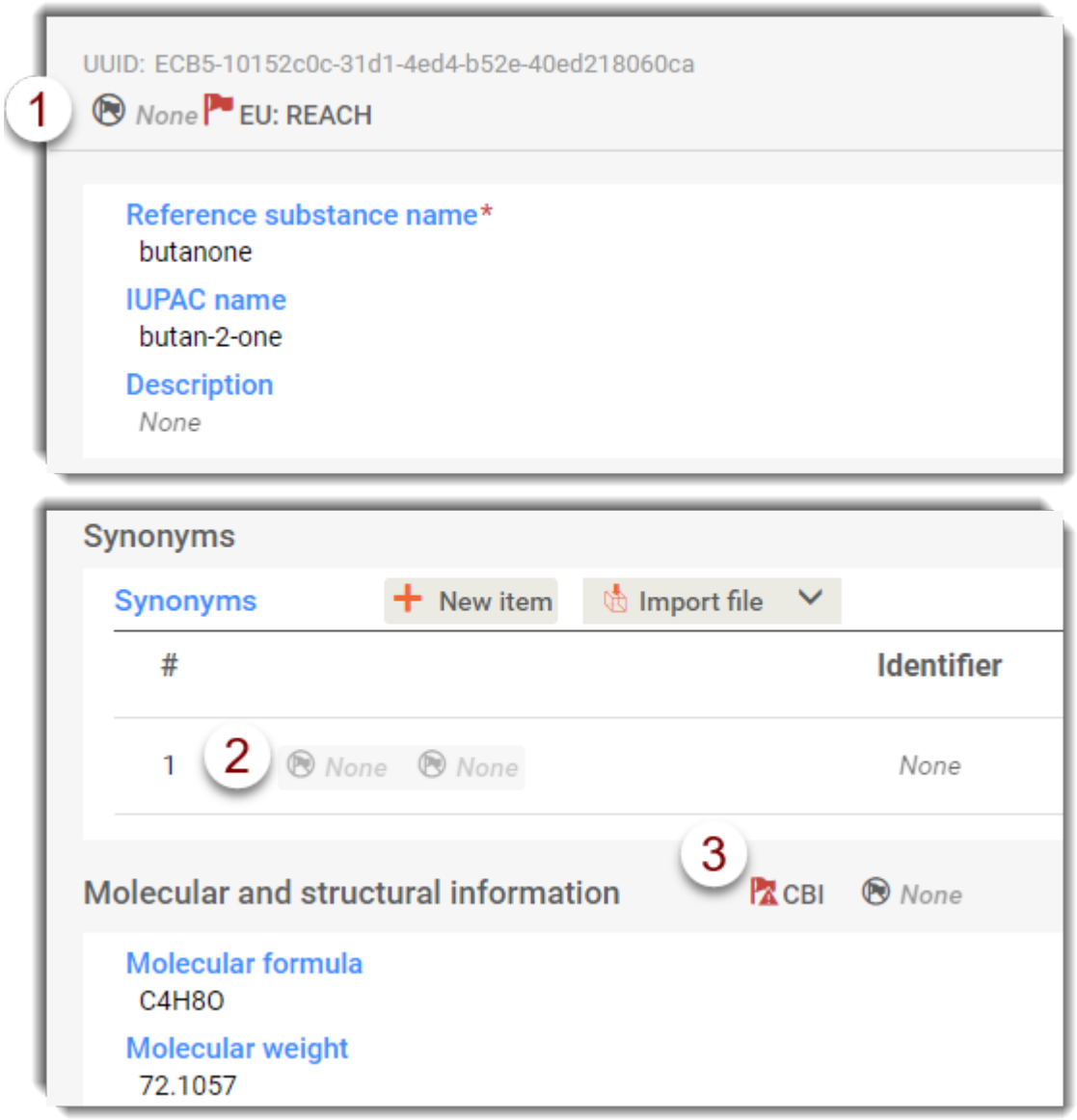
If an item is in a table, the flags are located in a dedicated column, as shown in the example below for *Impurities*.

Figure 28: Flags applied individually to items in a table



If flags can be set for a whole document, the flag icons are shown above the name of the document. An example is shown below for a *Reference substance*.

Figure 29: The extent of application of flags

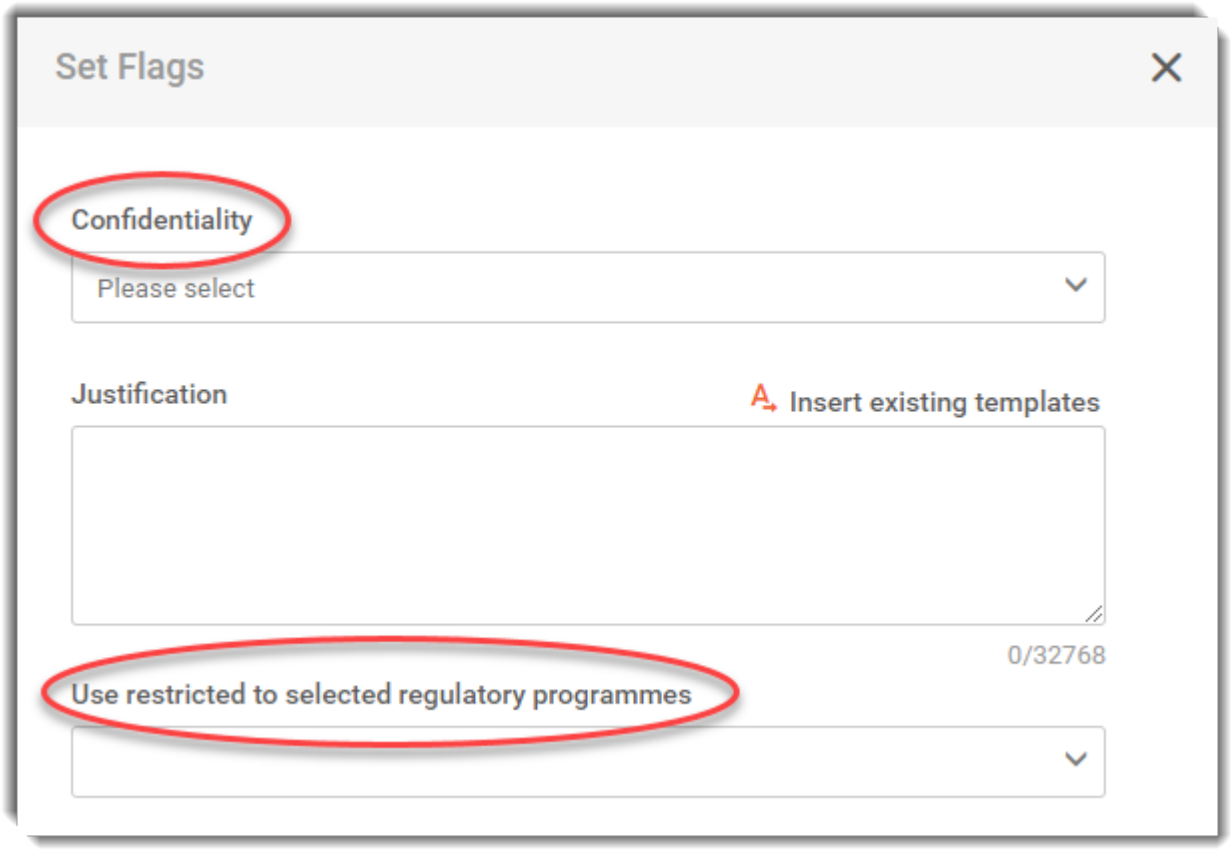


Legend for Figure 29

1. The flag (1) EU:REACH applies to the whole document, in this case, a *Reference substance*;
2. No flag is set for row 1 in the list. The flag set in (1) *EU:REACH* applies;
3. The flag *CBI* applies to only the data is this section. The flag set in (1) *EU:REACH* also applies.

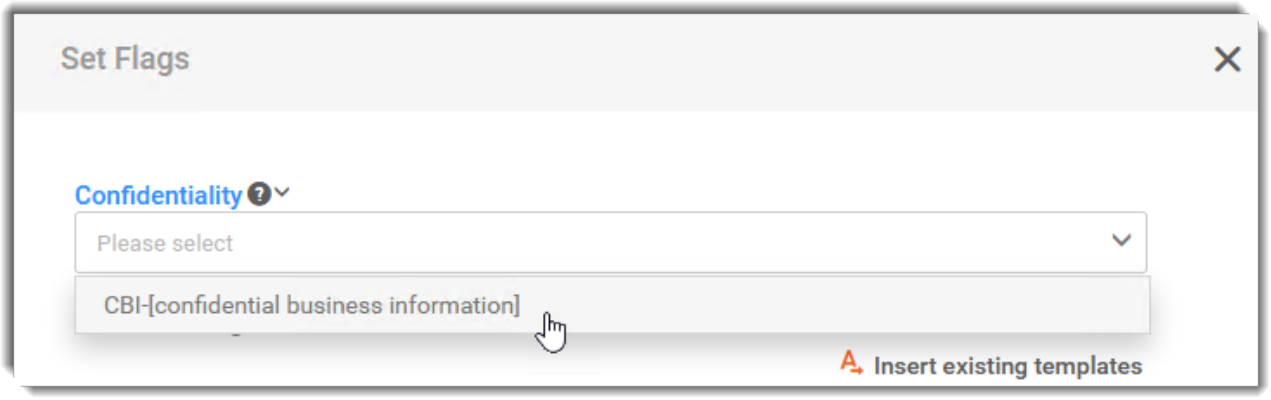
When a document is created, no flags are set. To edit a flag, click on either of the flag icons in its pair. The flag for confidentiality, and the flag for regulatory programme, are edited from the same page, as shown in the figure below:

Figure 30: Setting flags for confidentiality, and/or regulatory programme



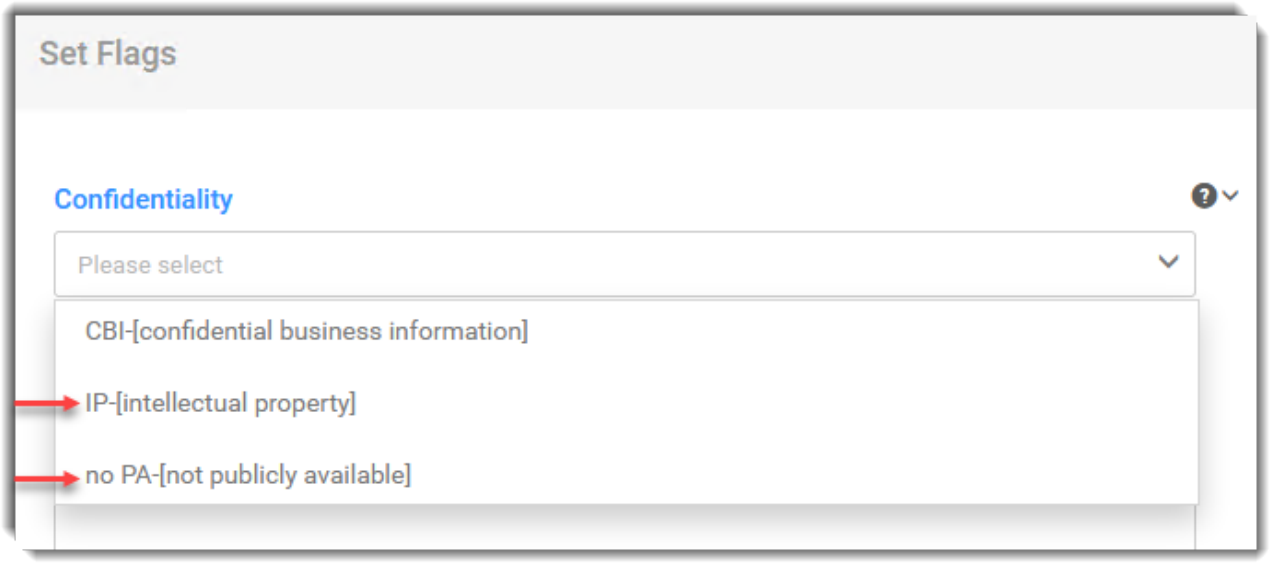
For confidentiality, select the type and then enter a justification. To ensure you select the correct type, read the help under the question mark icon. The type, *Confidential Business Information (CBI)* is being selected in the example shown below.

Figure 31: Setting a confidentiality flag



In this version of IUCLID the only option is CBI, but prior to IUCLID 6 version 6.0.0, there were two other options, as shown below.

Figure 32: Types of flags that are obsolete

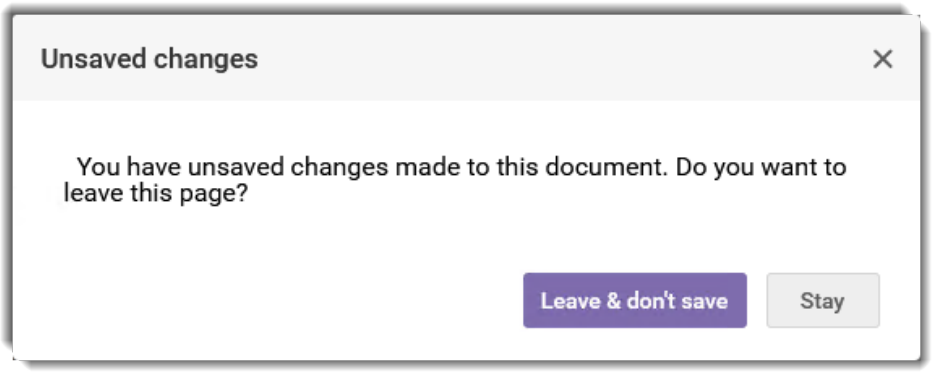


The options *IP-[intellectual property]* and *no PA-[not publicly available]* are obsolete. A flag set to either of those types, and then imported into the current version of IUCLID, is still visible, but it is read-only. An example of how obsolete flags appear is given below.

Figure 33: An obsolete flag that was set in an earlier version of IUCLID

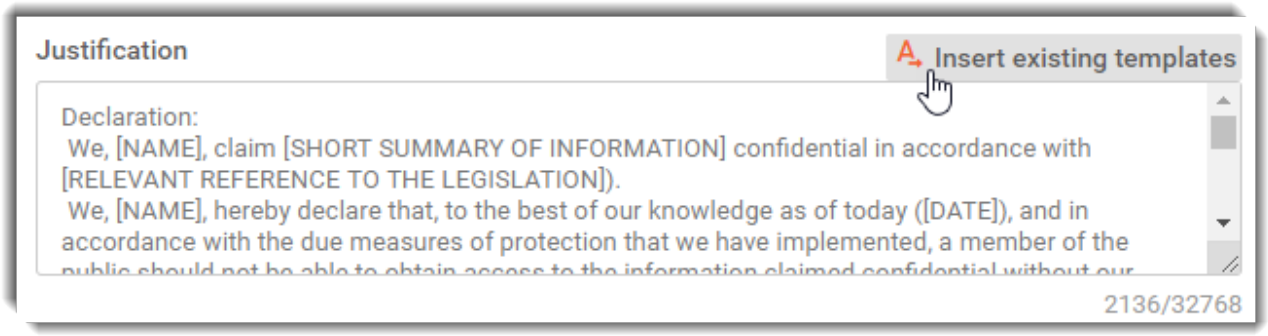
Note that selecting CBI from the menu, causes the obsolete value of the flag to disappear from the menu. If you do not want to change the value to CBI, close the window, navigate away from the documents without clicking on *Save*, and then select the option to not save the changes, as indicated below in the purple button.

Figure 34: Choose whether to save changes



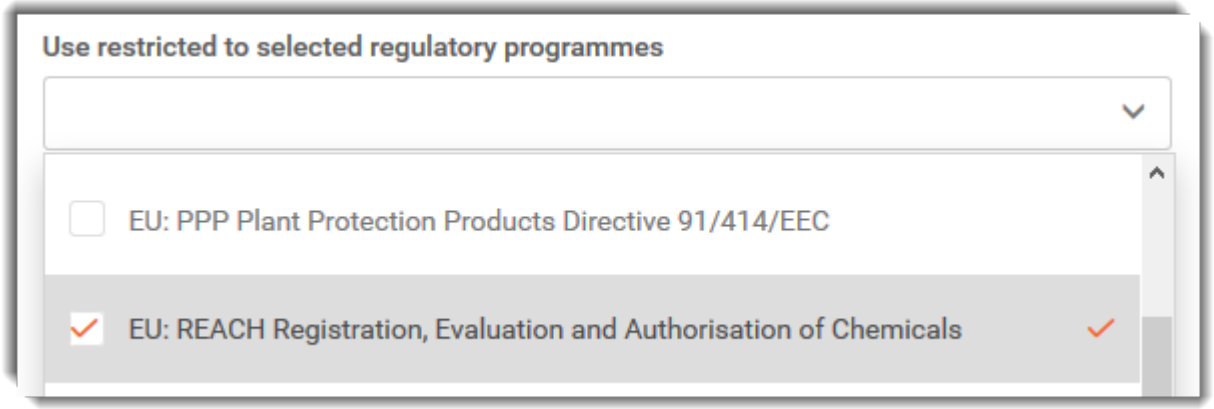
When setting a flag, if a justification of the confidentiality is required, enter it into the field *Justification*. The field has a free-text template, which contains suggestions as to what to enter. To open the free-text template, click on the icon that shows the letter A with an arrow at the bottom right, . To copy the text from the template to the field, click on the button labelled *Insert…* . Next, edit the text in square brackets, as required. An example is shown below.

Figure 35: Free-text template for the justification of a confidentiality claim



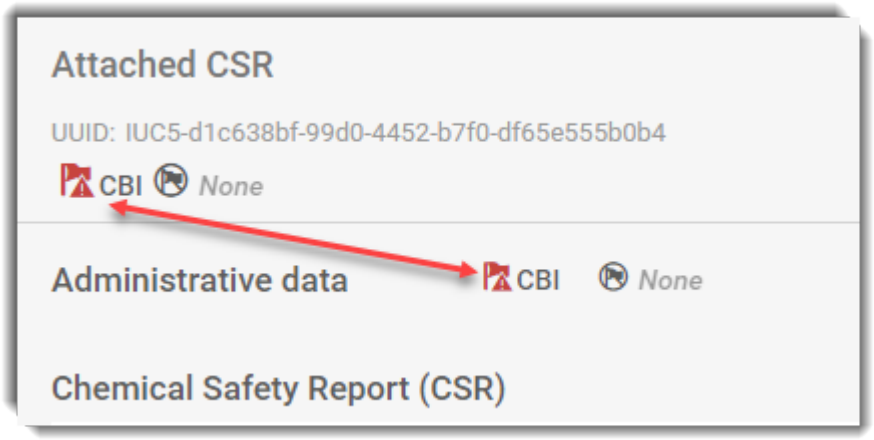
To set relevance to a particular programme or programmes, tick the box or boxes as required. In the example shown below REACH is selected.

Figure 36: Flag for relevance to a regulatory programme or programmes



Note that in many sections, setting a flag for *Administrative data* is taken as being applicable to the whole document. Where that is the case, the flag values are automatically propagated to those for the whole document, which are indicated above its name. One such example is for *Chemical Safety Report*.

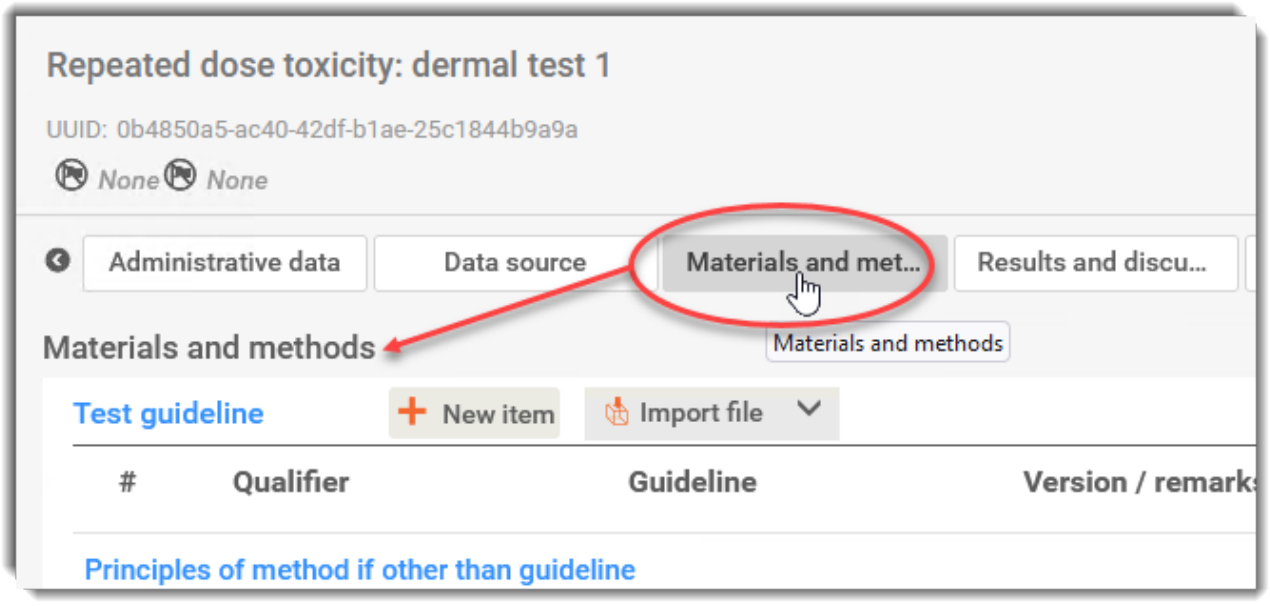
Figure 37: An example where the flags for Administrative data are set for the whole document automatically



1.7.8. Shortcuts to sections in a document

In the data area at the top of a document there is a set of buttons that are shortcuts to the sections. In the example below, the section *Materials and methods* has been brought to the top of the page by clicking on its button.

Figure 38: Shortcuts to sections in a document

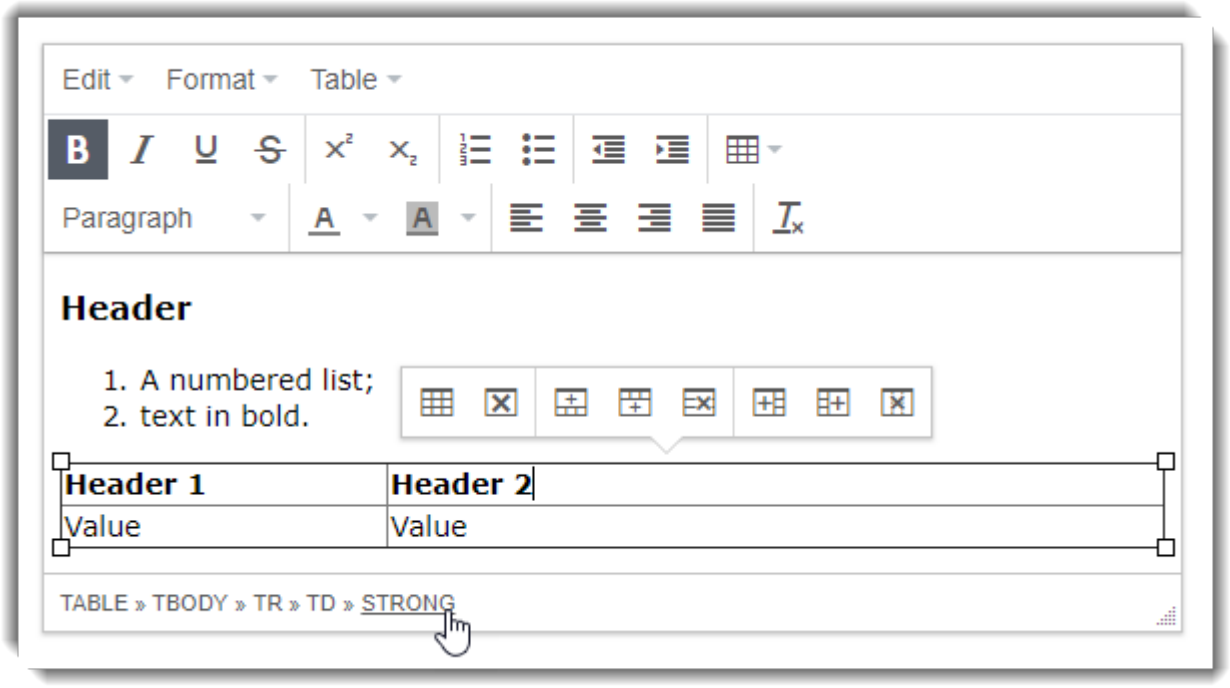


1.7.9. Rich text input

Some text fields allow text to be entered in rich text format, for example the executive summary in the results and discussion of endpoint study records. This allows for various types of formatting,

such as tables. A full description of rich text is out of the scope of this document, but see the example below in which a table has been created and is being edited.

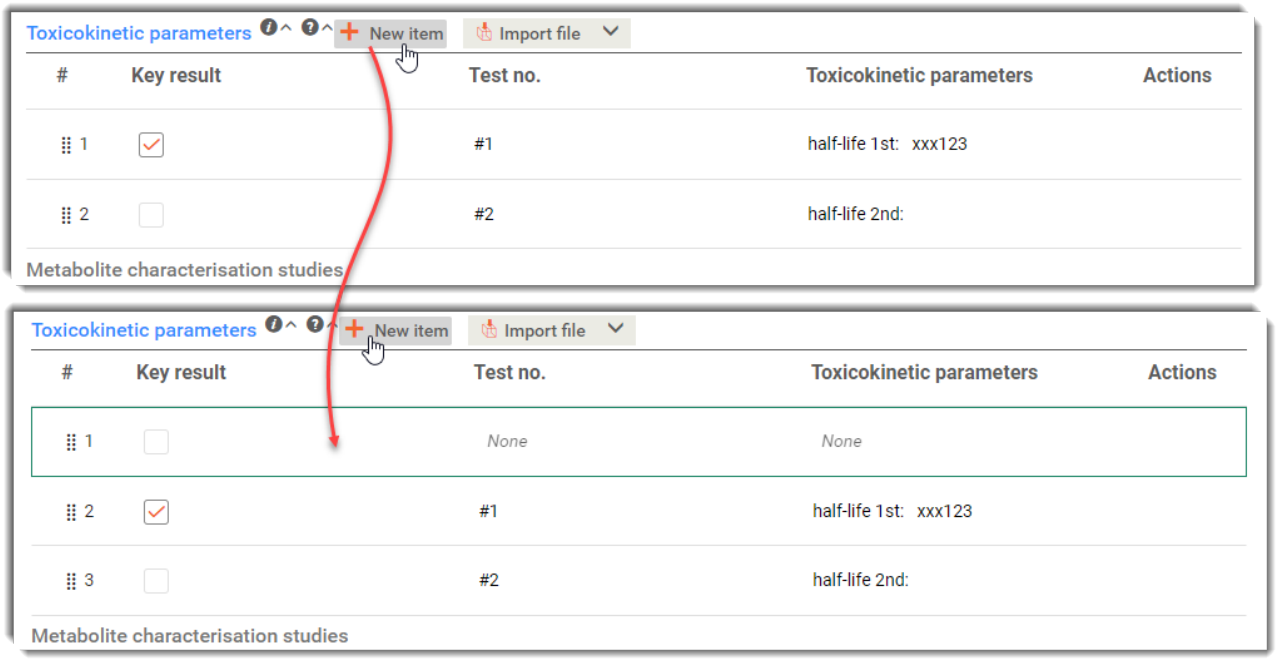
Figure 39: A rich text field



1.7.10. Tables

Some fields display data in tables that can have rows added and removed. The fields in the columns are defined by the IUCLID format, and therefore cannot be changed. An example is shown below, in which a row is being added:

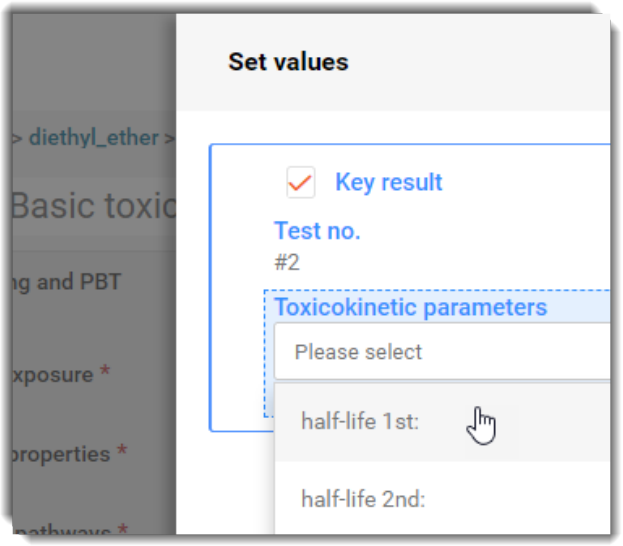
Figure 40: Add a row to a table



A new row contains empty fields. Empty fields are indicated by the word *None*, in pale grey italic text, or an empty check box. The value of such a field is not literally “None”.

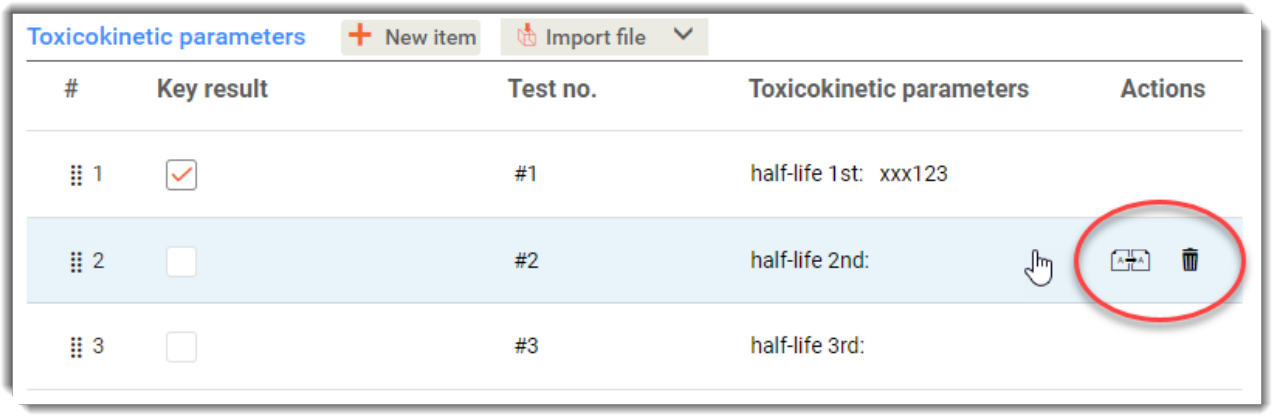
To edit any or all the fields in a row, click anywhere inside the row. The fields for that row are shown in a data entry window, as shown below.

Figure 41: Editing all the values in a table row



To delete or clone a row in the table, hover over the row and then click on the corresponding icon in the column *Action*.

Figure 42: Clone or delete a row in a table



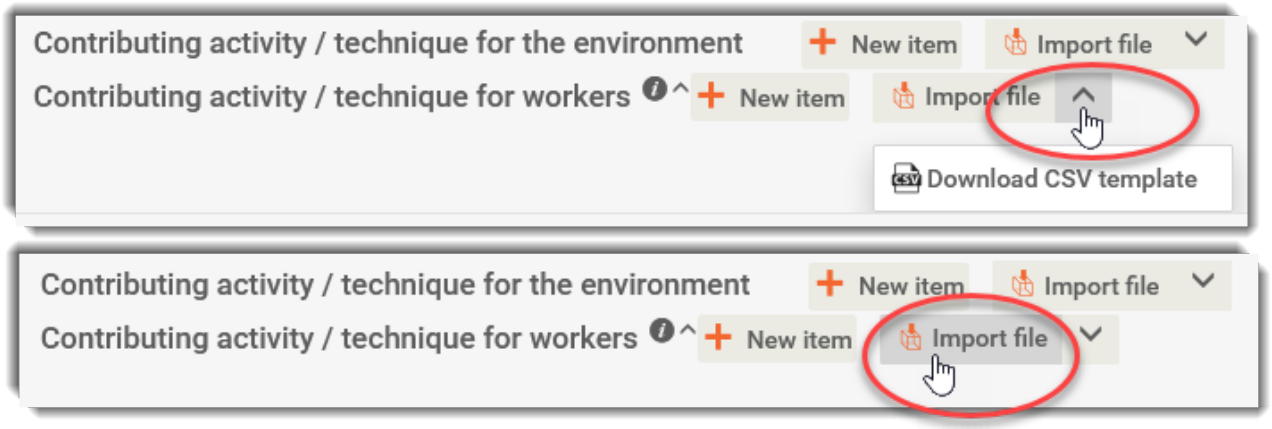
To record the new values in the view of the table, either click on the *Close* button at the bottom right, or click anywhere in the grey area to the left. When you have finished editing the table, remember to click on the orange button at the bottom right labelled *Save*. Changes to a table are written to the database only after clicking on *Save*.

1.7.10.1. Import data into a table from a text file

Some data can be imported into a table from a text file. This works for text values, phrases in single and multiple selection picklists, ranges, and cross-references within IUCLID. If a table contains an attachment or any value that cannot be imported, the import process ignores the fields it cannot populate, leaving the user to do it manually after import.

If you already have access to a file that can be imported, simply click on *Import file* and then select the file. New rows appear at the top of the table. If you are not sure of the format of the file, and/or you need to create a file, click on *Download CSV template*, as shown below.

Figure 43: Import file - Download CSV template



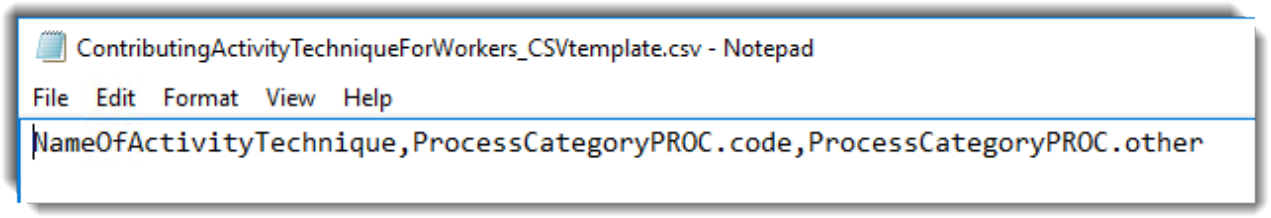
The import file is a table in text format, with each column separated by a comma (CSV). If a field can contain more than one phrase, the separator between the values is a semicolon ";". If the multiple values can have fields for *other:* or *Remarks* associated with them, the values can be added in dedicated columns which are also delimited by semicolon. The column names are terminated by *.other* and *.remarks*. An example is given in the figures below.

Text values can be surrounded by double quotes. Single quotes are treated literally, so placing them around a phrase will give an error. The template consists of the column headers in a single row of text. One header corresponds to one field. If a value cannot be imported into a field, the field has no corresponding column, and therefore no header. A template is specific to that table, which is reflected in its default name which begins with the last part of the IUCLID path of the table. For the example shown above, the file is named:

`ContributingActivityTechniqueForWorkers_CSVtemplate.csv`.

Data can be entered into the import file using any text editor or spreadsheet application. An example is shown below where the template has been opened in Notepad.

Figure 44: Template for import into a table

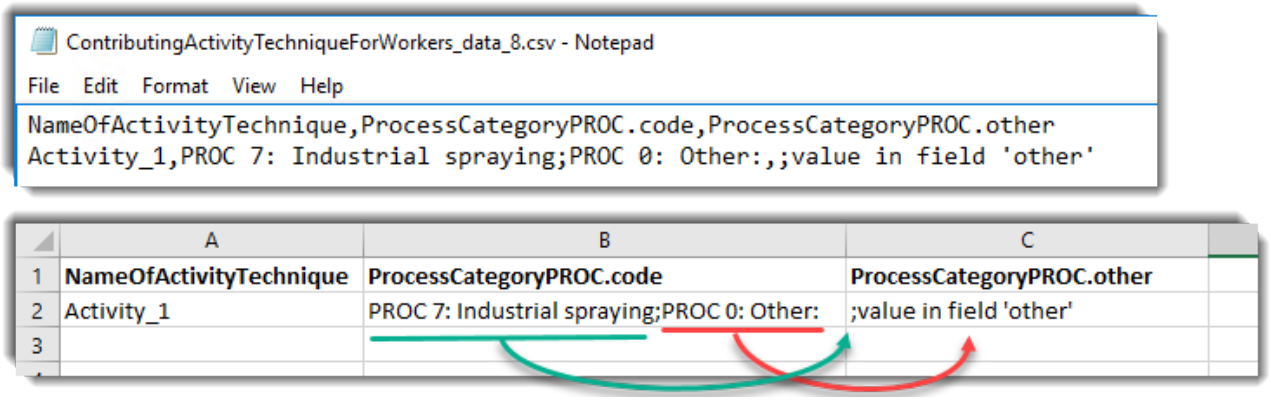


If a header ends in ".*code*" the value of the column must be either the value of a phrase that is valid for the field, or its code. Phrases can be copied from the IUCLID user interface, therefore using codes should not be necessary. Codes of phrase groups, and phrases, are sometimes referred to in error messages. For reference purposes, be aware that the codes of phrase groups and phrases are defined in the IUCLID format, which can be downloaded without charge from the IUCLID website. The codes are in the downloadable archive of the format, in a file named:

`IUCLID6_6_all_fields_<version>_<date>.xlsx`

For the example template above, some values have been added and the data are shown both in Notepad and Excel.

Figure 45: Example of the same CSV data file shown in Notepad and Excel

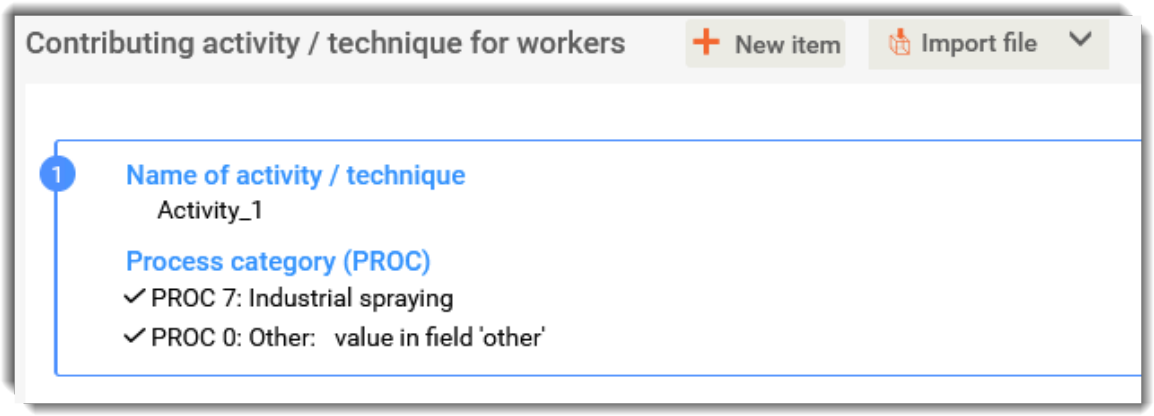


Note the headers are the same as those in the template file. The second column is for a field that can contain more than one phrase. In this example, two phrases are separated by a semicolon and Excel has been set to recognise comma as the column delimiter, so it is not shown. The third

column is for values of *other:*. The phrase marked in green cannot have a value for *other:*, so the value in column 3 is left blank. The phrase marked in red can have a value for other: , which in this example has the value, *value in field 'other'*.

After importing the file indicated above, the view in the IUCLID interface is shown below.

Figure 46: Example of data that has been imported from a file into a table



The imported data is at the top of the table. Note how the values have been mapped from the import file and where they have been placed.

Data values that are expressed as ranges can be imported. See the specific template for the fields. For example, for *BoilingPoint* the fields for the units are: *BoilingPoint.code*, *Pressure.code* and *DecompositionTemp.code*. The data must conform to the same rules that apply when entering the data directly into the user interface.

To tick a box that has a label beginning with *Key*, for example *Key result*, use the value *true*.

Figure 47: Entering boiling point data for a Key result with the data shown in Excel

	A	B	C	D	E	F	
1	KeyResult	BoilingPoint.lowerQualifier	BoilingPoint.lowerValue	BoilingPoint.upperQualifier	BoilingPoint.upperValue	BoilingPoint.code	Pre
2	TRUE	>	300	<	320	K	>

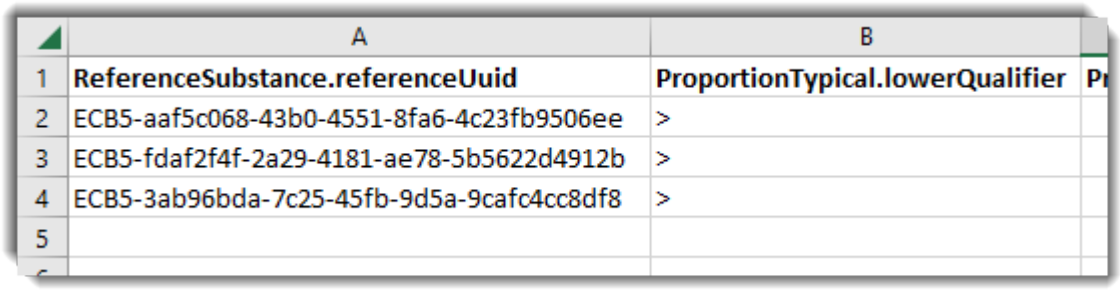
In some tables it is possible to create links to other entities or documents in the installation of IUCLID. Such a link is defined in an imported text file as the UUID of the document or entity. For example, the *Constituents* of a *Composition* can be imported all at once into section 1.2 under a working context for REACH. The output of the text template contains the following headers:

ReferenceSubstance.referenceUuid
ProportionTypical.lowerQualifier
ProportionTypical.lowerValue
ProportionTypical.code
ProportionTypical.other
Concentration.lowerQualifier
Concentration.lowerValue
Concentration.upperQualifier
Concentration.upperValue
Concentration.code
Concentration.other

Remarks

Into the first column, enter the UUID for each *Reference substance* in the *Composition* that is a *Constituent*. For example:

Figure 48: Import constituents in a composition from a text file



	A	B	
1	ReferenceSubstance.referenceUuid	ProportionTypical.lowerQualifier	Pr
2	ECB5-aaf5c068-43b0-4551-8fa6-4c23fb9506ee	>	
3	ECB5-fdaf2f4f-2a29-4181-ae78-5b5622d4912b	>	
4	ECB5-3ab96bda-7c25-45fb-9d5a-9cafc4cc8df8	>	
5			

Tips

If an attempt is made to import a phrase or its code that is not available for that field, an error message is returned. Check what the possible values are from the interface of IUCLID.

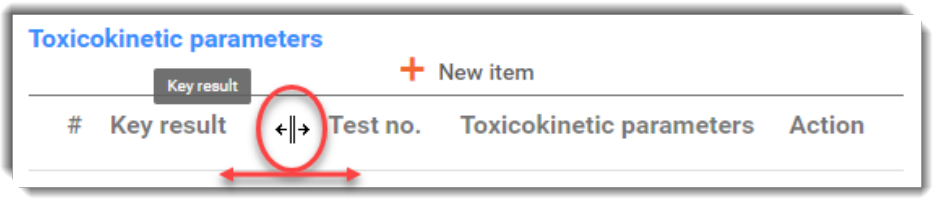
When saving data from Excel in Windows, be aware that the text delimiter is determined from the Windows menu indicated below:

Clock and Region > Region > Formats > Additional settings > List separator

This overrides the use of comma in *Save as* when using the format *CSV (comma delimited)*.

1.7.10.2. Column width

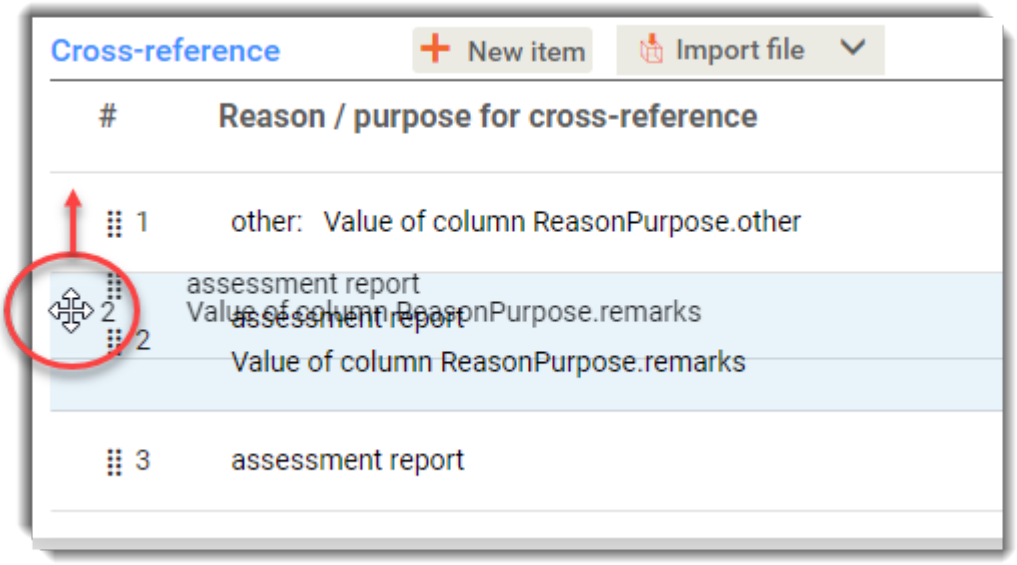
The distribution of column widths within a table is set by hovering in the table header until an icon of arrows appears, as shown below, and then moving it side to side.



1.7.10.3. Order within a table

Rows in a table can be moved up and down by dragging and dropping. The numbers in the column labelled # are always in order 1, 2, 3 …, so the values for the rows change if one is moved up or down. To select a row to be moved, hover to the left of the number until the cursor turns in to a set of compass points.

Figure 49: Moving a row up or down in a table.



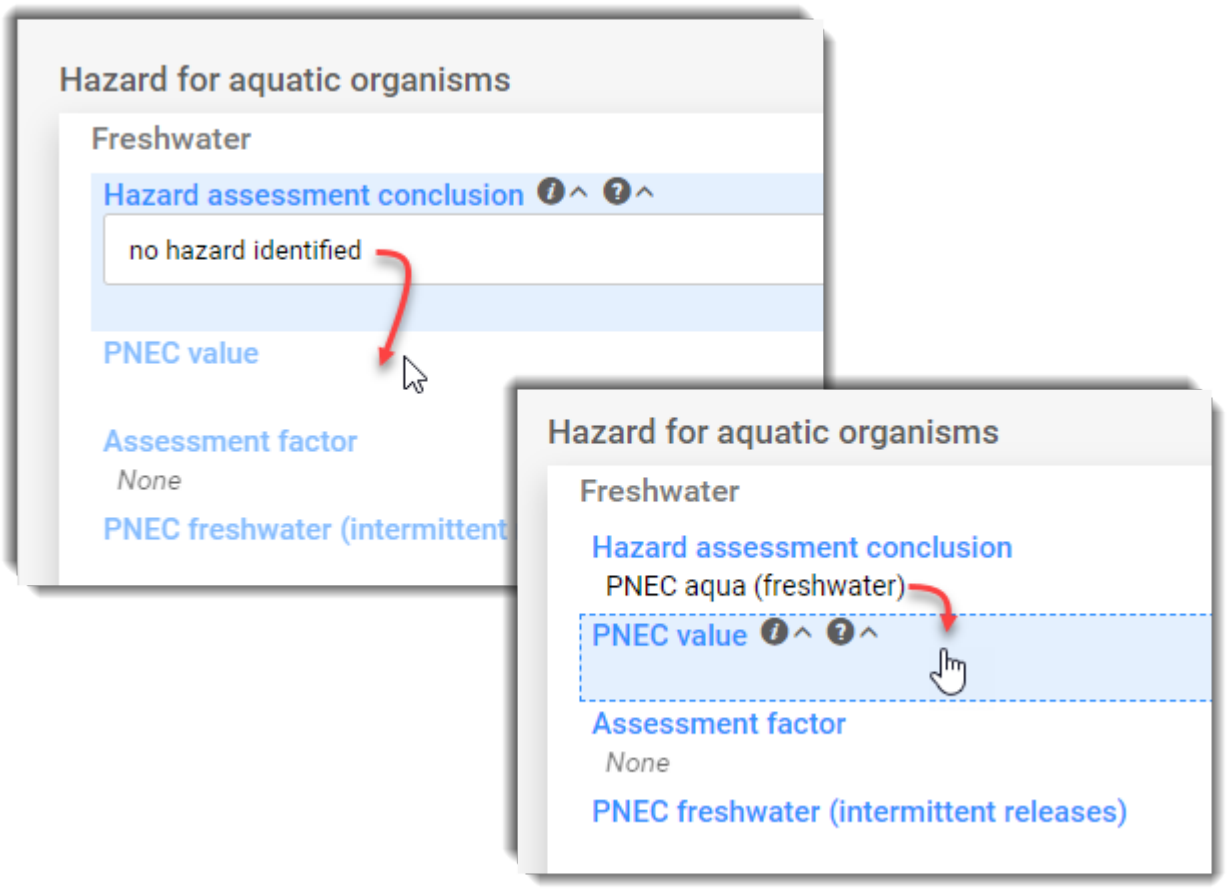
1.7.11. Dynamic content rules

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 it is illogical for a field to contain a value, entering data into the field is disabled, which is indicated by a lighter colour for the field label. If the value of a field is changed so that it breaks the rules for dynamic content, a warning message is displayed, and the data cannot be saved. The user must change what has been entered until it is logically consistent.

Examples

In the example shown below, on the left, 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 shown with a lighter field label, and no value can be entered. On the right, the field *Hazard assessment conclusion* has the value *PNEC aqua freshwater*. Therefore, the fields relevant to PNEC are shown with a darker field label and can be edited.

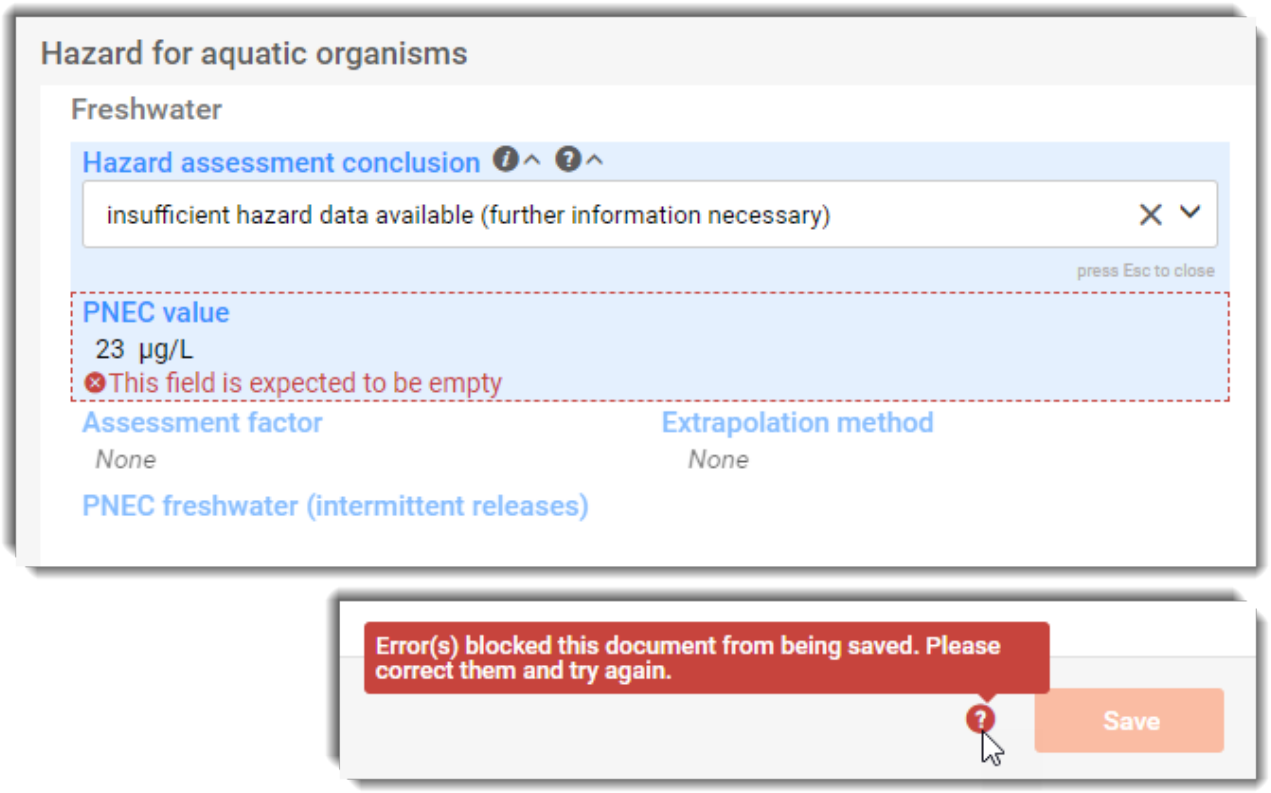
Figure 50: Dynamic content rules preventing fields from being edited



In the example shown below, whilst the field *Hazard assessment conclusion* had a value of *PNEC aqua (freshwater)*, the value of the field *PNEC value* was set to *23 micrograms per litre*. Then, the value of the field *Hazard assessment conclusion* was changed to *insufficient hazard data available…*, without deleting the value of *PNEC value*. This results in the error message “This field

is expected to be empty", and the *Save* button is inactivated. Under the red question mark icon there is a tip on how to proceed.

Figure 51: Effect of breaking a dynamic content rule



The rules for dynamic fields are applied to data that has been imported in to IUCLID and/or migrated from a previous version. If a rule has been broken due to a change in the IUCLID format, the data can still be imported, but on editing, it can be saved only when the rules are obeyed.

Example of dynamic content rules for imported migrated data

In the example shown below, the value of *Adequacy of study* (1) is inconsistent with the values for data waving (2). All the fields involved in the application of the dynamic rule are shown with an error message, and the data cannot be saved (3). The user must decide how to resolve the conflict. Removing the inconsistency by deleting the *Data waiving* (4) clears the error message from all the affected fields. The data can now be saved (5).

Figure 52: Dynamic content rules applied to imported migrated data

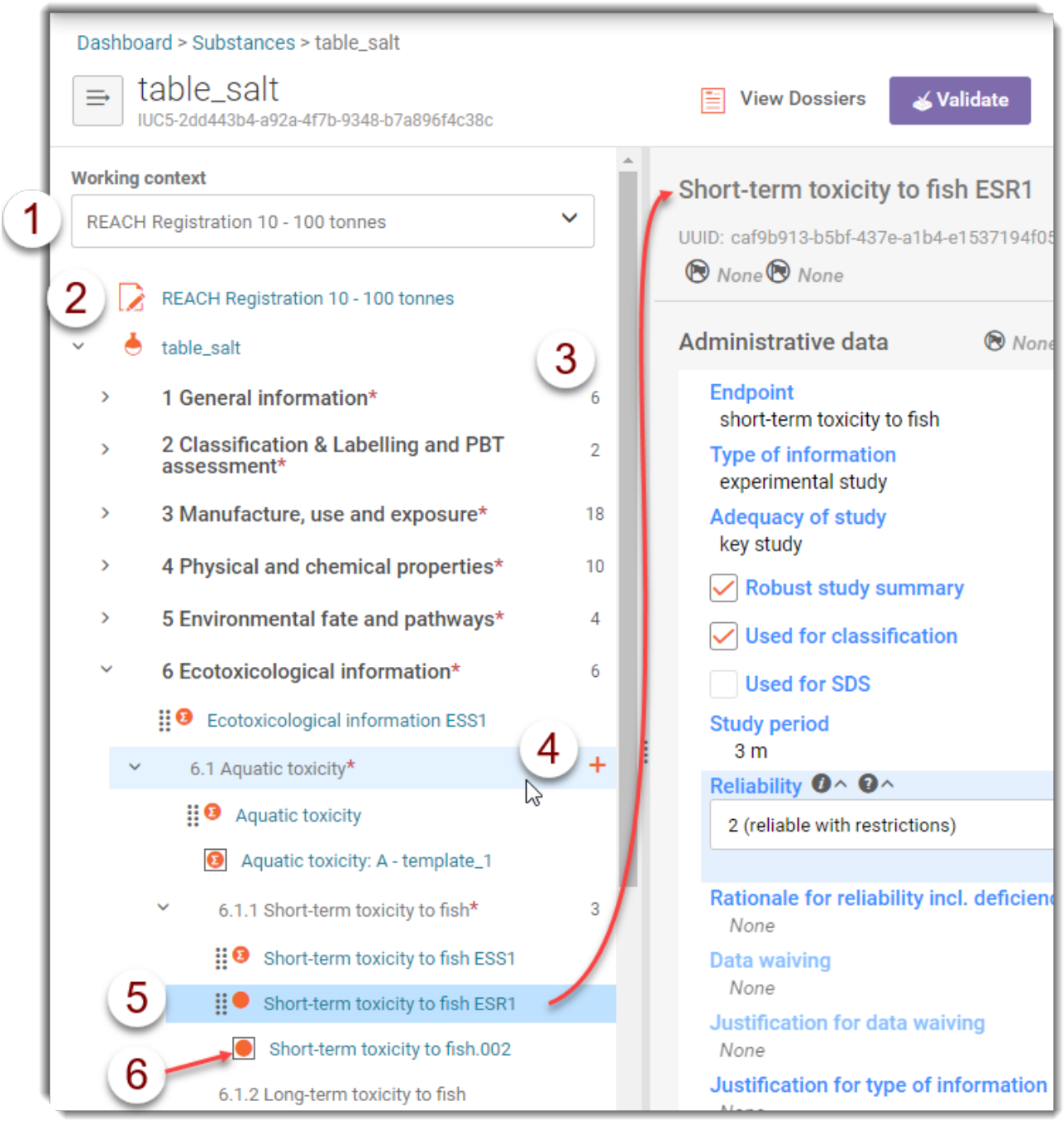
1.7.12. Table of contents

The *Table of contents* does the following:

1. Shows the structure of datasets and dossiers in a regulatory or other context, as defined by the *Working context*;
2. Indicates how many documents are in each section;
3. Provides management functionalities for documents in an entity.
4. Provides access to the draft dossier header of a raw dataset.

The figure below shows the *Table of contents* for a raw Substance dataset on the left of the interface, with a document opened in the data window on the right.

Figure 53: Table of contents with the data window in editing or viewing mode



Legend for Figure 53

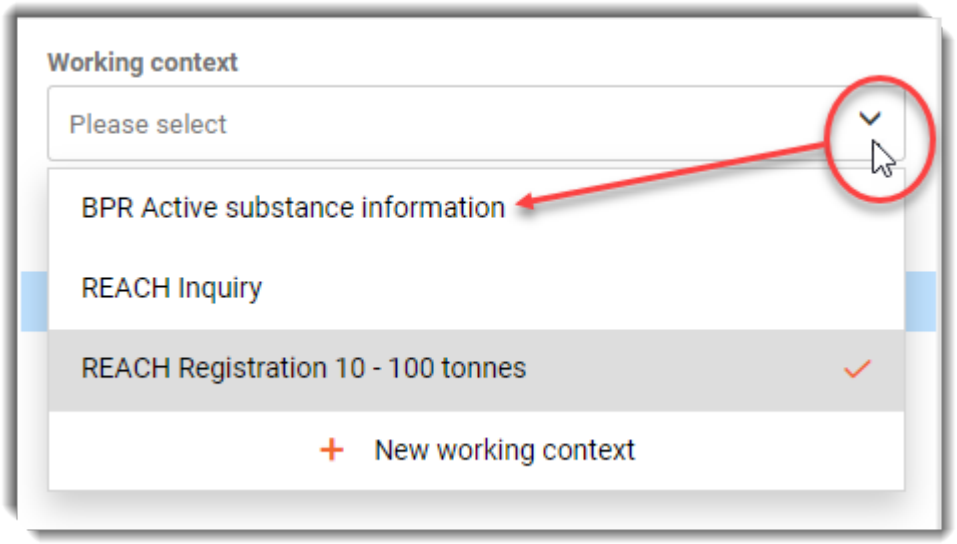
1. A working context of *REACH Registration 10 -100 tonnes* has been selected;
2. The first row gives access to the draft dossier header of a raw substance dataset, as indicated by the icon ;
3. The number of documents in a section;
4. On hovering over a section header, an orange cross (+) appears which is a clickable button to create a document in that section of the *Table of contents*. If only one type of document can be created in a section, the type is determined automatically. However, if more than one type is

possible, there is an option to choose the type, for example between *Endpoint study summary* and *Endpoint study record*. On hovering over a document, a dustbin icon ( ) appears which is a clickable button to delete the document.

5. The currently open document is high-lighted in the *Table of contents*. The working context is for the REACH regulation, therefore documents of type *Short-term toxicity to fish* are in section 6.1.1. Documents marked with the icon ⠿ can be moved up and down within a section or subsection by dragging and dropping.
6. Documents from a *Template* are placed below those created directly in the *Table on contents*, and marked with an icon in a box. Their order cannot be changed in the dataset, but the order within an individual *Template* can be changed, from the *Table of contents* of the *Template* itself;

The working context is selected from a drop-down menu of options that have been pre-selected by the user to form a personalised list. An example menu is shown below, where the button to open it is ringed in red.

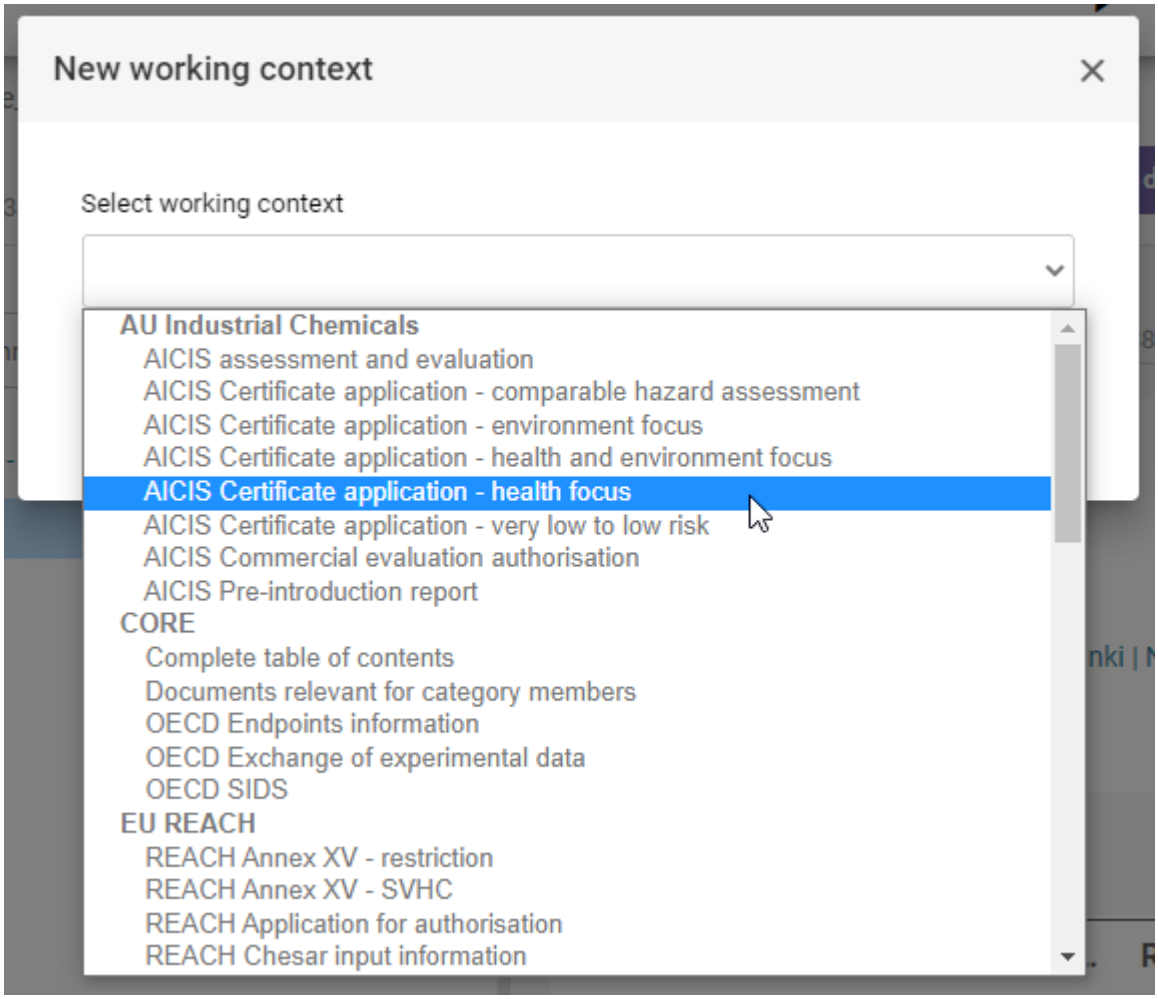
Figure 54: Selecting the working context



The current working context is shown in darker grey. Hovering over a menu item turns it pale grey, when it can either be selected as the new working context, or removed from the menu using the dustbin icon.

If the required working context is not on the menu, add it by first clicking on *New working context*, and then by selecting it from the predefined values. These include options that correspond to various dossier types for submission under a range of different regulatory programmes. In the example shown below, *AICS Certificate application – health focus* is being added to the menu.

Figure 55: Add a working context to the personalised menu



The *working context* typically, but not always, corresponds to a specific type of *Dossier* used to submit information under a regulatory programme. An example of a working context that is not used for data submission is *REACH Complete*, which shows all the documents that have any relevance to the REACH regulation. It uses the structure that is common to all *Dossiers* submitted under REACH. Also, it refers to no specific type of *Dossier*, so no document is marked as mandatory.

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

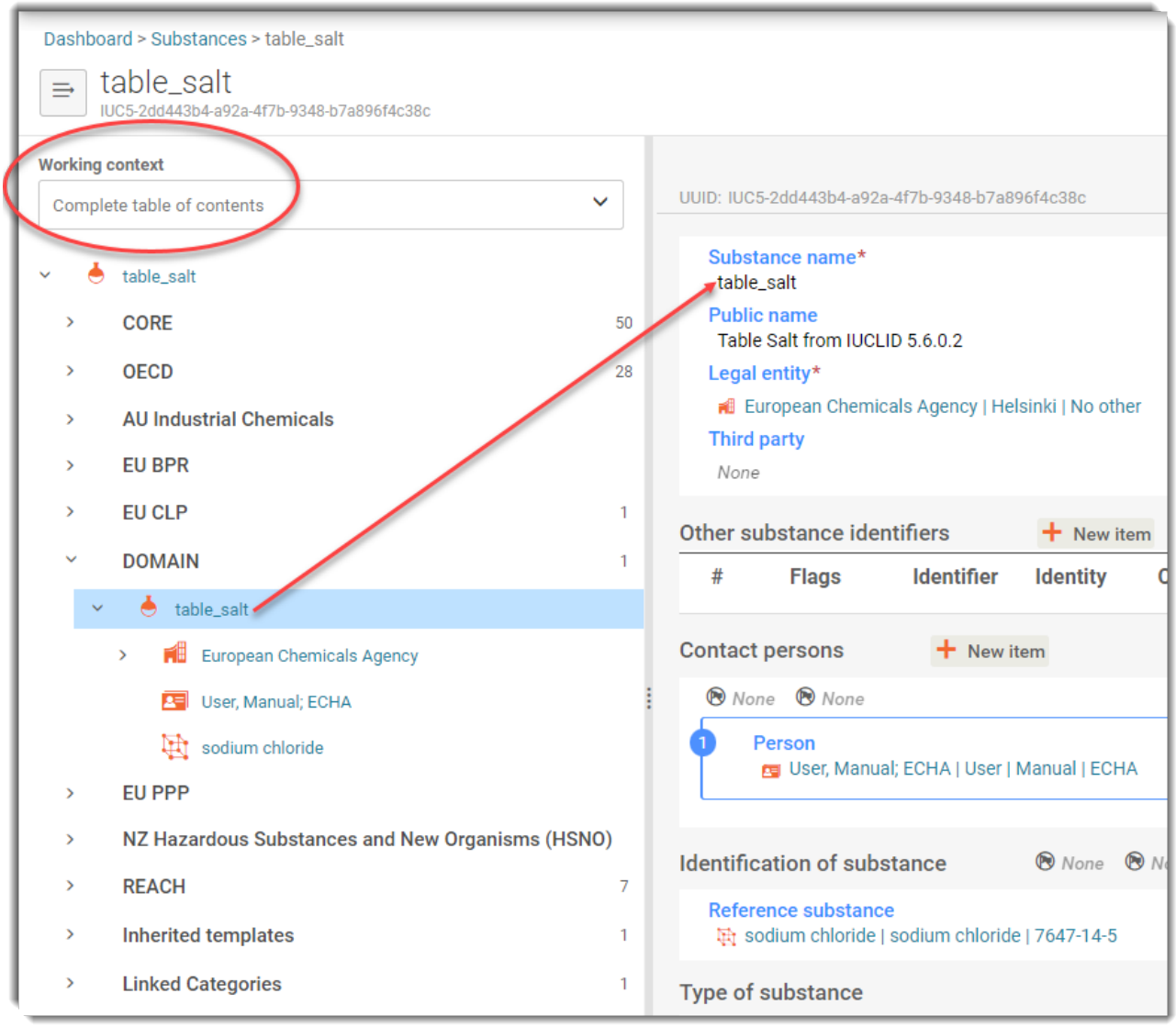
1.7.12.1. Complete table of contents

For the *working context* of type *Complete table of contents*, documents are displayed in sections that are determined by the origin of their definitions. Documents that are defined by OECD harmonised templates are under OECD. Documents that are not defined for a specific legislation and are not under OECD are either under *CORE* or DOMAIN. DOMAIN contains the definition of the entity at the highest level in the table of content for the dataset, for example an entity of type *Substance*. In addition, IUCLID 6 is supplied with sections dedicated to documents that are defined under the legislations: *AU Industrial Chemicals*, *EU BPR*, *EU CLP*, *EU PPP*, *NZ Hazardous Substances and New Organisms (HSNO)* and *REACH*. For a complete list, see the menu displayed when adding a working context to your personalised list.

Example

In the example shown below for a *Substance* dataset there is one document under DOMAIN because there is a single top-level definition of the *Substance* entity, which has its own UUID. There are 43 documents in CORE, including a *Composition* document, which is in CORE because its definition is not specific to a legislation, and it is not defined by an OECD harmonised template. There are 29 documents that are defined by OECD harmonised templates, and 7 documents are specific to the REACH legislation. Inherited Templates are at the foot of the table.

Figure 56: Complete table of contents



The section under which a document is shown in *Complete table of contents* may be different from that used for a particular legislation. *Endpoint study summaries* and *Endpoint study records* documents that are in the same section under a particular legislation, may be in different sections from each other when viewed in *Complete table of contents*.

Example

An example of where the sections are the same is for a working context of *REACH Registration 10 – 100 tonnes*, where if a *Site* is added to section *3.3 Sites*, it appears under *Complete table of contents* in *CORE / section 3.3 Sites*.

Example

Under the working context of *REACH Registration 10 – 100 tonnes*, documents of type *Endpoint study summary* and *Endpoint study record* are under the same top-level section.

Under the working context of *Complete table of contents*, the same documents are no longer in the same top-level section. *Endpoint study summaries* are under CORE, and *Endpoint study records* are under OECD.

An example is shown in the figures below.

REACH Registration 10 – 100 tonnes

Endpoint study summary	*6.1.1 Short-term toxicity to fish*
Endpoint study record	*6.1.1 Short-term toxicity to fish*

Complete table of contents

Endpoint study summary	CORE *6.1.1 Short-term toxicity to fish*
Endpoint study record	OECD *C Effects on biotic systems, 41 Short-term toxicity to fish*

Figure 57: Example location in table of content: Short-term toxicity to fish under 'REACH'

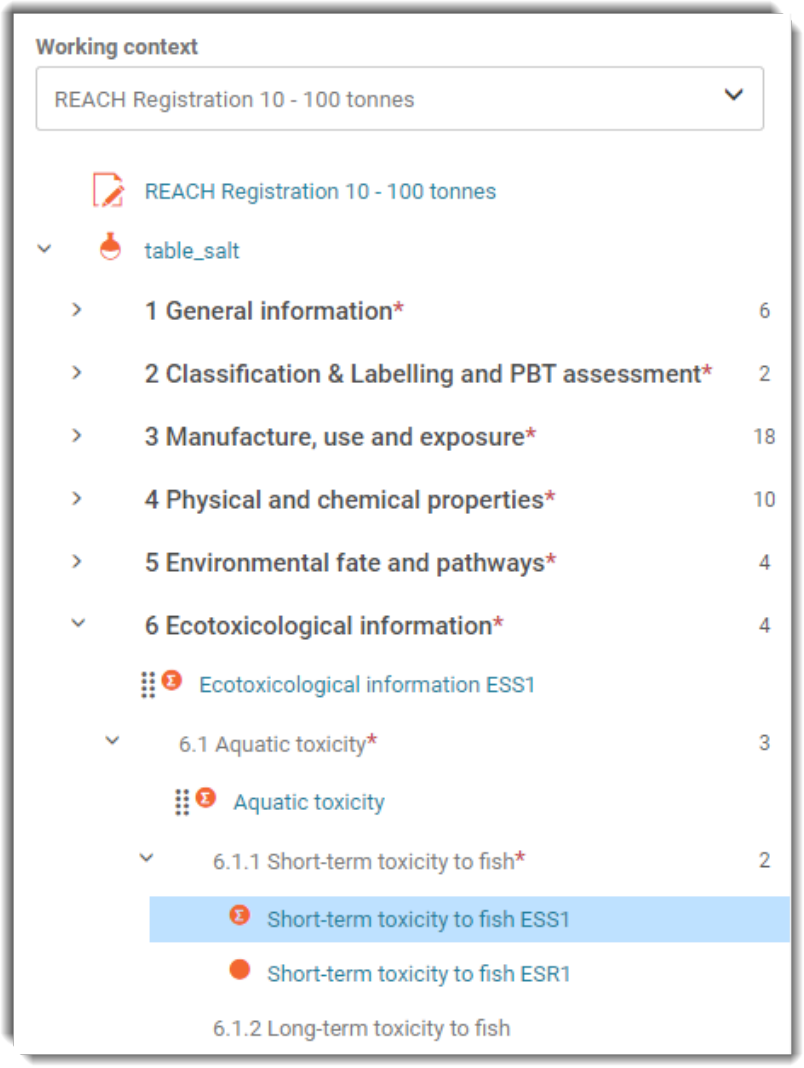
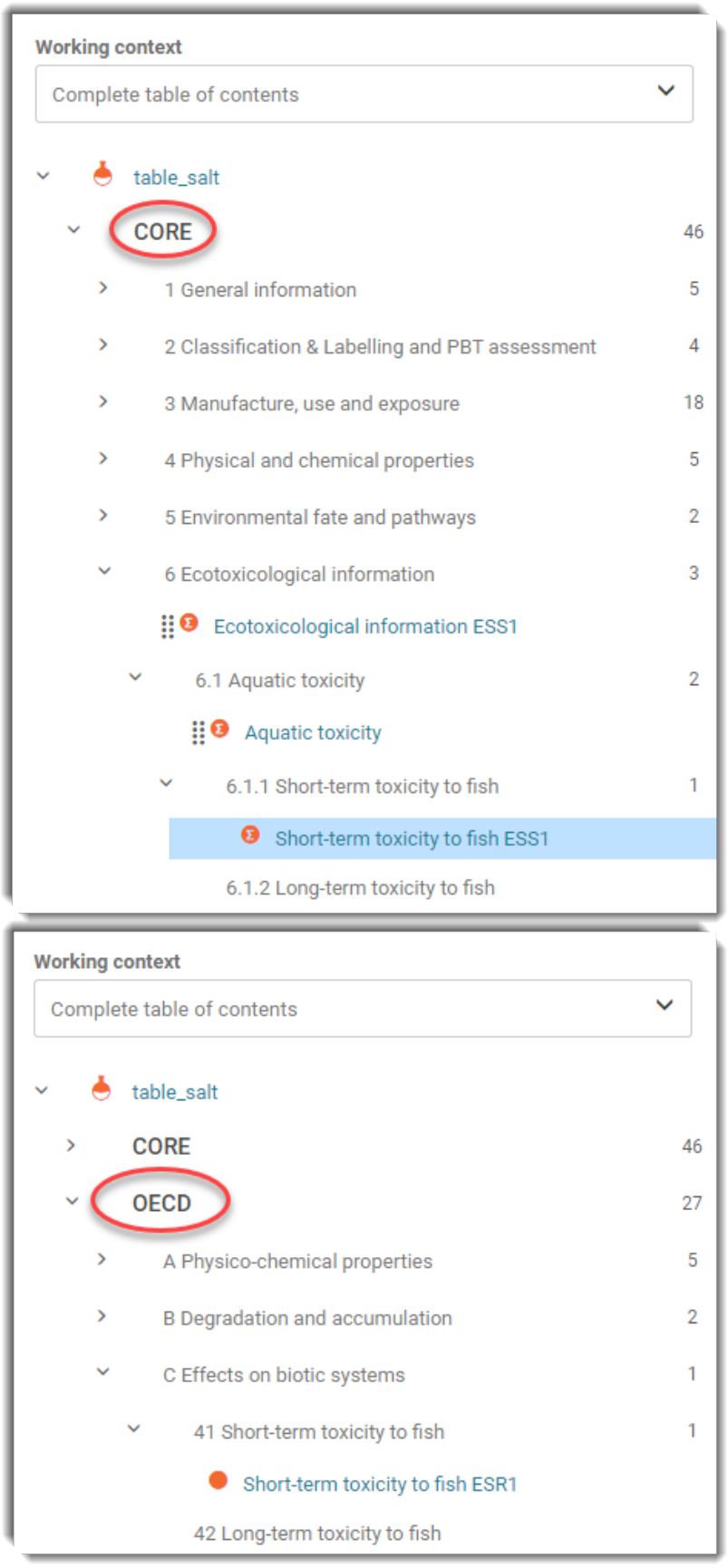
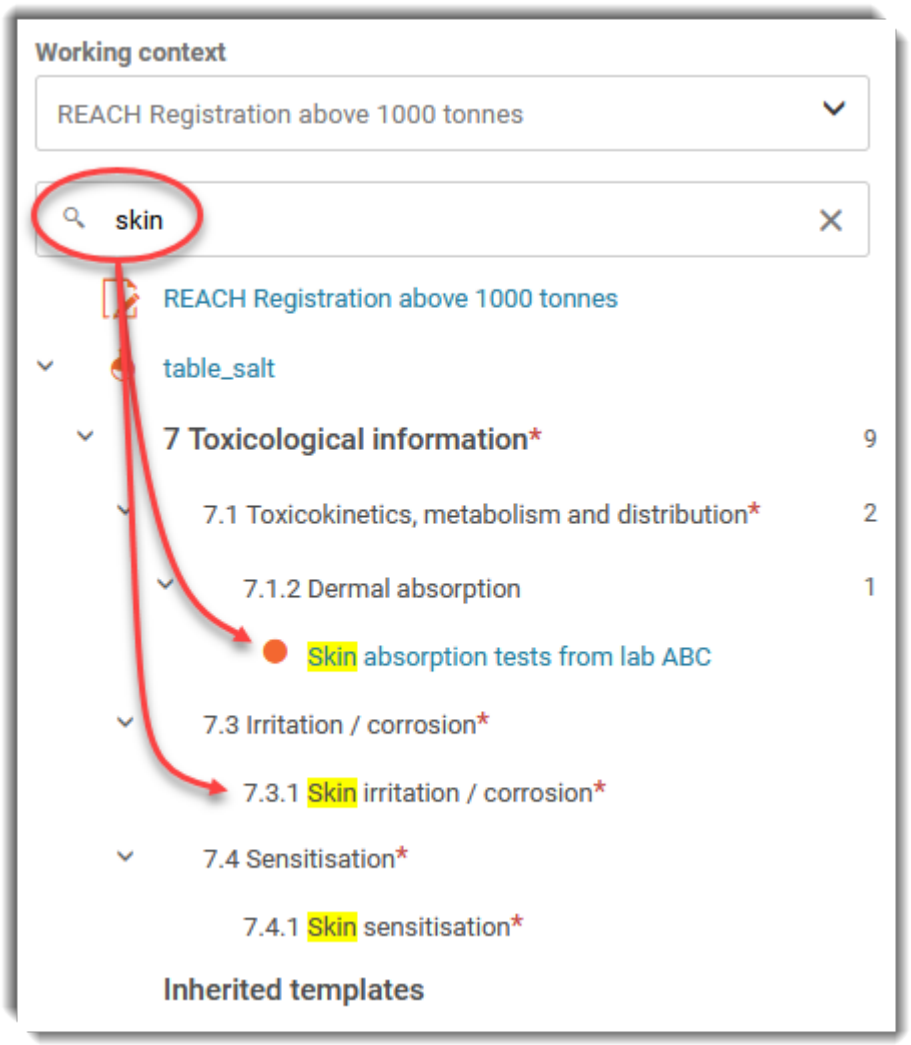


Figure 58: Example location in table of content: Short-term toxicity to fish under 'Complete table of contents'



The *Table of contents* can be filtered by text, whereby the only sections and documents shown are those whose titles contain the search term. It is not case sensitive. An example is shown below for the text *skin*, in which sections and a document match.

Figure 59: Filtering a table of contents



1.7.12.2. 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. All entries under the OECD harmonised templates are *endpoint study records*.

An example of an *endpoint study record* is *Long-term toxicity to fish*.

1.7.12.3. Endpoint summary

An *endpoint summary* provides a means of grouping *endpoint study records* from within the same subsection, 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)*.

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.

1.7.12.4. Record

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

e.g. Under REACH, section *1.2 Composition*, section *1.6 Sponsors*.

1.7.12.5. Summary

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

e.g. Under BPR section *13 Summary and evaluation*.

1.7.12.6. Fixed record

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

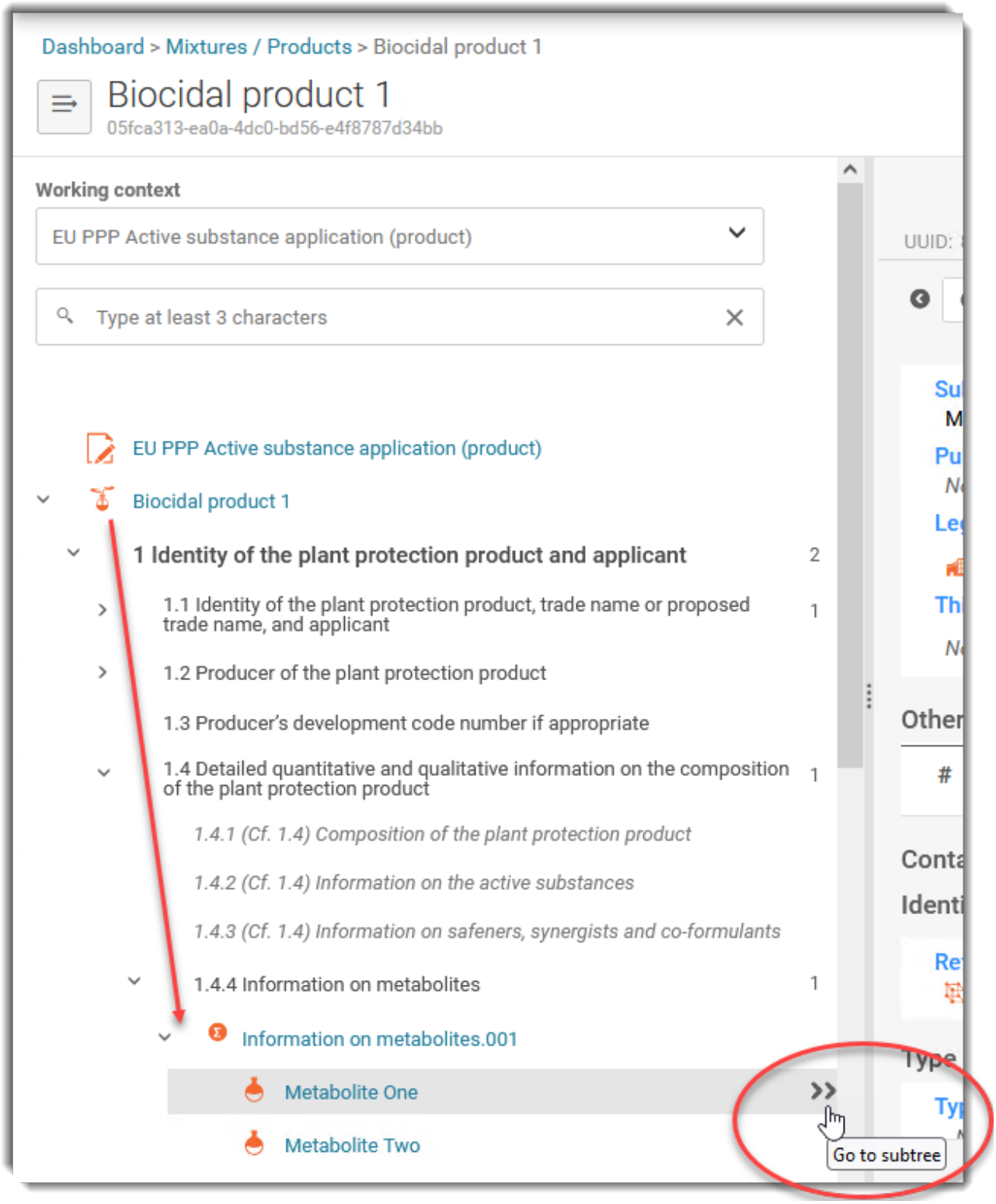
e.g. Under REACH, section *14 Information requirements > Downstream user report*.

1.7.12.7. Sub-trees in the table of contents

In some working contexts, the table of contents can contain references to one or more datasets. The question is, how to view the tables of contents of such datasets, whilst still being able to see where you are in the overall picture. The approach taken, is to allow the table of contents of referenced datasets to be opened in a sub-tree. Links into and out of a subtree are provided under double arrow icons in the table of contents. *In*, or *down*, has an icon (>>) at the right of the name of the referenced dataset. *Out*, or up, has as icon (<<) at the top left of the subtree. At the top of the subtree, the path to it is indicated so that users can see the context in which they are working.

The feature sub-tree is relevant for only certain working contexts. The example shown below is for the working context *EU PPP Active substance application (product)*. *Biocidal Product 1* is a *Mixture* that refers in section *1.4.4 Information on metabolites* to a *Substance* named *Metabolite One*. To view the table of contents of *Metabolite One* in a sub-tree, select its name, and then click on the icon **>>**.

Figure 60: Opening a sub-tree in the table of contents

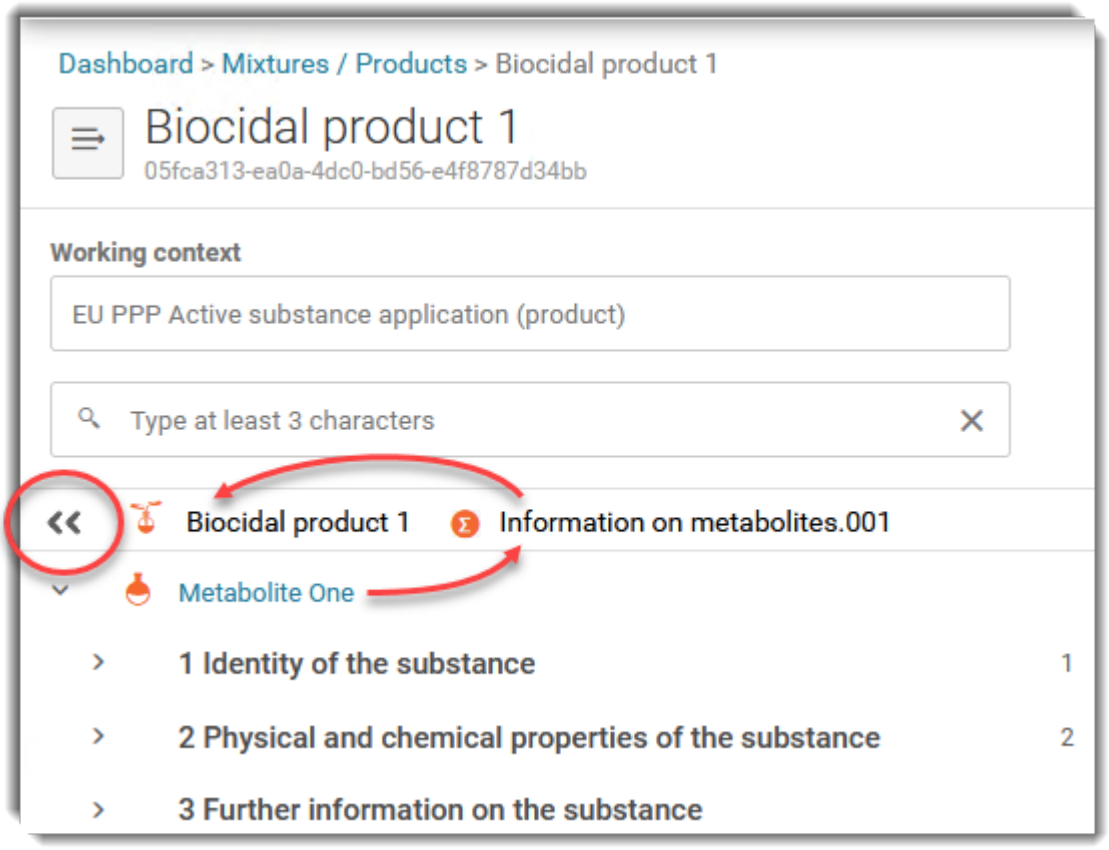


The path to the dataset shown in the subtree is indicated at the top of the sub-tree:

Biocidal Product 1 > Information on metabolites.001

To go back to the table of contents of *Biocidal product 1*, click on the icon **<<**.

Figure 61: Closing a sub-tree in the table of contents

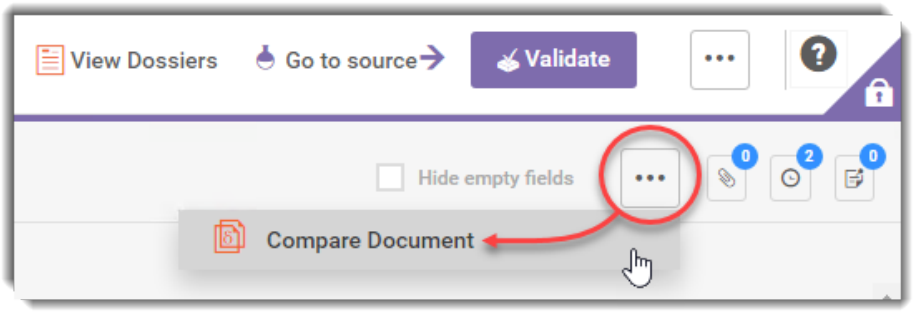


1.7.13. Compare Document

Compare Document compares two individual documents that are of the same type. For example, compare two versions of an endpoint study of type *short-term toxicity to fish* that are in different Dossiers. The output is an HTML file that can be viewed in a web browser, for example by opening it in a tab alongside the user interface of IUCLID.

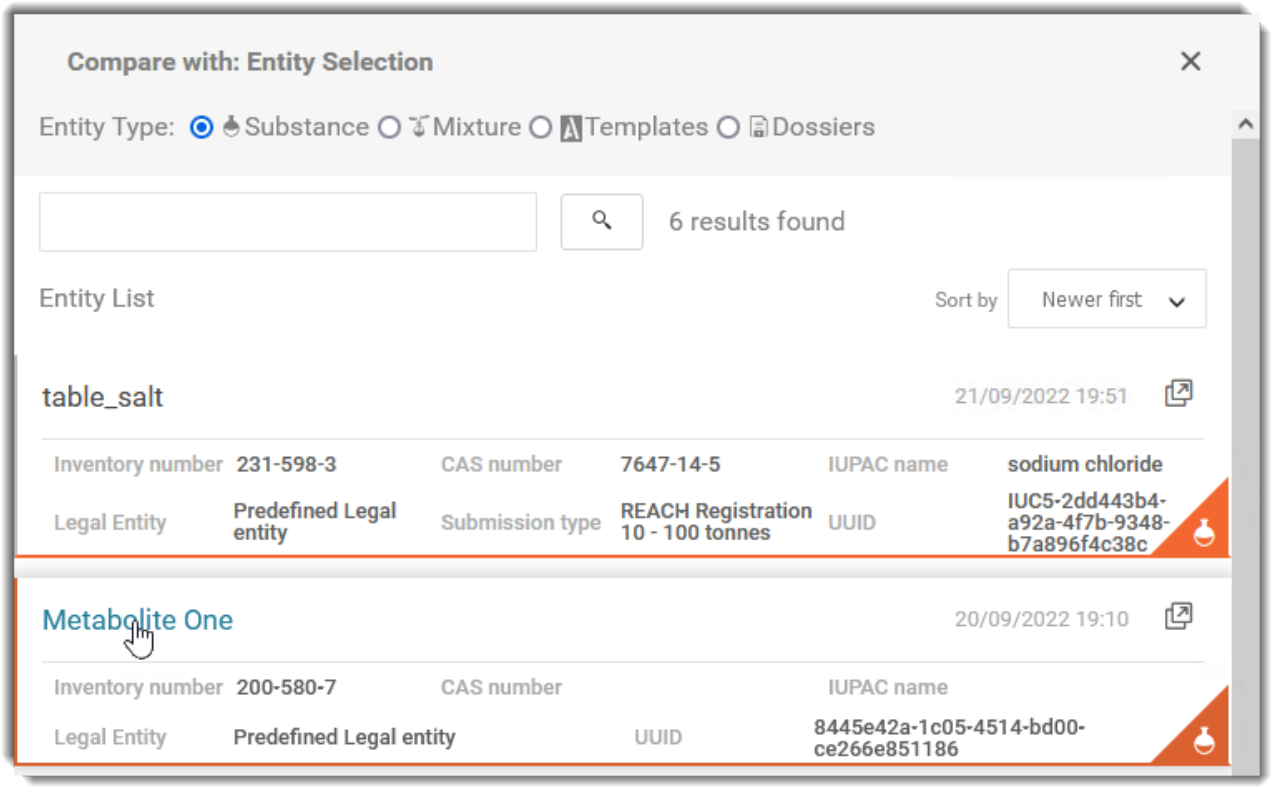
Start by viewing the record of the *source* document against which the comparison will be made. From the three-dot menu at the top righthand corner of the data window, select *Compare Document*, as shown below.

Figure 62: Open the feature that compares two documents



Select the entity that contains the other document, which is known as the *target*.

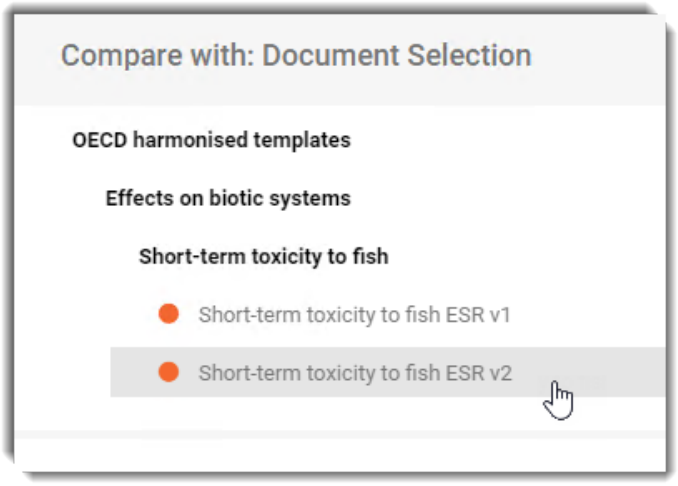
Figure 63: Select the entity that contains the other document to be compared



This opens a view of the table of contents at the same section as the source document from where the comparison was started. It shows only documents of the same type. To select a document for

comparison, click on it. In the example below, the comparison is made with *Short-term toxicity to fish ESR v2*.

Figure 64: Select a document to be compared

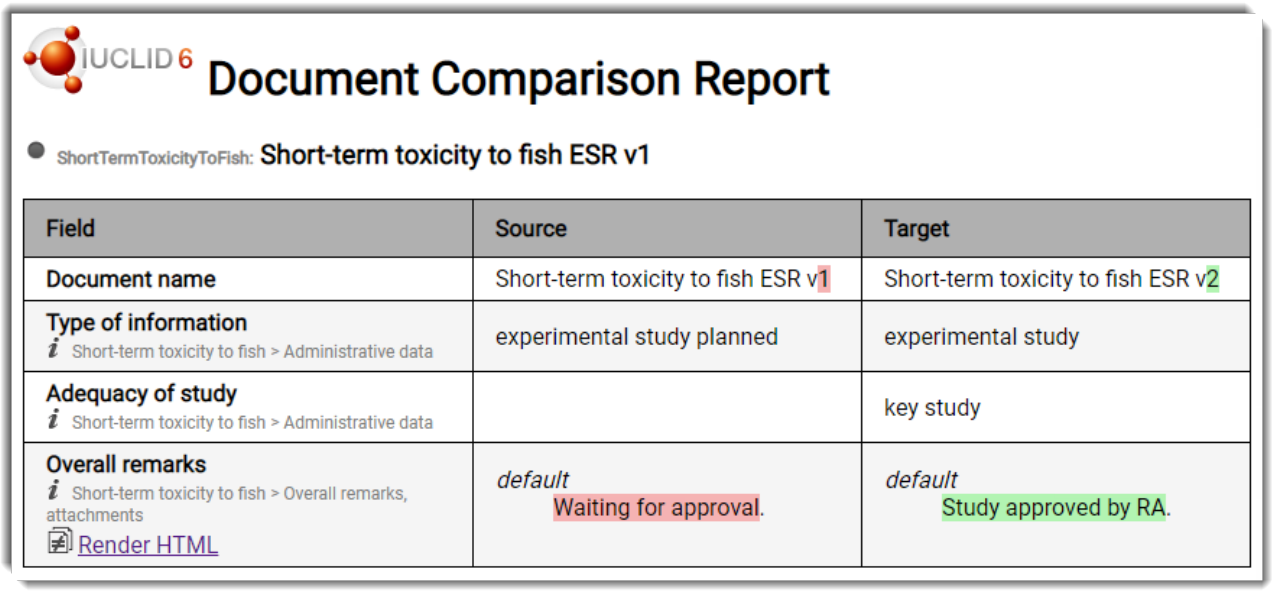


A document comparison report is generated in HTML format. Download the file, then view it with a web browser. The comparison report is similar to the section for fields when comparing whole dossiers and datasets, which is described in section *6.5 Compare*.

The changes are highlighted in red for the source, and green for the target. In the example below, the source document is *Short-term toxicity to fish ESR v1* and the target is *Short-term toxicity to fish ESR v2*.

For rich-text fields, which are encoded in HTML, the content can be viewed either according to the HTML, or with the differences highlighted in colour. To switch between the two views, click on either *Highlight differences*, or *Render HTML*. In the example below, the differences in *Overall remarks* are highlighted in colour.

Figure 65: A document comparison report



IUCLID 6

Document Comparison Report

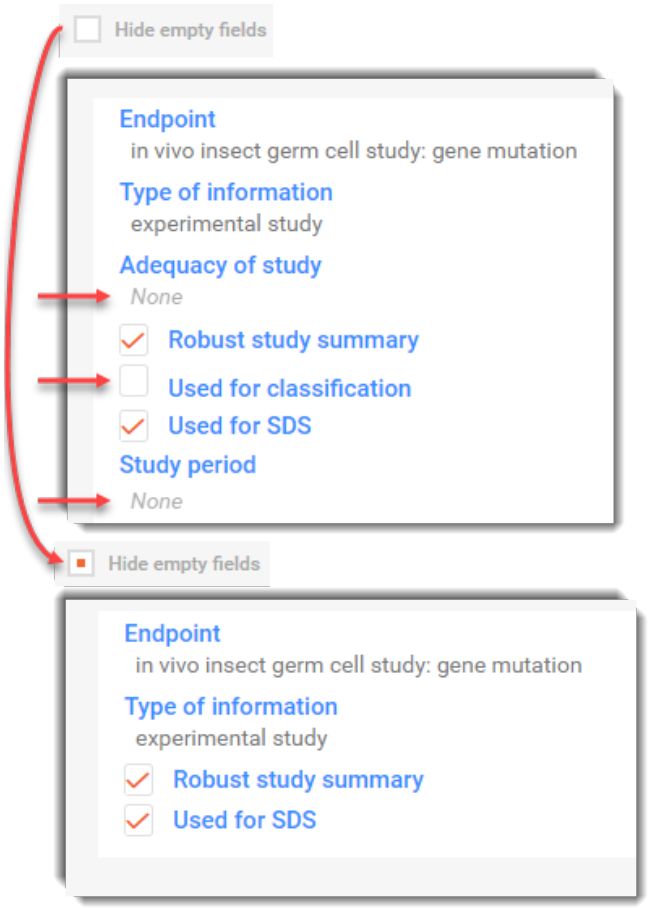
ShortTermToxicityToFish: **Short-term toxicity to fish ESR v1**

Field	Source	Target
Document name	Short-term toxicity to fish ESR v1	Short-term toxicity to fish ESR v2
Type of information Short-term toxicity to fish > Administrative data	experimental study planned	experimental study
Adequacy of study Short-term toxicity to fish > Administrative data		key study
Overall remarks Short-term toxicity to fish > Overall remarks, attachments Render HTML	*default* Waiting for approval.	*default* Study approved by RA.

1.7.14. Hide empty fields

Empty fields can be hidden when viewing a *Dossier*. An example is shown below.

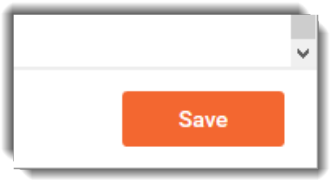
Figure 66: Hide empty fields



1.7.15. Save

After editing a document, click on the *Save* button at the bottom right of the interface:

Figure 67: Save



For a few seconds after clicking on *Save*, an option to view the record page of what was saved is presented in a green box, as shown below.

Figure 68: Option to view a document that has just been saved

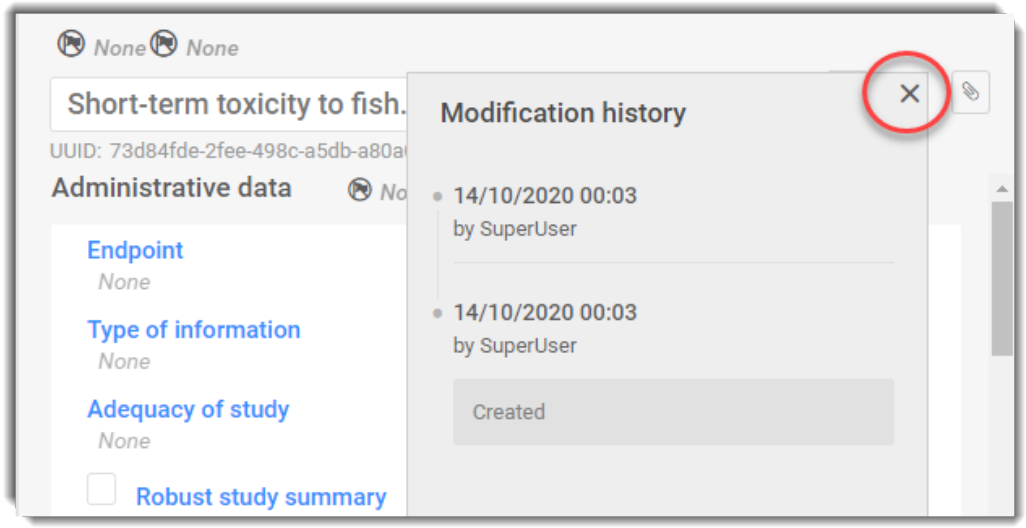
1.7.16. Modification History

The modification history for a document is available whilst the document is open in the data window. It is accessed via a button at the top right of the data window, as shown in the example below. The number of items in the history is indicated in a superscript:

Figure 69: Access to the modification history

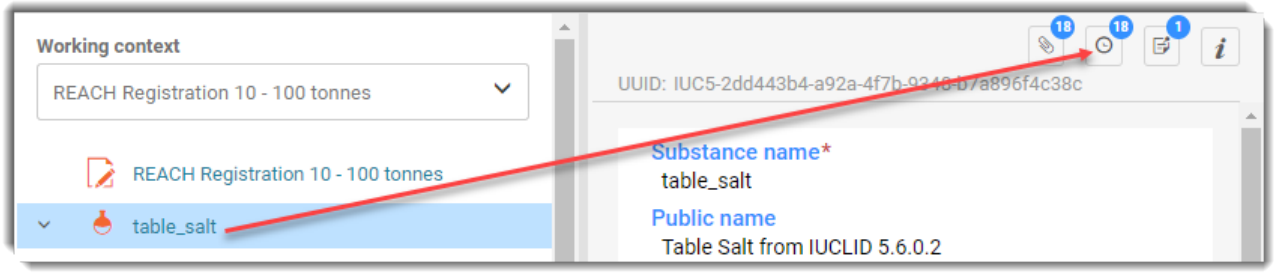
For each event, the history shows a timestamp, the IUCLID *User* that carried out the action, and for some cases, a description of the event. The example below shows the modification history of an *Endpoint study record* immediately after it has been created. Note that the document is open in the data window.

Figure 70: Modification history of an Endpoint study record



The modification history of a top-level entity such as a *Substance* or *Mixture/Product* is accessible from the document that defines its name. For example, the document that defines the name of a *Substance* under REACH is section *1.1 Identification*, as shown in the example below.

Figure 71: Access to the modification history of a Substance



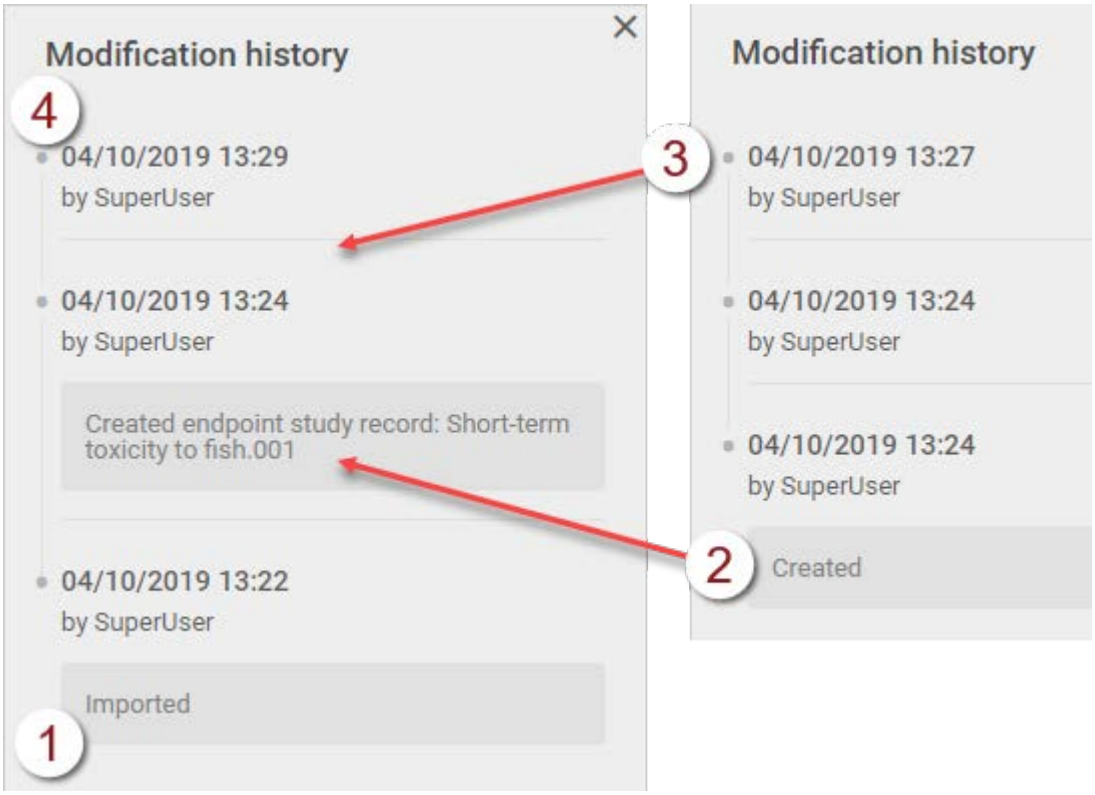
When the content inside a IUCLID document is edited, the edit does not appear in the modification history of a IUCLID document or entity that refers to it. For example, when the value of a field is changed inside an *Endpoint study record*, the event does not appear in the modification history of a *Substance* dataset that contains it.

Each import action is recorded as an event, even where the import did not result in a change to the data as a result of migration from a previous version. If the modification history does not start with a *Creation* event, but *Import* instead, it means that the document had been exported from IUCLID with the modification history excluded.

A description for an event is given, in a grey box below the timestamp, if a reference to a IUCLID document is changed, or the action was an import. If only the value of a field is changed in a document, no description is given.

An example of the modification histories for a *Substance* and an *Endpoint study record* inside it is given below.

Figure 72: Example modification histories for a Substance and an Endpoint study record inside it



Legend for Figure 72

1. 13:22 *Substance* was imported from an i6z file;
2. 13:24 An *Endpoint study record* was created with the default name, *Short-term toxicity to fish.001*;
3. 13:27 The value of a field was changed in *Short-term toxicity to fish.001*. Note that it is not shown in the history of the *Substance*;

4. 13:29 Name of the *Substance* was changed. Note that it is not shown in the history of the *Endpoint study record* named *Short-term toxicity to fish.001*;

1.7.17. Bookmarks, hyperlinks, and the sharing of entities and documents

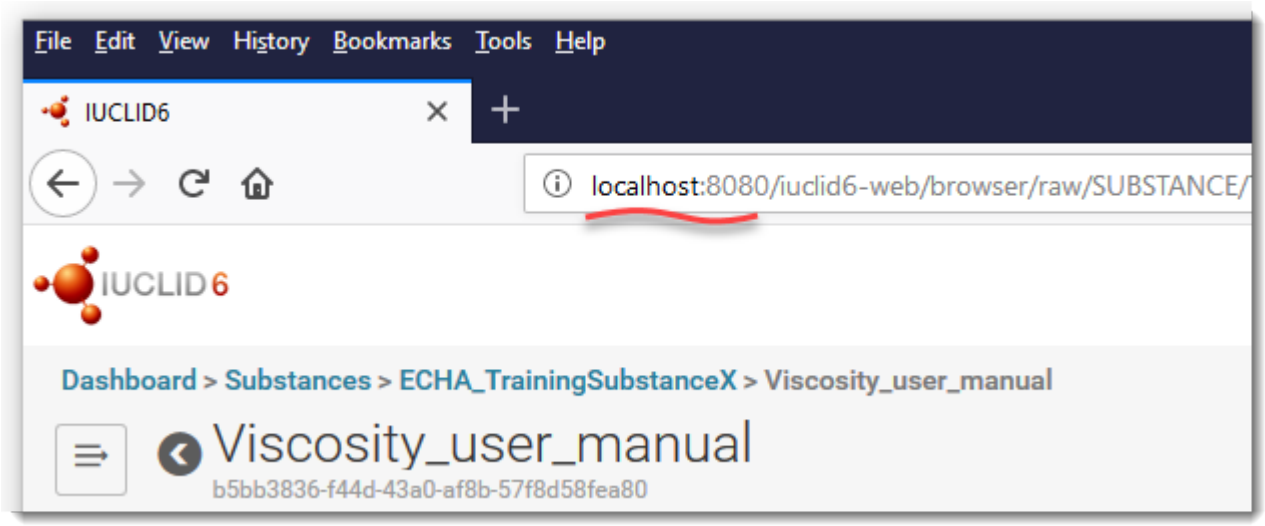
The web technology behind the interface means that it is possible to create a hyperlink that points to any document or entity. Such links can be saved as bookmarks, and then shared between colleagues. To create a bookmark that links to an entity, view the entity, and then create a bookmark in the browser. The exact steps depend on the browser. The bookmark will contain the address that is displayed in the navigation bar of the browser. That address can be copied, pasted, and shared.

Remember that you must take into consideration the address of the instance of IUCLID. For example, links can be shared without modification between any two *default* instances of IUCLID 6 Desktop. The same goes for colleagues sharing access within a single instance of IUCLID 6 Server. However, if the addresses of the instances of IUCLID differ, modifying the link is a simple matter of changing the first part of the link up until the start of the following code:

```
/iuclid6-web/…
```

The part of the address to change is indicated in the screenshot below, underlined in a wavy red line.

Figure 73: The part of a link to an entity or document that depends on the instance of IUCLID



A link to a *Dossier* is of the form:

```
<protocol><server>/iuclid6-web/browser/dossier/<dossier uuid>
/DOSSIER/<dossier uuid>
```

Example 1

An address from a default instance of IUCLID 6 Desktop is adapted to an instance of IUCLID 6 Server.

Default instance of IUCLID 6 Desktop:

https://iuclid6.echa.europa.eu

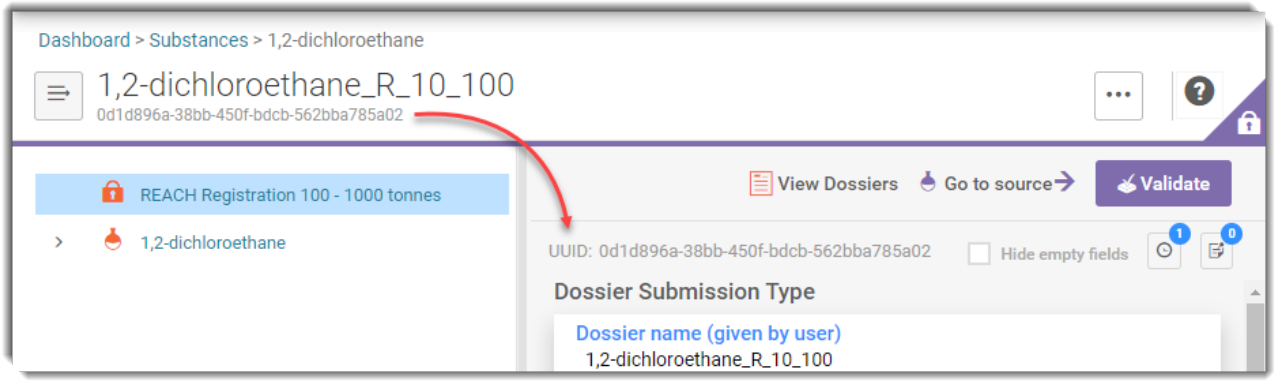
```
http://localhost:8080/iuclid6-web/browser/raw/SUBSTANCE/...
```

Changes to:

```
https://echa.europa.eu.house/iuclid6-web/browser/raw/SUBSTANCE/...
```

Example 2

A link to a *Dossier*. This requires the *Dossier* UUID, and the location of the installation of IUCLID. The *Dossier* UUID can be copied from the record page of the *Dossier*, where it is stated just under the name. The location of the UUID is indicated below.



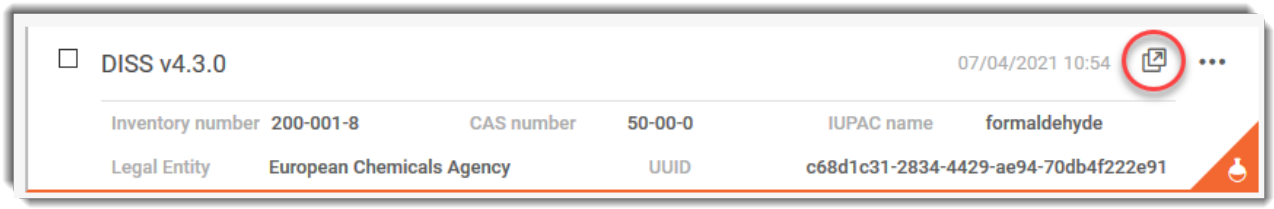
Link to the *Dossier* in a local instance of IUCLID.

```
http://localhost:8080/iuclid6-web/browser/dossier/0d1d896a-38bb-450f-bdcb-
562bba785a02/DOSSIER/0d1d896a-38bb-450f-bdcb-562bba785a02
```

1.7.18. Open in new tab

An entity or document can be opened in a new browser tab from the following icon . An example is shown below for the list page of *Substances*.

Figure 74: Open in new tab from a list page

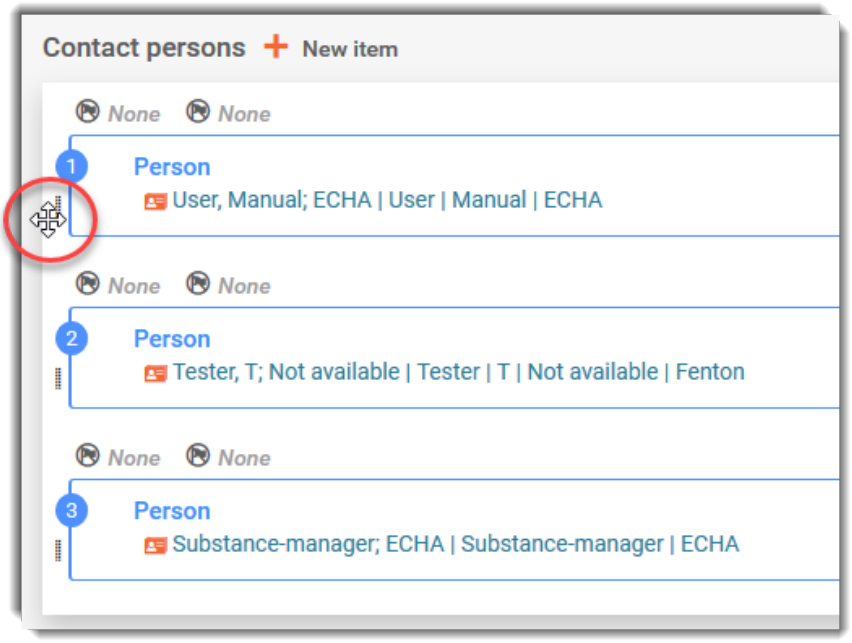


1.7.19. Re-order repeatable blocks

Repeatable blocks of data in numbered lists can be reordered by dragging and dropping the following icon .

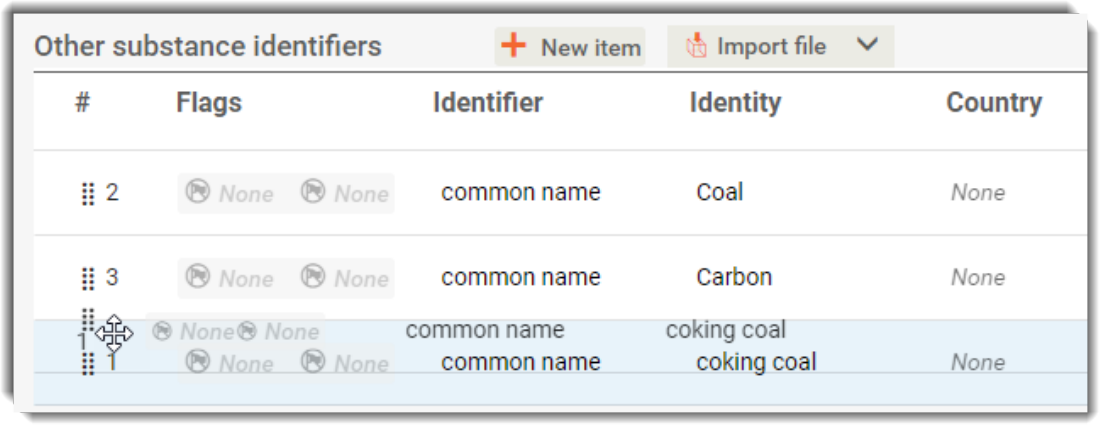
In the example below, a *Contact* is about to be moved from position 1 to further down the list.

Figure 75: Re-order repeatable blocks in a numbered list



In the example below, a numbered table row has been moved from position one to three.

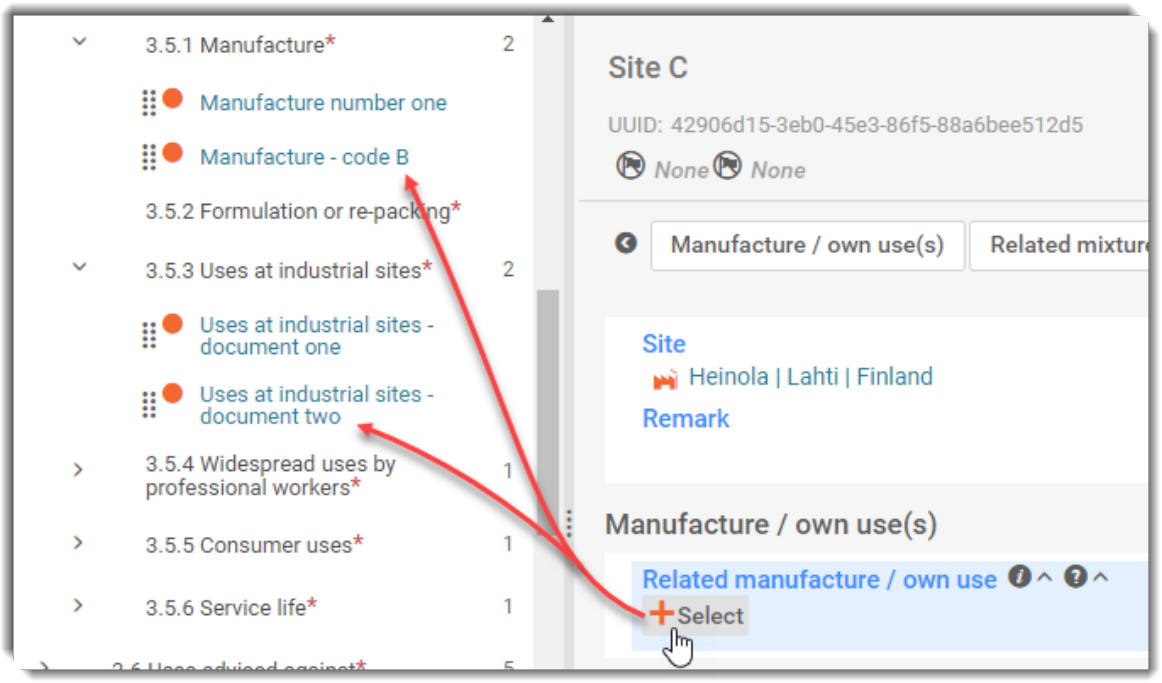
Figure 76: Re-order numbered table rows



1.7.20. Cross reference

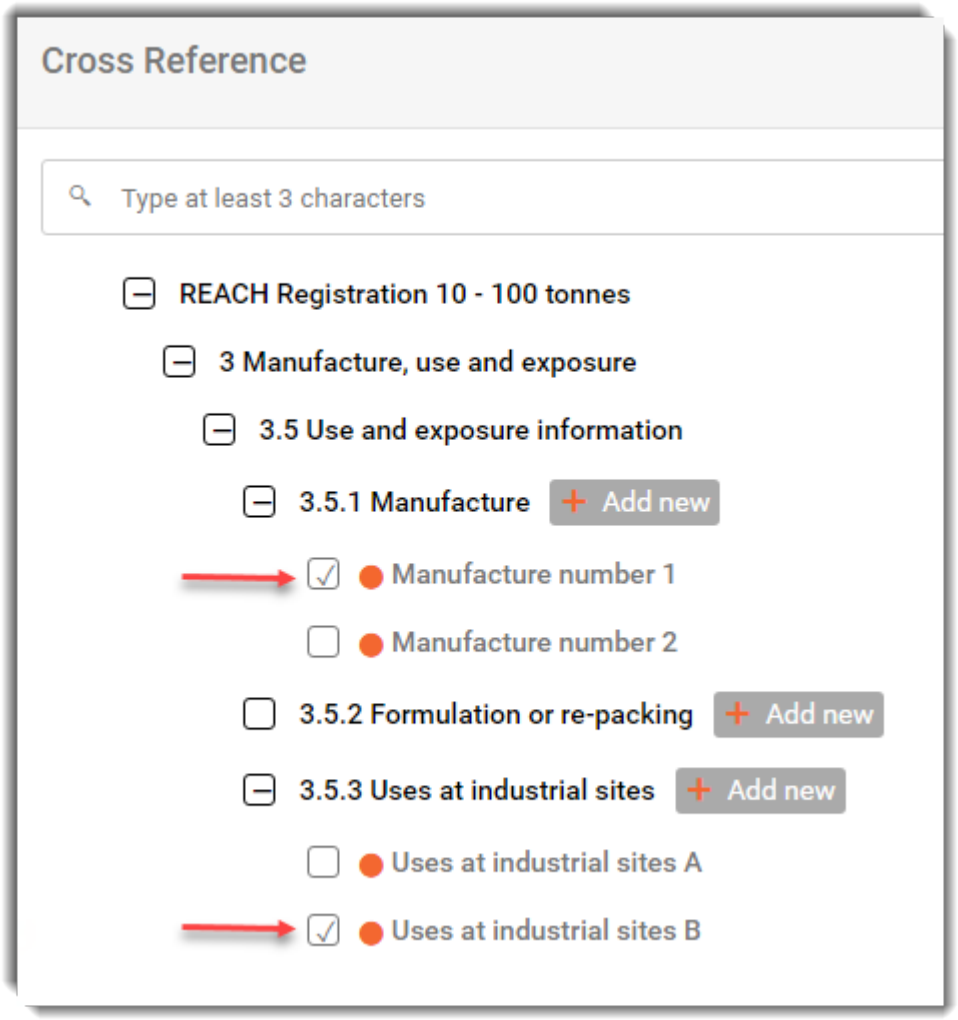
Some fields in a document consist of one or more references to other documents. In that case, clicking in the field to edit its value opens the window *Cross reference*, which displays the relevant documents in a tree view from which they can be selected. An example is shown below for the file *Manufacture / own use(s)*. The arrows point to the location of the required documents in the *Table of contents*.

Figure 77: Creating references between documents



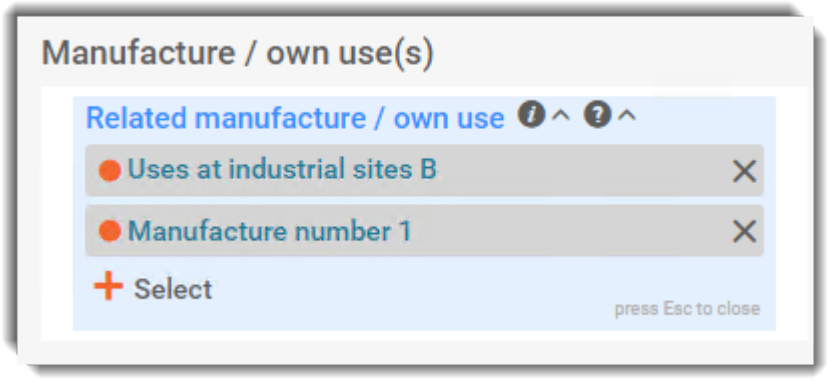
A document is selected from the tree by ticking its box. There can be multiple selections. The button *Add new* can be used to create a document directly from the selection window.

Figure 78: The Cross Reference window



On clicking on *Select*, the references are shown in the document.

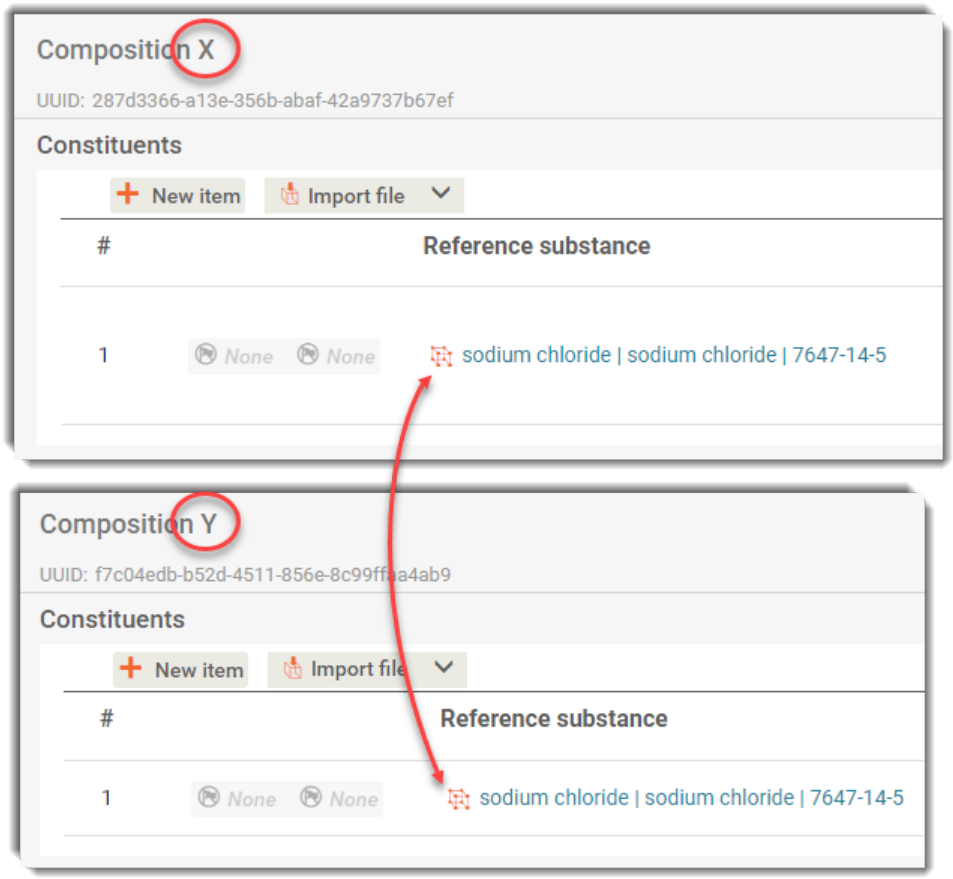
Figure 79: Cross references between documents



1.8. Inbound references

The ability of IUCLID to refer to an entity from more than one entity or document, is convenient and efficient because entities can be re-used, thereby avoiding duplication and inconsistency. An example is shown below in which a *Reference substance* is used in two different *Compositions*. If the *Reference substance* is edited, the changes automatically appear in both *Compositions*.

Figure 80: Example of an inbound reference



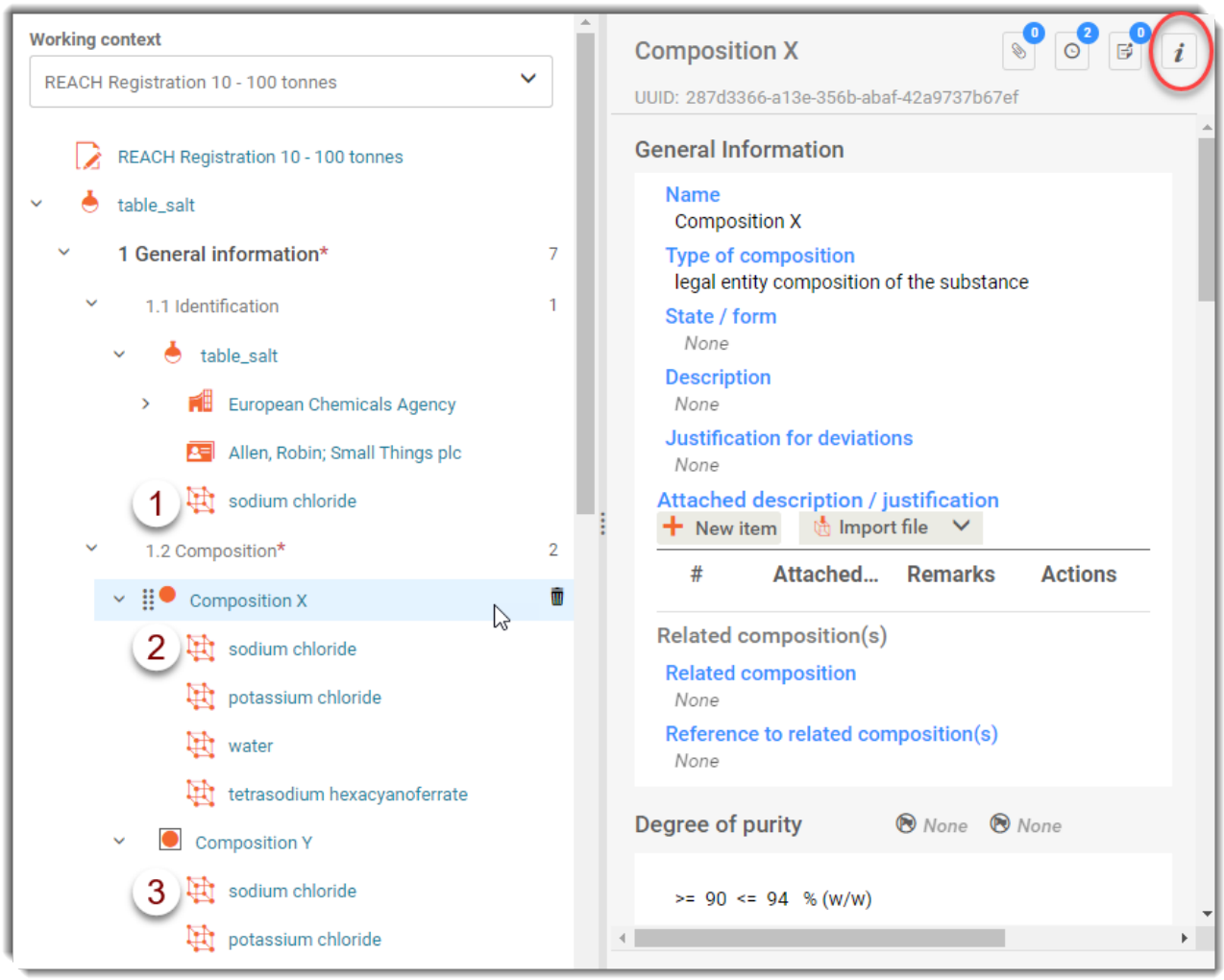
An entity that is directly linked to or referred to as shown in the example above is said to have an *inbound reference*.

Keeping track of the references can become complex, and needs to be taken into consideration when editing data, and especially when deleting entities. This process is made easier by the feature, *Inbound references*, which shows a listing per entity of the entities and documents that refer to it, and provides easy access to them. It is opened from the icon with an i , which is on the righthand side of the header in the data window. Associations between documents and entities that are not created in the way shown in the example above are not classed as inbound references. For example, an endpoint study record in a *Substance dataset* does not have an inbound reference from the *Substance*. The instance of the endpoint study record is unique to the *Substance* and not used elsewhere, even if its content has can been copied elsewhere.

Inbound references is not available for *Dossiers*.

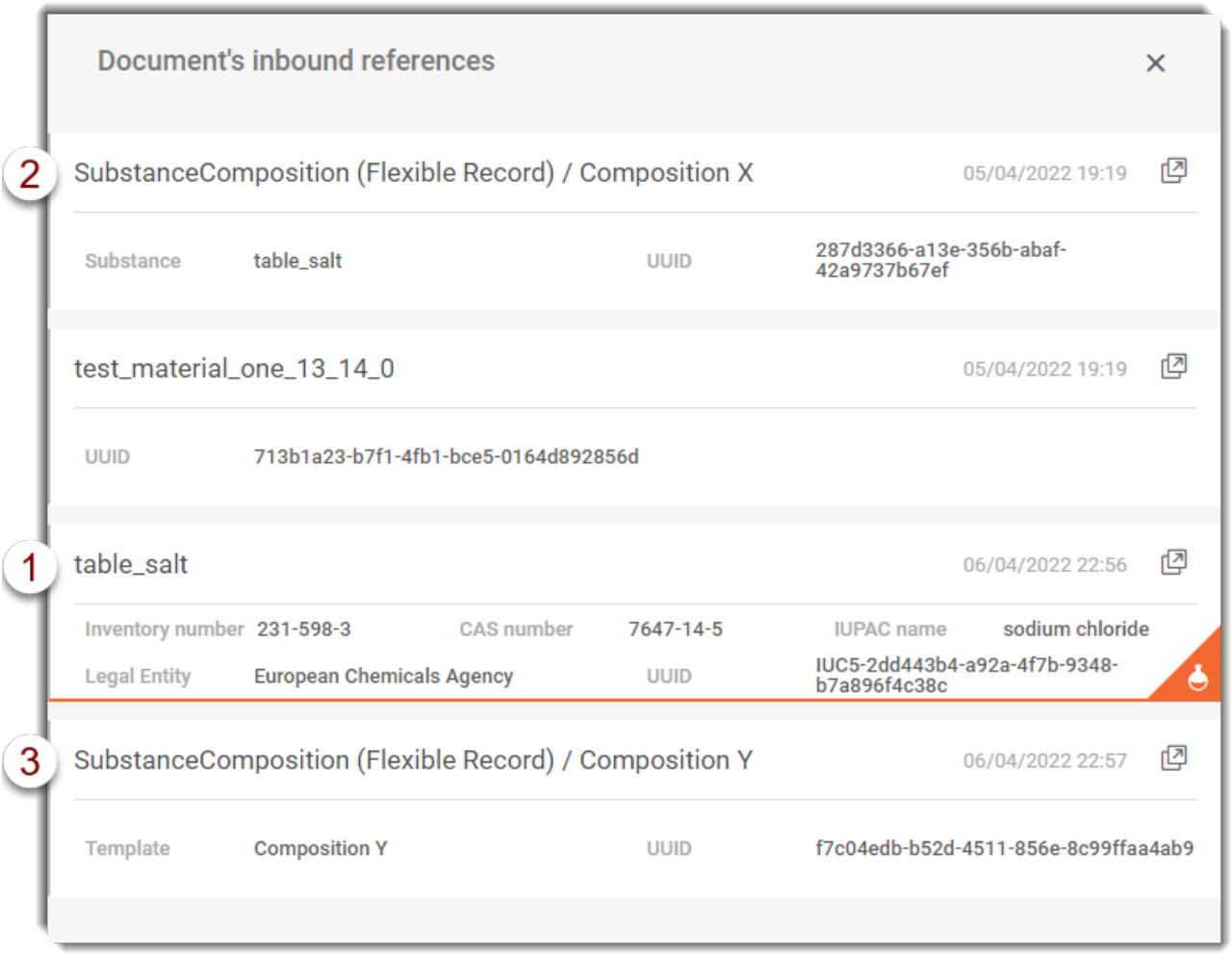
An example is shown below for a *Reference substance* that is referred to by a *Substance dataset* (1), a *Composition* directly in the *Substance* (2), and a *Composition* in an inherited *Template* (3). It is also linked to from a *Test material* but that cannot be seen from the view below.

Figure 81: An example of inbound links to a Reference substance from a Composition and a Substance



Opening *inbound references* from each of the three instances of the *Reference substance* shown above shows the same *inbound references* because they represent the same entity. The references are shown below.

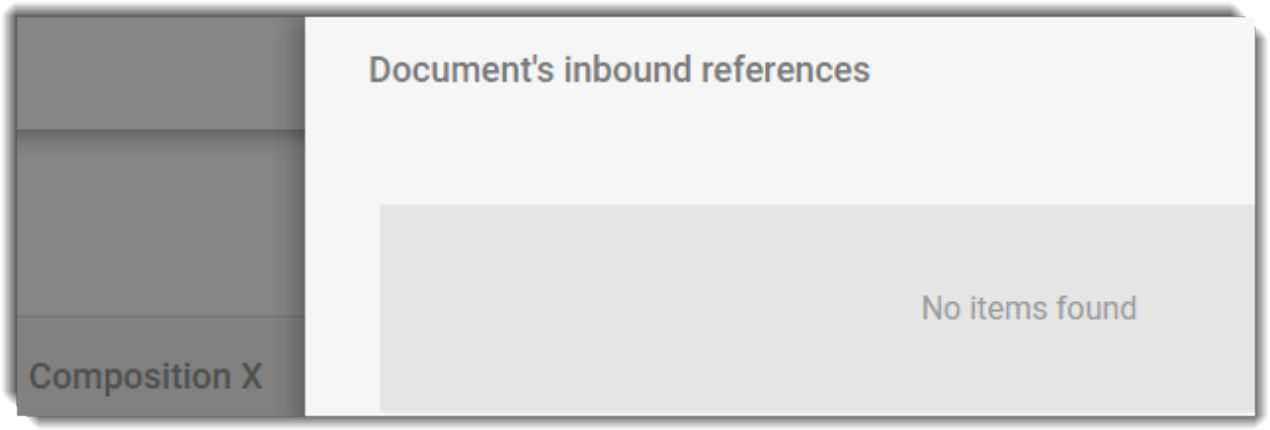
Figure 82: The inbound links for the Reference substance shown in the example above



The referring entity or document can be opened in a new browser tab from the arrow icon .

The *Reference substance* Sodium chloride is referred to, or linked to directly, by two *Compositions*, a *Substance* and a *Test material*. It cannot be deleted because that would break the links, which can be edited only from the referring entity. By contrast, the *Composition* shown selected above can be deleted, hence the dustbin icon. After deleting the *Composition*, the *Reference substances* in the *Composition* and the *Substance* that used to contain the *Composition* would still exist. The *Compositions* here have no *inbound references*, as shown below.

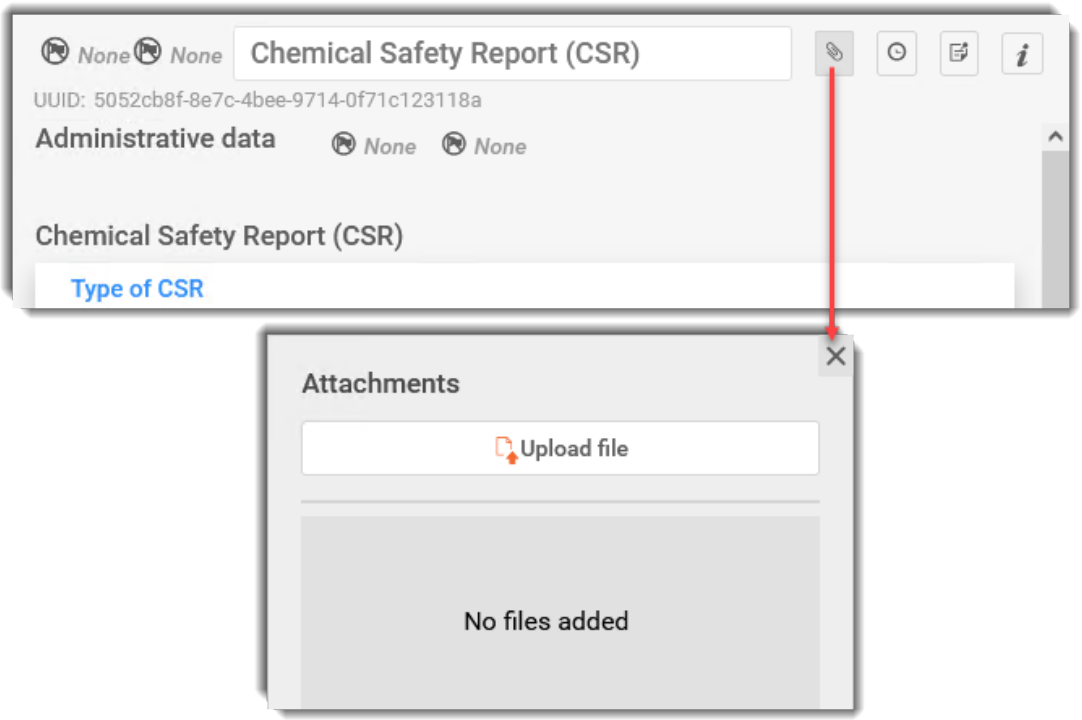
Figure 83: Documents with no inbound references



1.9. Attachments

An attachment is a file external to IUCLID, that has been included in a IUCLID document. This is done either for convenience, or because the data cannot be entered directly in to a IUCLID field. A file can be attached either to a whole document at its top level, or within a field. All the attachments for a document can be viewed from an attachments window which is opened from the paperclip icon ( ) in the application bar, as shown below.

Figure 84: Open the attachments window

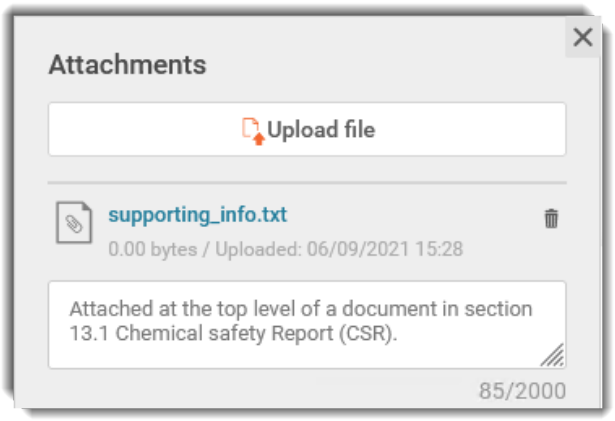


1.9.1. Attachments at the top level of a document

Files can be attached at the document level, only via the attachment window. To attach a file, click on *Upload file*, and then select a file. To remove a file, click on its dustbin icon in the attachments window. A remark can be added for each attachment by clicking on the icon .

An example of attachment to a whole document is shown below.

Figure 85: Attaching an attachment to a whole document



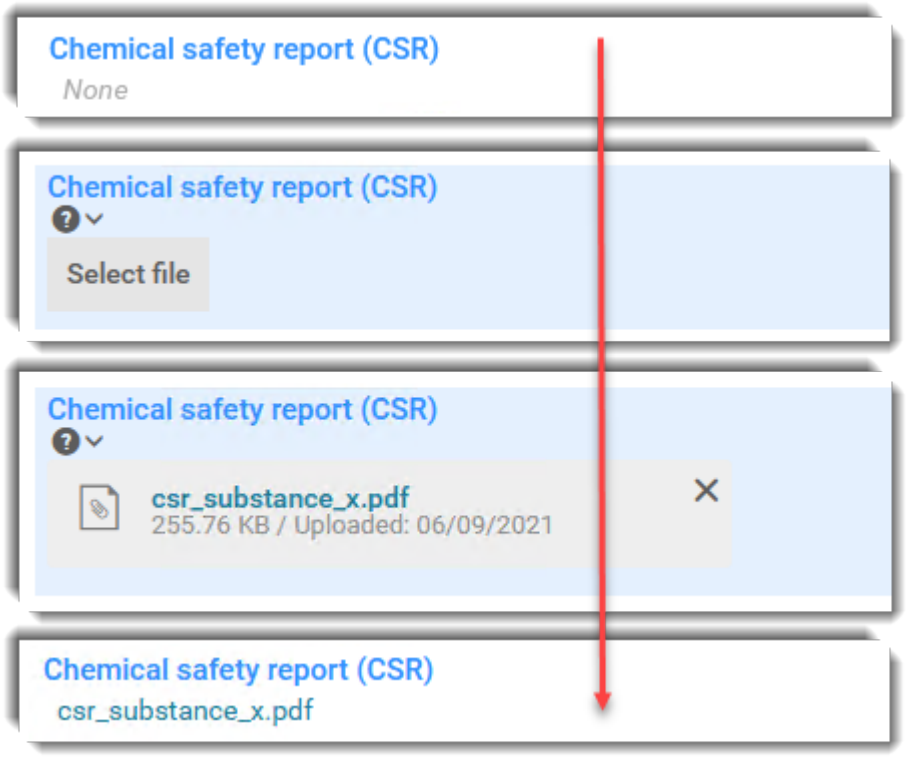
The draft dossier header and whole datasets behave as their own separate documents. Files can be attached at their top level, and they are accessible only from there, in the attachments window. Note that a file attached to a whole *Substance* dataset is accessible from the section *Identification*, and a file attached to a whole *Mixture/Product* dataset is accessible from the first section under the identity of the *Mixture/Product*.

1.9.2. Attachments at the field level

At the field level, a file is attached by clicking in the field to enter edit mode, and then by clicking on the box labelled *Select file*. Once attached, a file can be removed by entering edit mode, and then clicking on the x icon.

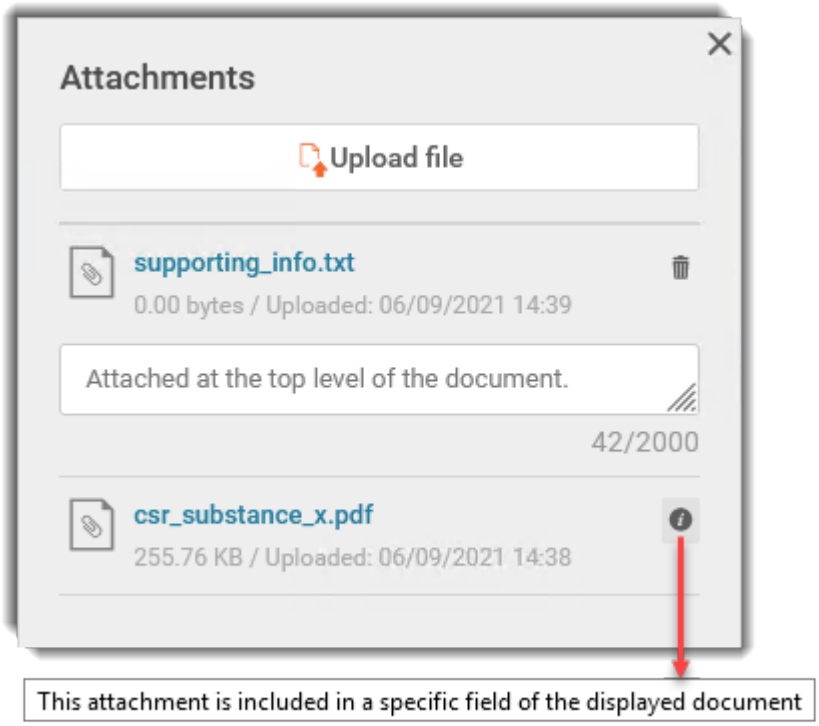
An example of attachment within a field is shown below for the attachment of a Chemical Safety Report in section *13 Assessment reports*, under REACH.

Figure 86: Attaching an attachment within a field



The file name of an attachment in the data window is a link to the file, from which it can be downloaded. Opening the attachments window shows the attachment at the field level, underneath those at the document level.

Figure 87: At attachment at the field level in the attachments window



Note how unlike the attachment at the level of the document, the attachment at field level cannot be deleted via the attachments window. That can be done only from the field.

1.9.3. Attachments created on migration

If a migration of data across different versions of IUCLID involves the transfer of data into a version of IUCLID that has no equivalent field in which to place it, the data is not lost, but is automatically placed into a new text file that is then attached to the document. The file name of such attachments is of the form:

…<source version>-to-<destination version>_migration_<date>.txt

1.10. Search in a list of entities

The lists of entities accessed from the main menu all contain a simple search function, and an *Advanced search* function. Both types are described below. Remember that on the dashboard there is also *Search entities and dossiers by UUID*.

1.10.1. Simple search in a list of entities

To do a simple search within a list on entities, enter a search term into the box at the top left of the list, and then click on the button with the magnifying glass. The search can match any of the values shown in the list, which for example, can contain chemical identifiers.

If a value starts with the search term, it matches. The wild card * can be used to represent one or more of any character.

Example

Search for the *Reference substance* Sodium iodide in the figure below.

Terms that match:

Sodium

sodium

*iodide

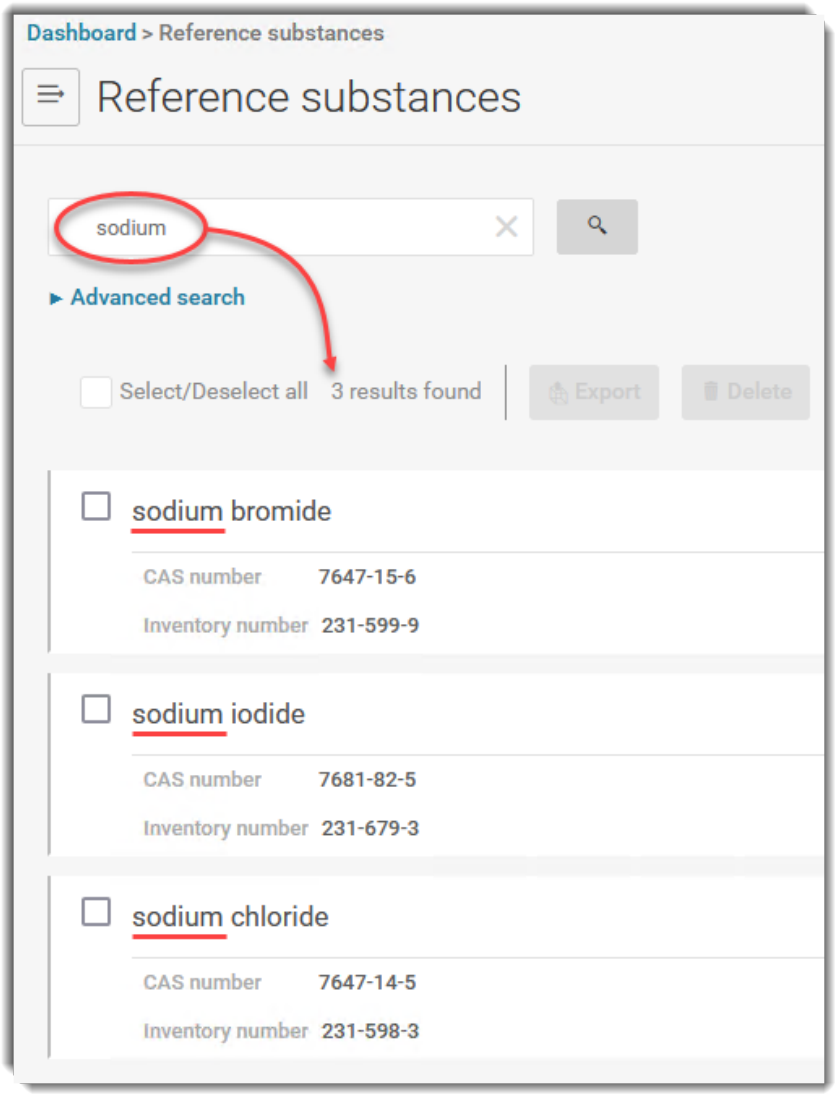
Sodium *ide

231-679-3

Terms that do not match:

iodide

Figure 88: Search for an entity



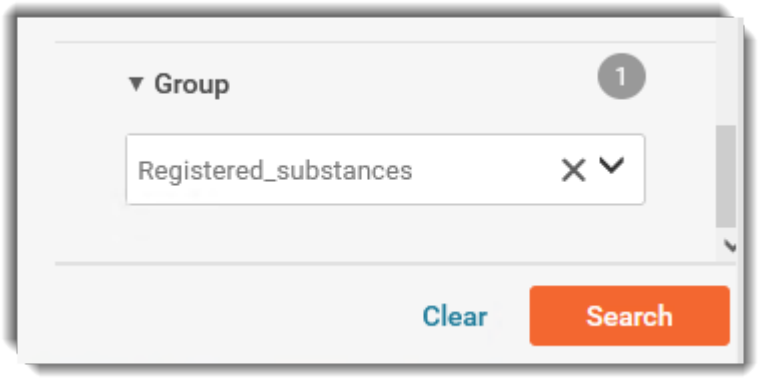
1.10.2. Advanced search in a list of entities

Each type of entity has an advanced search on its list page. The searchable fields available depend on the type of entity, although they all have *Modification date*. Multiple criteria can be added to which Boolean logic applies. A grey horizontal line between criteria is interpreted as AND. The operator between multiple items of the same type is OR. The number of criteria for each type of data is shown in a round icon to the right of the criteria. The total is shown in the header of the search results. The search results have the same functionalities as the list page.

For *Substance*, the AND operators are applied across multiple *Compositions* in such a way that there does not have to be a single *Composition* that satisfies all the criteria applied to *Constituent*, *Impurity* and *Additive*.

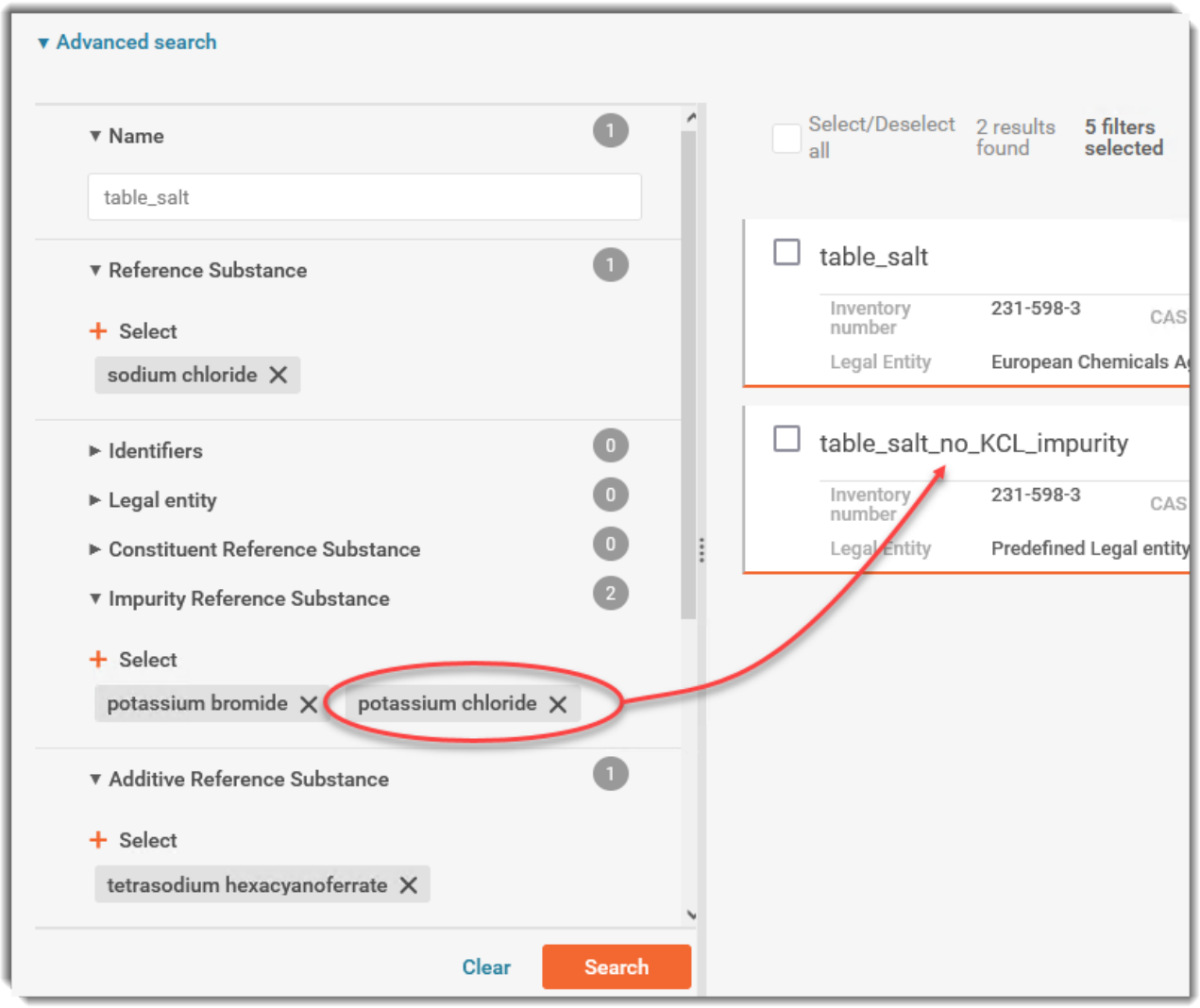
If *Instance Based Security (section 24.4)* is in use for the instance of IUCLID, a search criterion for a single security *Group* can be added. The search is limited to items that have been shared to the security *Group* with at least read access, and where the *User* is a member of the security *Group*. An example is shown below for a security *Group* named *Registered_substances*.

Figure 89: Search by security group



An example search for *Substances* is shown below.

Figure 90: Advanced search for entities in a list page - Example for Substances



Example above

The name of the *Substance* must begin with "table_salt" and other characters can follow it.

The *Reference substance* in section 1.1 of the *Substance* must be Sodium chloride.

In an *Impurity* in a *Composition* of the *Substance*, there must be *Reference substances* of either Potassium chloride **or** Potassium bromide. Thus, there is a search hit that does not contain Potassium chloride as an impurity.

In an *Additive* in a *Composition* of the *Substance*, there must be a *Reference substance* of Tetrasodium hexacyanoferrate.

The criteria stated above for *Impurity* and *Additive* do not have to be satisfied by the same *Composition*.

2. Substance

A *Substance* is a type of 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 the identity of the chemical substance and a broad range of different types of information relevant to its regulation. The fields are organised in a *Table of contents*. For more information see 1.7.12 Table of contents.

In the table of contents, 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*.

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.

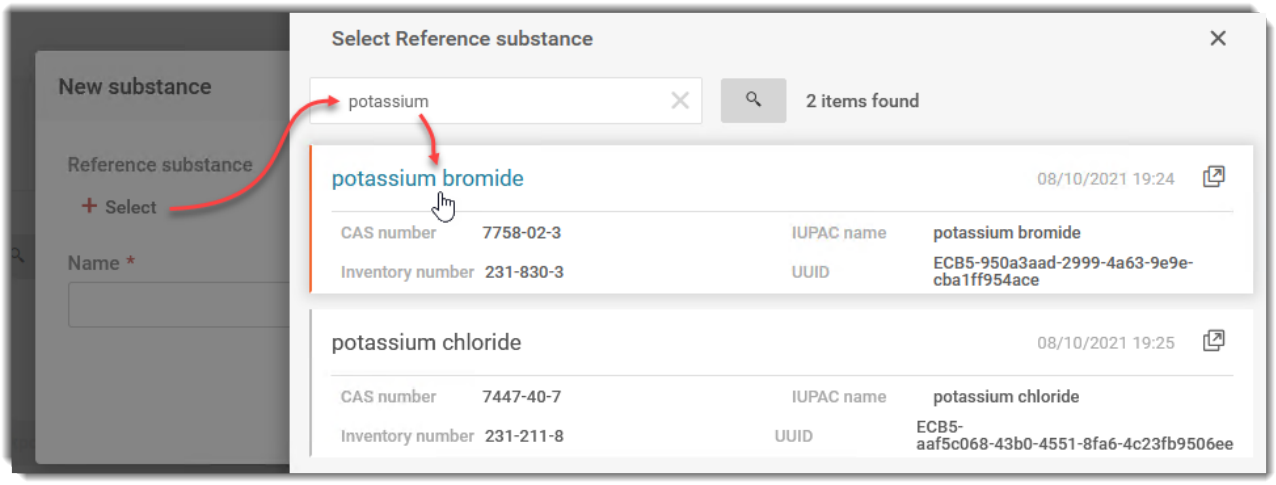
http://echa.europa.eu/manuals

A *Dossier* used to submit information on a chemical substance to a regulatory authority contains a read-only copy of a *Substance* dataset. IUCLID can be used to create such *Dossiers* directly from a *Substance dataset*. A read-only copy of a *Substance* dataset within a *Dossier* is indicated in the IUCLID interface by placing a lock icon next to the *Substance* icon, as shown below:

The list of *Substances* can be accessed from the *Dashboard* and the *Main menu*. The viewing of *Dossiers* that refer to *Substances* is described in section *6.3 Viewing Dossiers and Substances or Mixture/Products*.

On creation of a *Substance*, it must be given a name that is unique in the instance of IUCLID. In the first step, there is an option to define which *Reference substance* will be referred to in the field *Identification of substance*, because that field must be filled in if the *Substance* is to be used in a regulatory context. For more information about *Reference substances* see section *9 Reference substance*. A *Reference substance* can either be selected from those already in the instance of IUCLID, or one can be created. An example of selection is shown below for Potassium bromide.

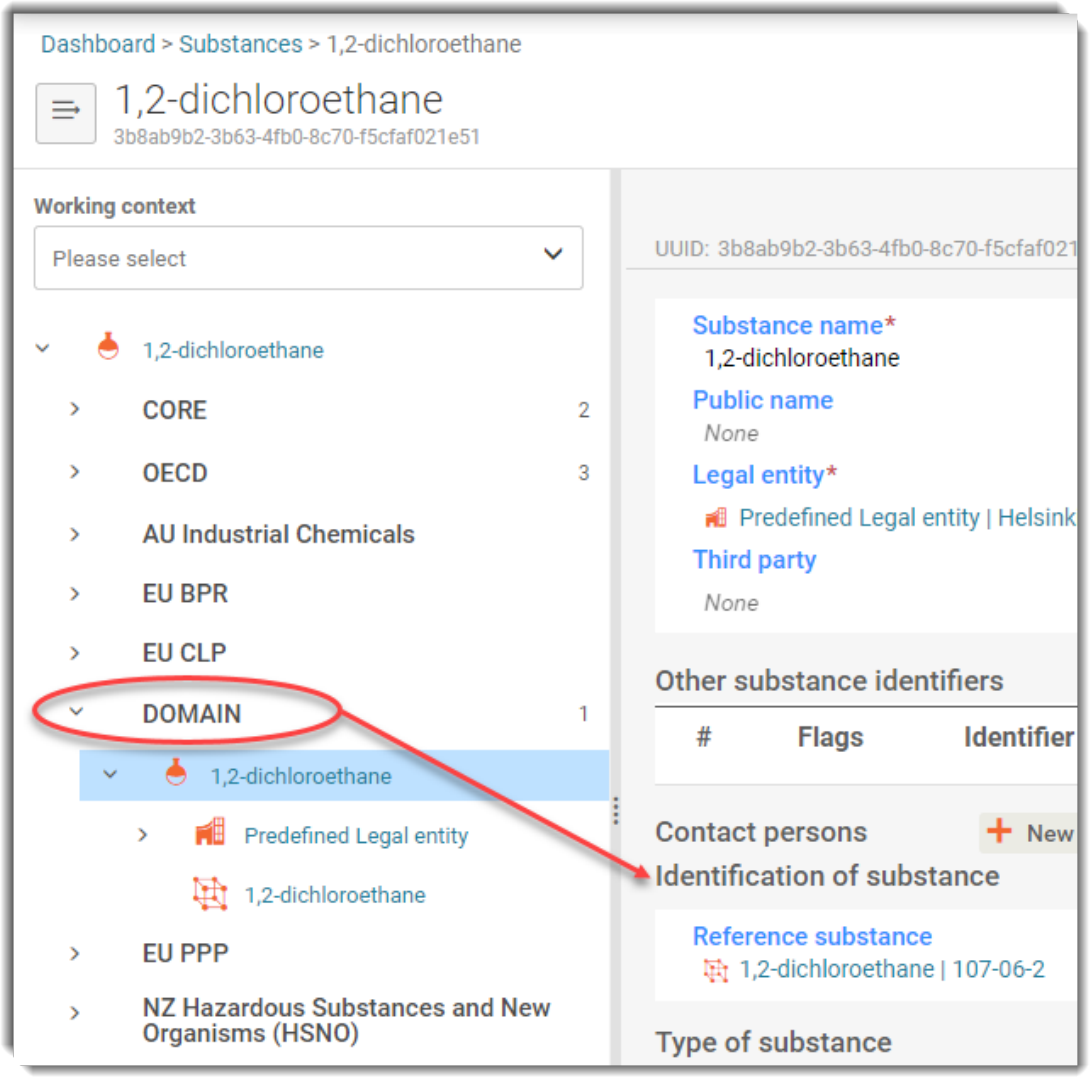
Figure 91: Whilst creating a Substance, select the Reference substance that identifies it



If no value is entered for the name of the *Substance*, if possible, the name is set to be the name of the *Reference substance*. On creation, a *Substance* is automatically associated with the working *Legal entity* of the IUCLID *User*. This can be changed later, if required. The default is *Predefined Legal Entity*, which is delivered with IUCLID.

The location of the field *Identification of substance*, and therefore the *Reference substance* is determined by the working context. If no working context is set, the *Reference substance* is under DOMAIN, as shown below.

Figure 92: Location of the identifying Reference substance of a Substance where no working context is set



2.1. The Assessment entity

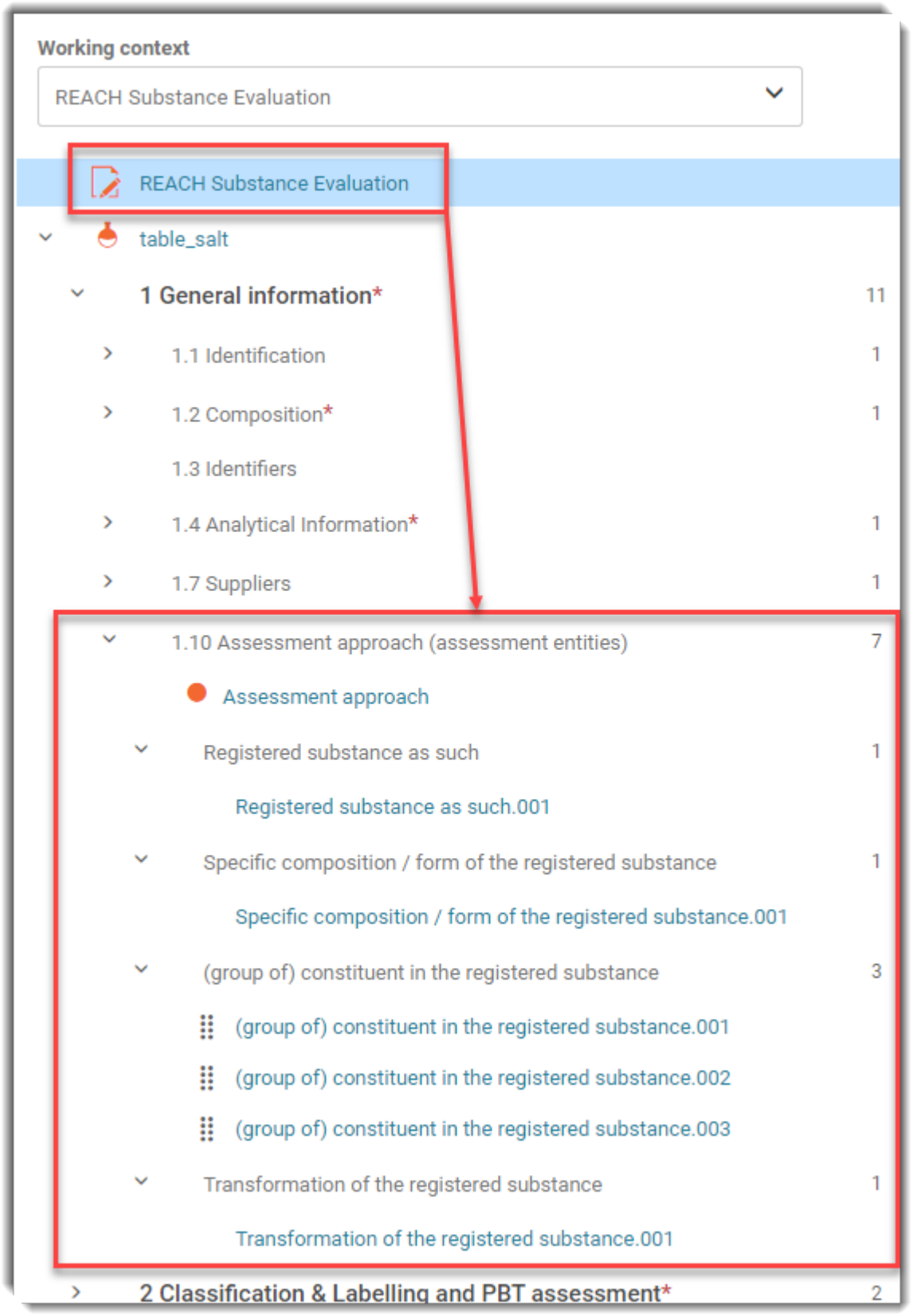
An *Assessment entity* can be thought of as a wrapper for a set of substance property data, across endpoints, that is used for assessment purposes. It enables the definition of consistent sets of properties that are relevant to the assessment of specific compositions/forms of the substance whether placed 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, where only one document can be created, and four subsections under which multiple records can be created. An example is shown below.

Figure 93: Assessment entities in the table of contents



2.1.1. 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.

2.1.1.1. 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*.

2.1.1.2. Approach to fate/hazard assessment - public information

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

2.1.2. Types of assessment entity

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

5. Registered substance as such
6. Specific composition/form of the registered substance
7. (group of) constituent in the registered substance
8. Transformation of the registered substance

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

2.1.2.1. Assessment entity confidentiality claim

A flag can be set that applies to all of an individual *assessment entity* document. A flag is set by clicking on the flag icon to the left of the name in the application bar. For a full description of flags, see section *1.7.7 Flag*.

2.1.2.2. 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.

2.1.2.3. Relation to the registered substance

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

2.1.2.4. 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*]

2.1.2.5. 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*.

2.1.2.6. 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.

2.1.2.7. 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 or summaries 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.

2.1.2.8. Reaction schema

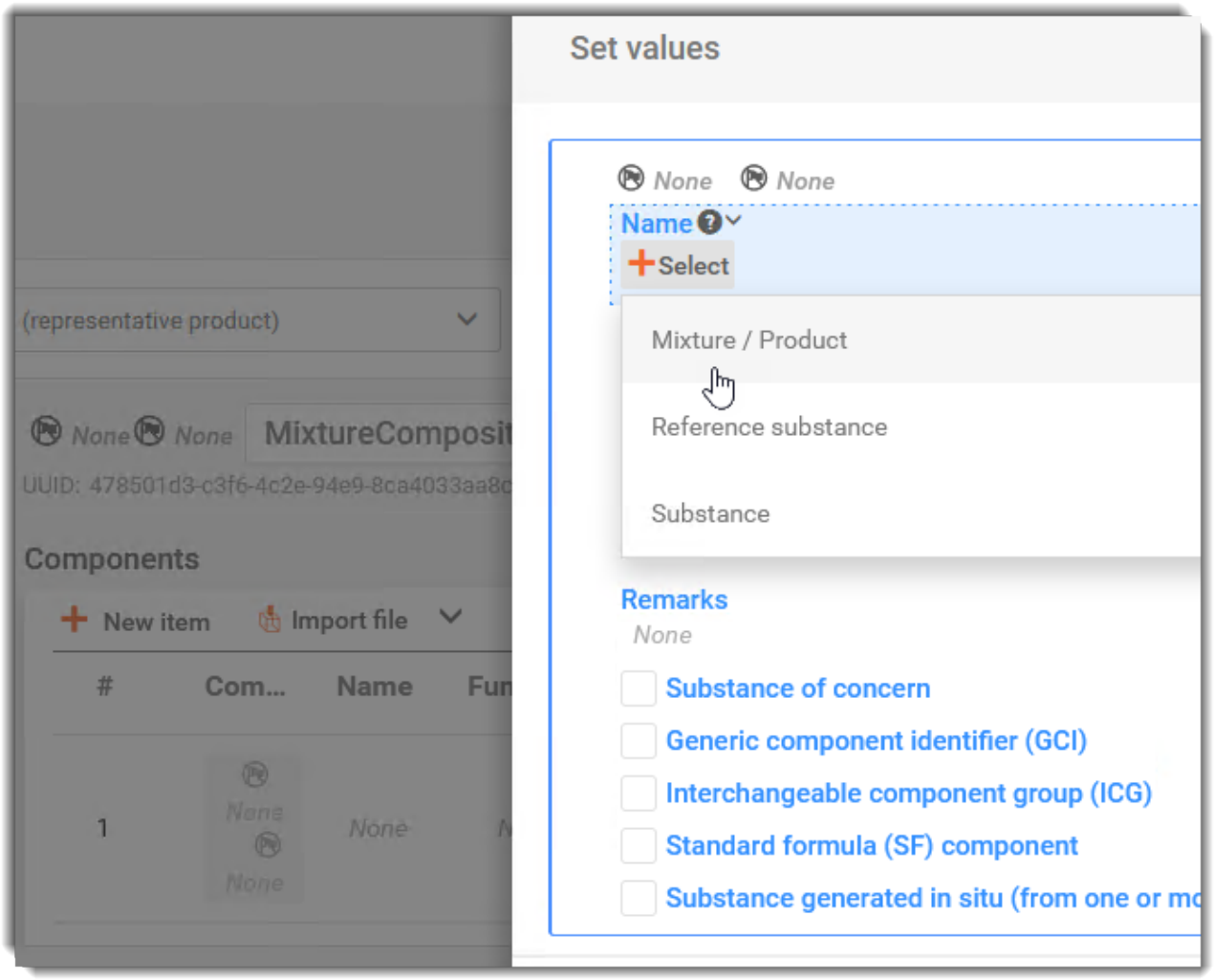
Upload the image of the reaction schema when needed [for *Transformation of the registered substance*].

3. Mixture/Product

A *Mixture/Product* is a type of entity in IUCLID that is used to store information on a chemical substance that is considered to be in a regulatory context, either a mixture, or a product, or both. An example is the concept of *Mixture/Product* under the BPR regulation.

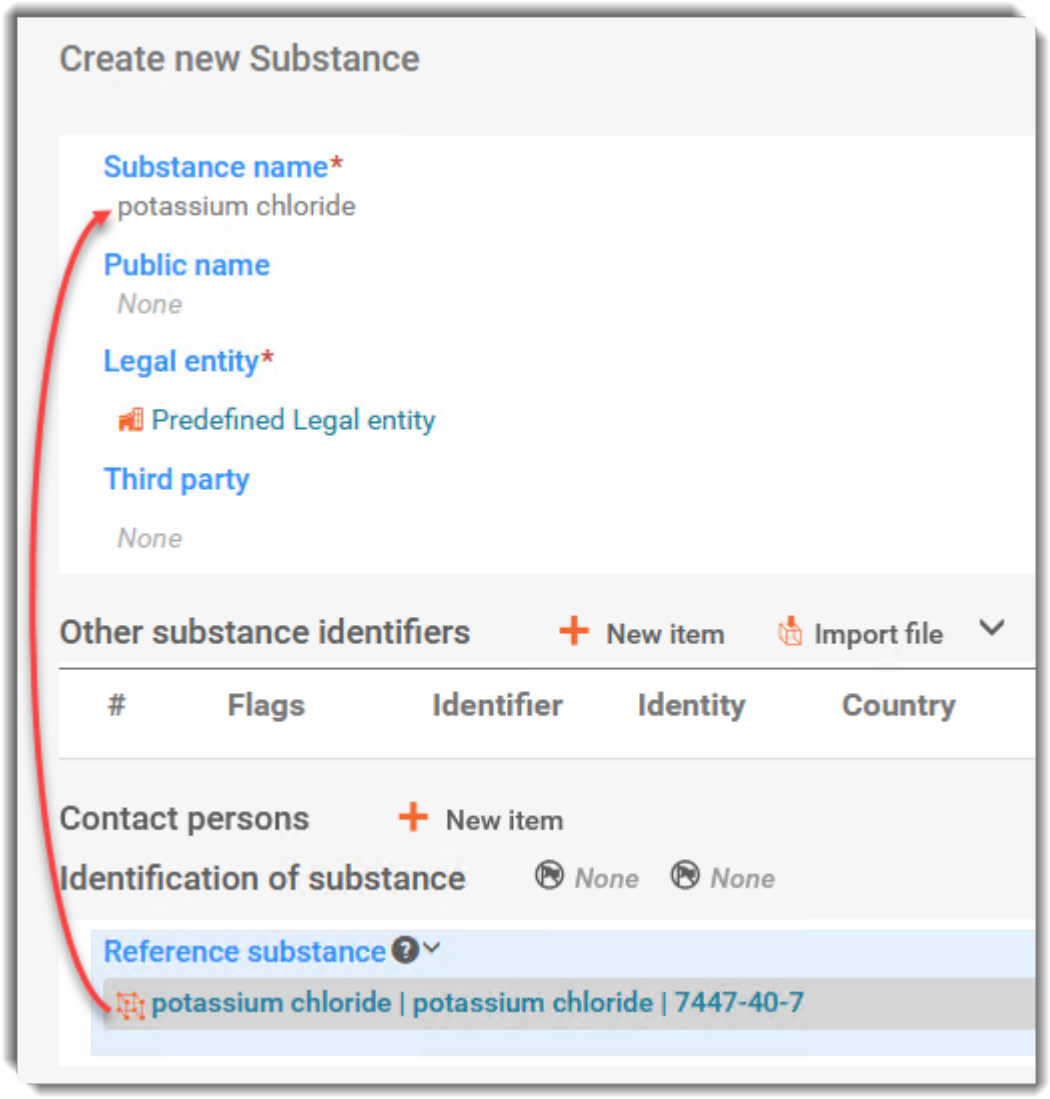
Like a *Substance* a *Mixture/Product* has a *Composition* but it contains an additional field named *Formulation type* which is relevant to *Products*. In addition, the *Mixture/Product* contains *components* instead of *constituents*. A *component* refers either to a *Reference substance*, a *Substance* or another *Mixture/Product*. The type of entity is selected from within the *Name* field of the component, as shown below for the addition of a *Mixture/Product*.

Figure 94: Adding a Mixture/Product as a component in a Mixture/Product



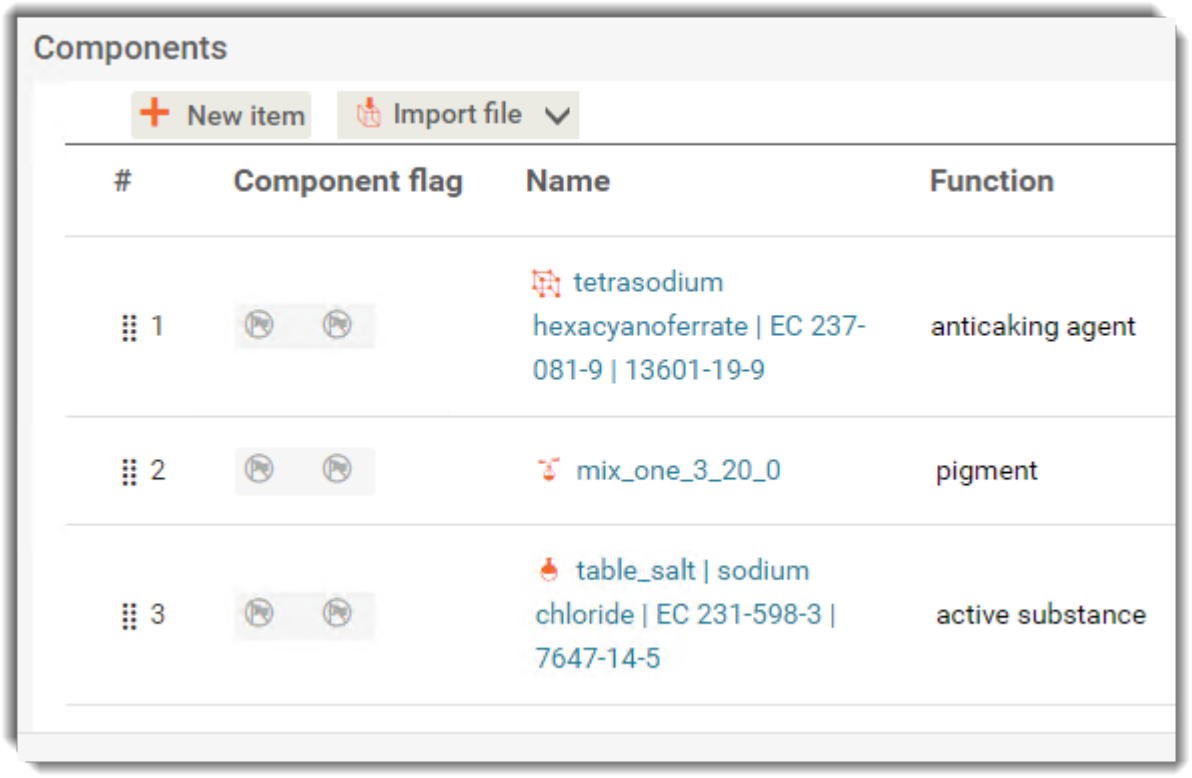
After the type of entity has been selected, it is possible to select existing entities, or to create them. For example, whist creating a *Substance* a *Reference substance* can be selected that is used as the basis for the *Substance*. This is similar to the functionality when creating a *Substance* from the list page of *Substances*. In the example shown below, a *Reference substance* named Potassium chloride has been selected, which has caused the *Substance* to be named potassium chloride automatically. The *Legal entity* of the *Substance* is automatically set to the working *Legal entity* of the IUCLID *User*.

Figure 95: Mixture/Product component - create a Substance based on a Reference substance



In a *Mixture/Product*, *components* are shown in a numbered list, which can be re-ordered by dragging and dropping. An example of the list is shown below.

Figure 96: Components in a Mixture/Product



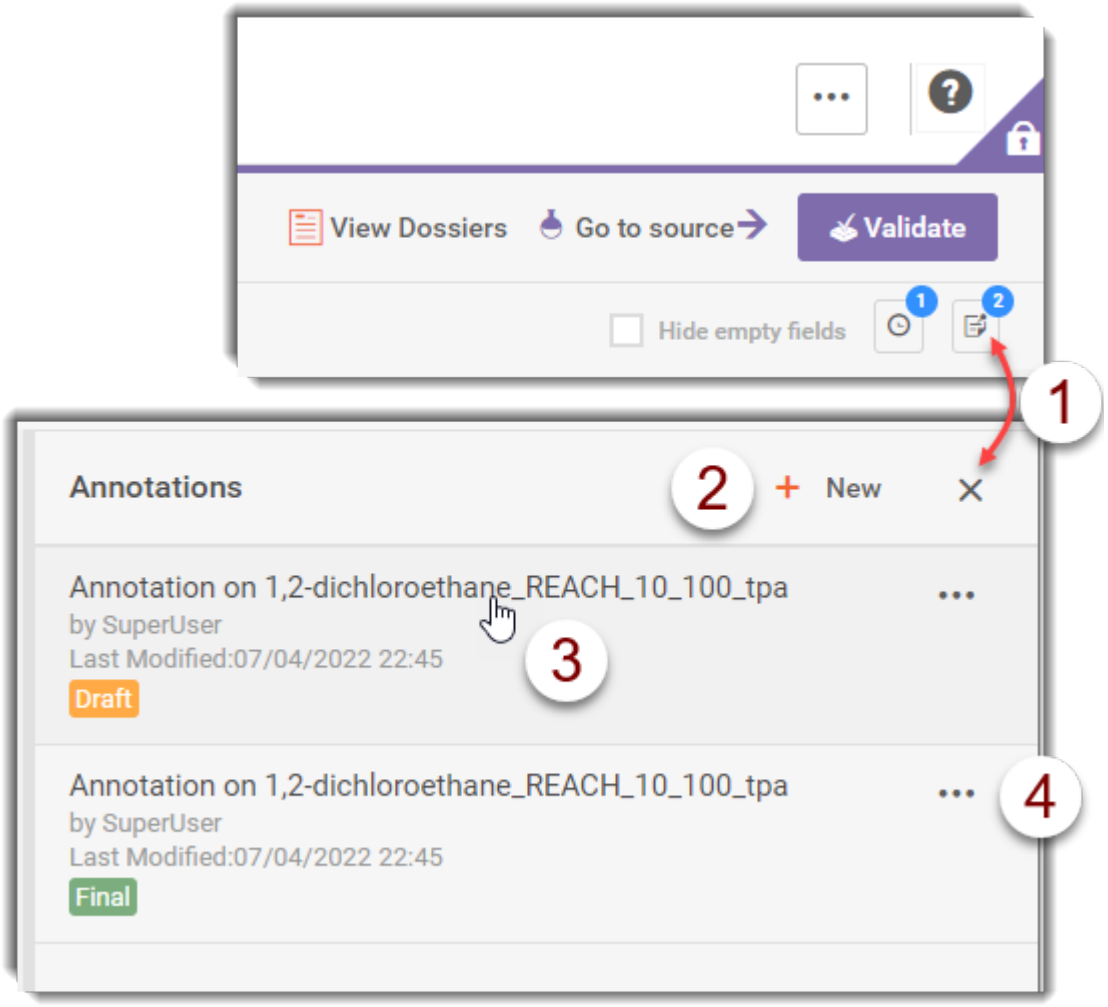
Mixture/Product can be accessed from the *Dashboard* and the *Main menu*. The way they are viewed is linked to the viewing of *Dossiers* that refer to them, as described in section *6.3 Viewing Dossiers and Substances or Mixture/Products*.

4. 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 provides more functionality than using an attachment because the data is structured within IUCLID. An *Annotation* is applied to an individual document. A document can have more than one *Annotation* applied to it, and an *Annotation* can be applied to more than one document.

The *Annotation(s)* applied to a document are accessed and managed via a link at the top right of the record of the document, as indicated in the figure below.

Figure 97: Viewing and managing the Annotations applied to a document



Legend for Figure 97

1. Open and close the list of *Annotations* for the document by clicking on the *Annotation* icon and the cross, respectively;
2. Create an *Annotation* for the current document;
3. Edit an *Annotation* by clicking on its record in the list. The value of the *status* field for the *Annotation* is shown with a colour code;
4. Actions that apply to only the specific *Annotation* are accessed via the three-dot icon, for example, delete.

There are two sections in an *Annotation*, as described below.

4.1. Annotation - 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*.

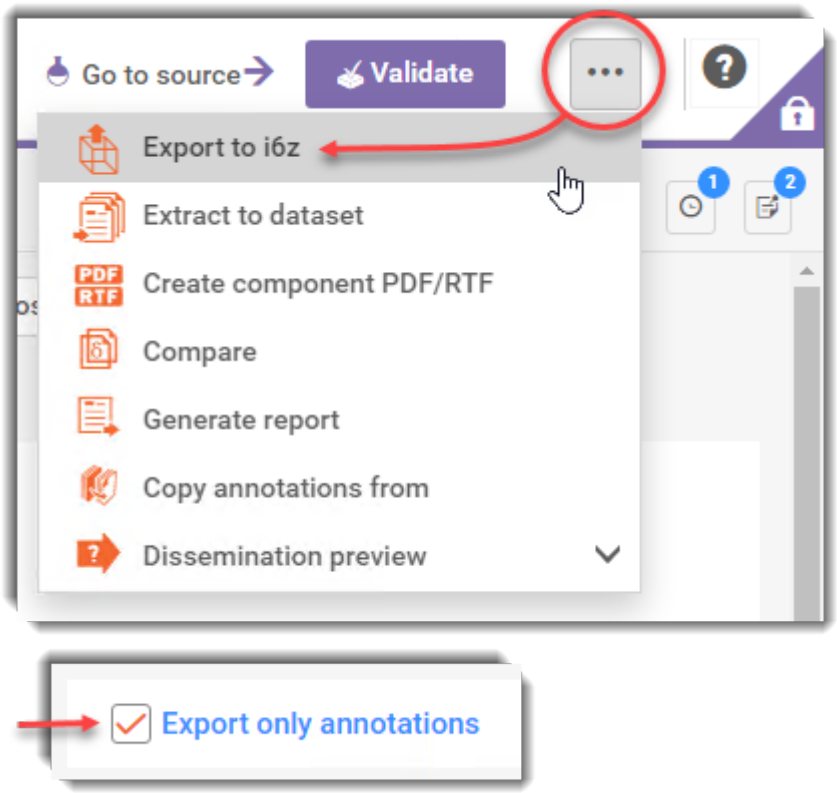
4.2. Annotation - Dataset data

This section 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 a free-text template. To open the free-text template, click on the icon that shows the letter A with an arrow at the bottom right, . To copy the text from the template to the field, click on the button labelled *Insert…* . Next, edit the text in square brackets, as required.

4.3. Annotation - Export to i6z

The *Annotations* for a *Dossier* can be exported all at once in a `zip` archive that contains an `i6z` file per *Annotation*. The option *Export to i6z* is on the menu shown in the application bar whilst viewing the record of the *Dossier*. Select the option *Export only annotations*.

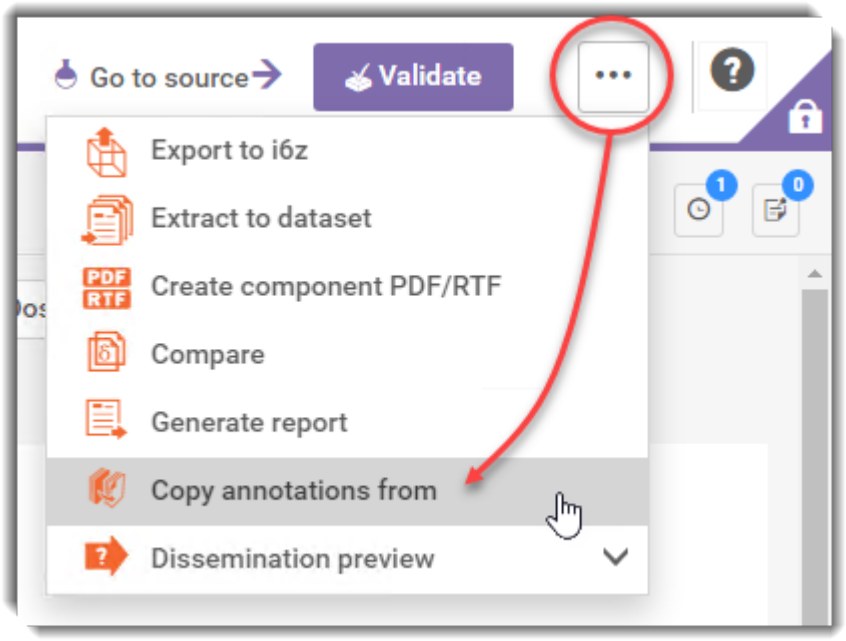
Figure 98: Export the Annotations from a specific Dossier



4.4. Copy annotations from

This is used to copy *Annotations* between *Dossiers*. The target *Dossier* is the currently selected one. Select the source *Dossier* from the list.

Figure 99: Copy annotations from



5. Template

A *Template* is a type of entity that allows data from multiple sections to be inserted into a *Substance* or *Mixture/Product* dataset all at once, without having to manually recreate all the sections individually, and re-enter the data. *Templates* can be managed from their list view, which is accessible via the main menu.

5.1. Data from a Template in a Substance or a Mixture/Product

Data from a *Template* can be transferred to a *Substance* or *Mixture/Product* dataset, either by copying from the Template, or by inheriting the *Template*.

5.2. Copy data from a Template

The function *Copy data from …*, may be used to copy either all or a selection of documents from a *Template* to a *Substance* or a *Mixture/Product.* There is no link to the *Template*. The function is described in its own section *22 Copy data from … .*

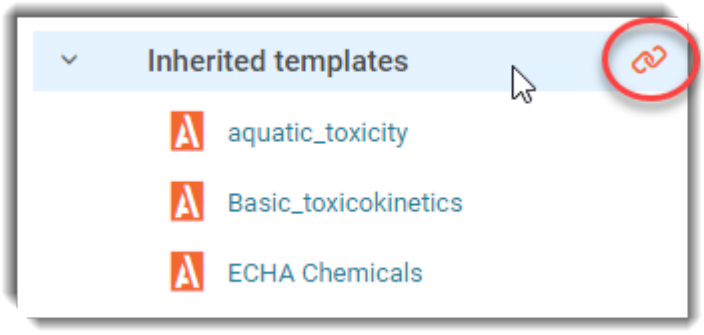
A document copied in this way can be modified in the *Substance* or *Mixture/Product* to which it was copied. Changes to the data in the *Template* do not affect the *Substance* or *Mixture/Product* to which it was copied. If a *Template* is copied more than once to the same *Substance* or *Mixture/Product*, new extra copies of the documents are added to the table of contents, without over-writing data. Documents copied from a *Template* are added to the table of contents 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.

5.3. Inherit a Template

There are dynamic links between all the data in an inherited *Template*, and the *Substance* or *Mixture/Product* that inherits it. A *Template* can be inherited by more than one *Substance* or *Mixture/Product* at the same time. Modifications made in the *Template* are available immediately in the *Substance* or *Mixture/Product*.

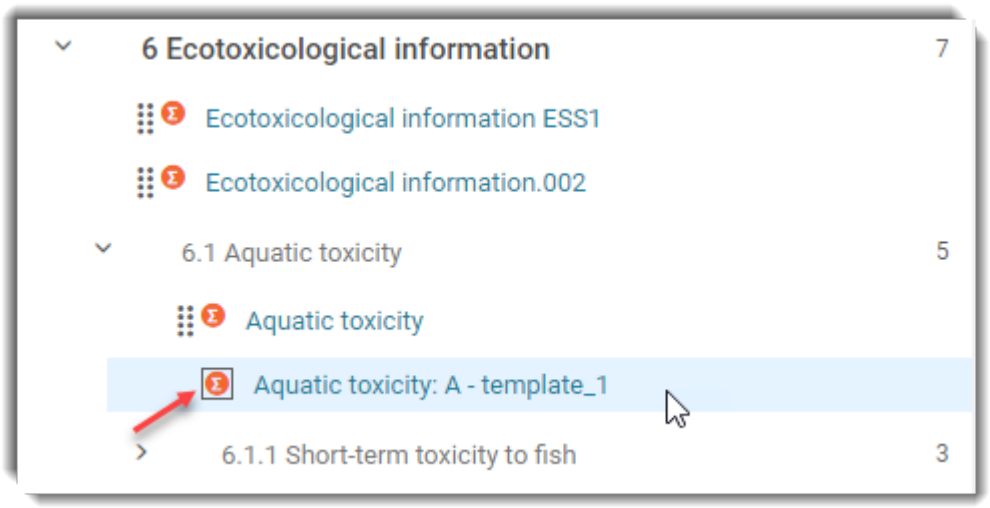
The inheritance is managed from the foot of the *Table of contents* of a *Substance* or *Mixture/Product*. To create an inheritance, click on the orange link icon, and then select one of the available *Templates*. To remove an inheritance, click on the struck-through orange link icon to the right of the Template.

Figure 100: The inherited Templates for a dataset



Documents inherited from a *Template* are visible in the *Table of contents* of the *Substance* or *Mixture/Product*. They are shown beneath non-inherited documents, marked out by an icon that has a box surrounding the standard icon, as shown below.

Figure 101: A document from an inherited Template in the table of contents



Note how the inherited documents do not have delete buttons and the order of listing cannot be changed from the dataset. They can be removed only by deleting them from the *Template*, or by removing the inheritance.

The data in a *Template* can be accessed for editing from the *Table of contents* of a dataset that has inherited it. Where that is done, the following warning is given:

6. Dossier

A *Dossier* is used to submit data to a regulatory authority to satisfy a legal obligation arising from a legislation, for example REACH.

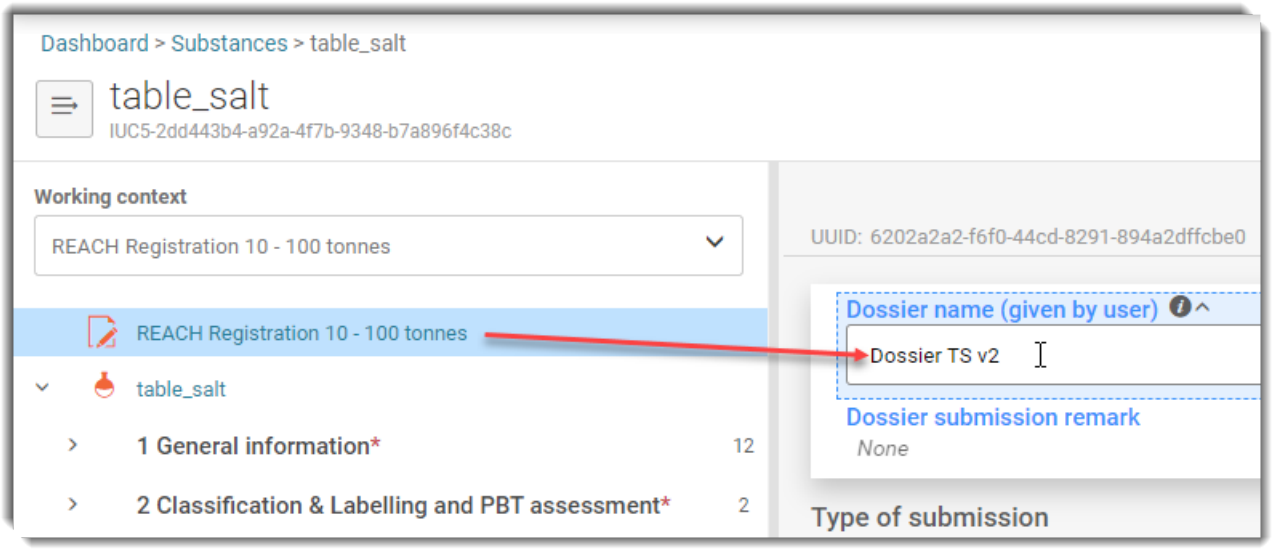
A *Dossier* contains a read-only copy of a header for storing administrative data, and a read-only copy of either a *Substance* or a *Mixture/Product* dataset. *Dossiers* are created starting from the *Substance* or *Mixture/Product* dataset which they will contain. The functionality described in this section applies to both *Substances* and *Mixture/Products*.

6.1. Dossier header

A *Dossier* header is a set of fields used to store administrative information that is relevant to the submission of data under a particular regulation. The fields present are determined by the *Working context*. Each *Substance* dataset has a *Dossier* header associated with it which can be edited at any time, including during *Dossier* creation. When a *Dossier* is created, a read-only copy of the *Dossier* header is placed into the *Dossier*.

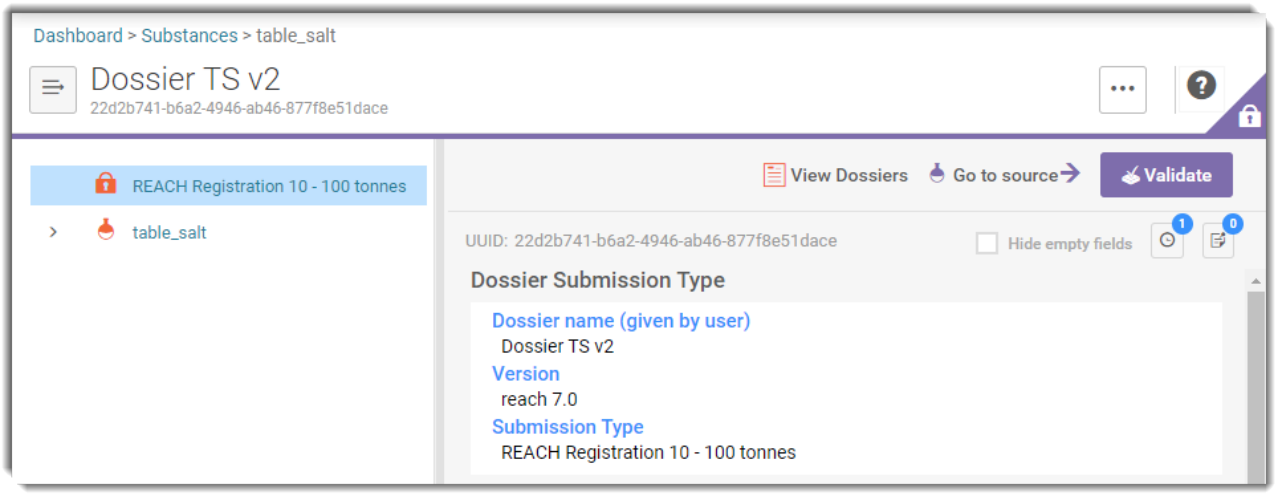
The *Dossier* header is accessed independently of *Dossier* creation from the top of the *Table of contents*, as shown in the figure below.

Figure 102: Editing the Dossier header independently of Dossier creation



During *Dossier* creation, the first step is to review and/or edit the *Dossier* header. See the section on *Dossier* creation for more information. Once a Dossier has been created, its read-only *Dossier* header can be viewed at the top of the table of contents, as shown in the example below.

Figure 103: View the read-only Dossier header in a completed Dossier



The values to be entered into the *Dossier* header depend on the specific circumstances under which data is to be submitted to a regulatory authority. For example, for advice on how to fill out the header under the REACH regulation, see the manual *How to prepare registration and PPORD dossiers*, which is available on the ECHA website here. Translated versions of that manual, and other manuals on *Dossier* preparation under the REACH and CLP regulations are available on the ECHA website at the following address:

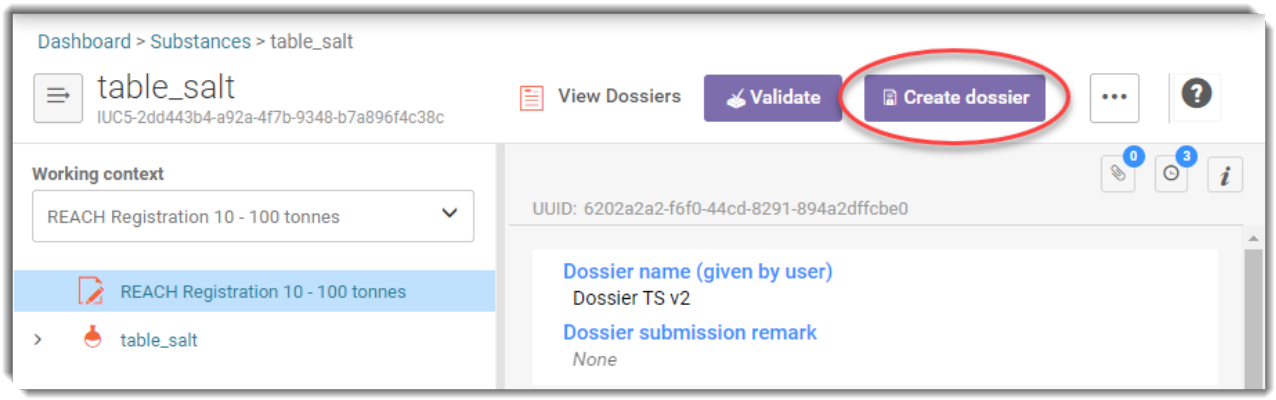
http://echa.europa.eu/manuals

6.2. Creating a Dossier

Before creating a *Dossier*, a *Working context* must be selected. This allows the IUCLID interface to present to the user at the start of *Dossier* creation, either a pre-filled or blank *Dossier* header of the correct type. Entering data into the *Dossier* header is an essential part of creating a *Dossier*, for the reasons described in section *6.1 Dossier header*.

Dossier creation is started by clicking on the button labelled *Create dossier*, which is shown at the upper right of the record of a dataset. If the button is dimmed and cannot be clicked on, select a *Working context*. An example where to find the *Create dossier* button is shown below for a *Substance* dataset.

Figure 104: Start Dossier creation for a Substance dataset



Fill out the *Dossier* header, and then click on one of the buttons at the foot of the page. To use default settings, click on *Create dossier*, in which case you can skip the next section. To use advanced settings, click on the button labelled with three dots, as described in the next section.

Figure 105: Enter values into the Dossier header during creation of a Dossier

6.2.1. 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*. To use advanced settings, click on the button labelled with three dots, as ringed in red in the screenshot below.

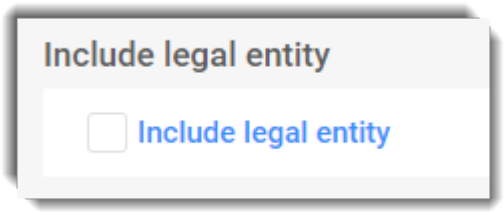
Figure 106: Enter values into the Dossier header during Dossier creation

After editing the advanced settings, click on *Create dossier*.

6.2.1.1. *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**, which is the setting shown in the screenshot below.

Figure 107: Include/Exclude legal entity from a Dossier

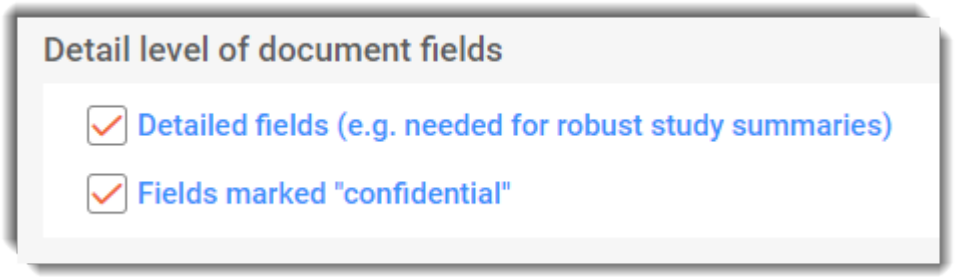


6.2.1.2. *Detail level of document fields*

Unticking the box labelled *Detailed fields (e.g. needed for robust study summaries)* excludes the fields needed for robust endpoint summaries, for example *Details on test animals* or *Details on study design*.

Unticking the box labelled *Fields marked as "confidential"* excludes from a *Dossier* the fields that are labelled as being confidential by having the text *(confidential)* and the icon (⚠) appended to the name of the field. Note that these fields are handled completely separately from fields for which flags may be set.

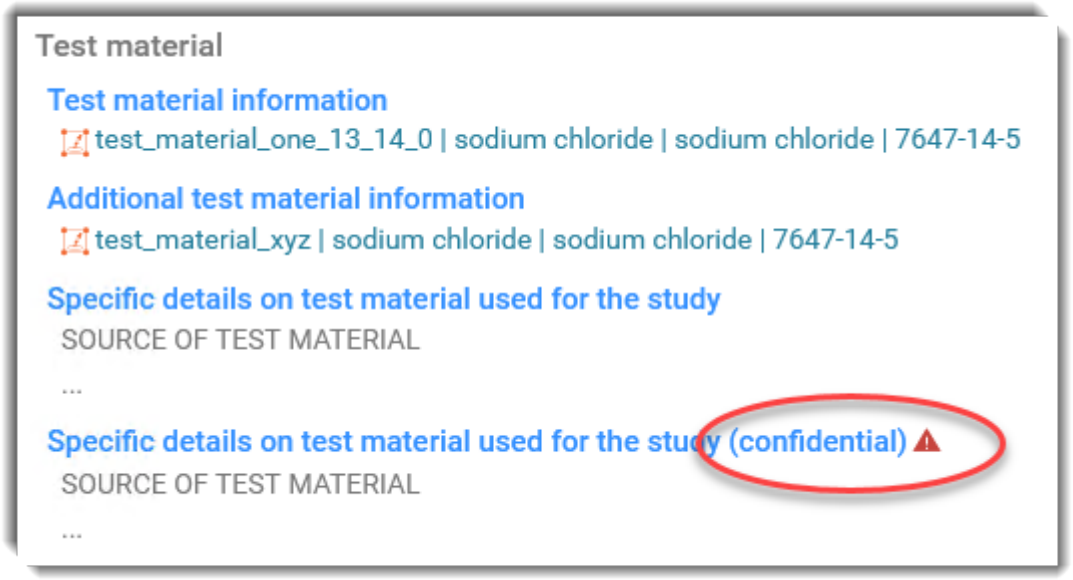
Figure 108: Detail level of document fields, to be included in a Dossier



Example

The figure below shows an example of a field that can be excluded. It is in an endpoint study record where information can be supplied about a *Test material*. There is a similar field in a *Test material* entity.

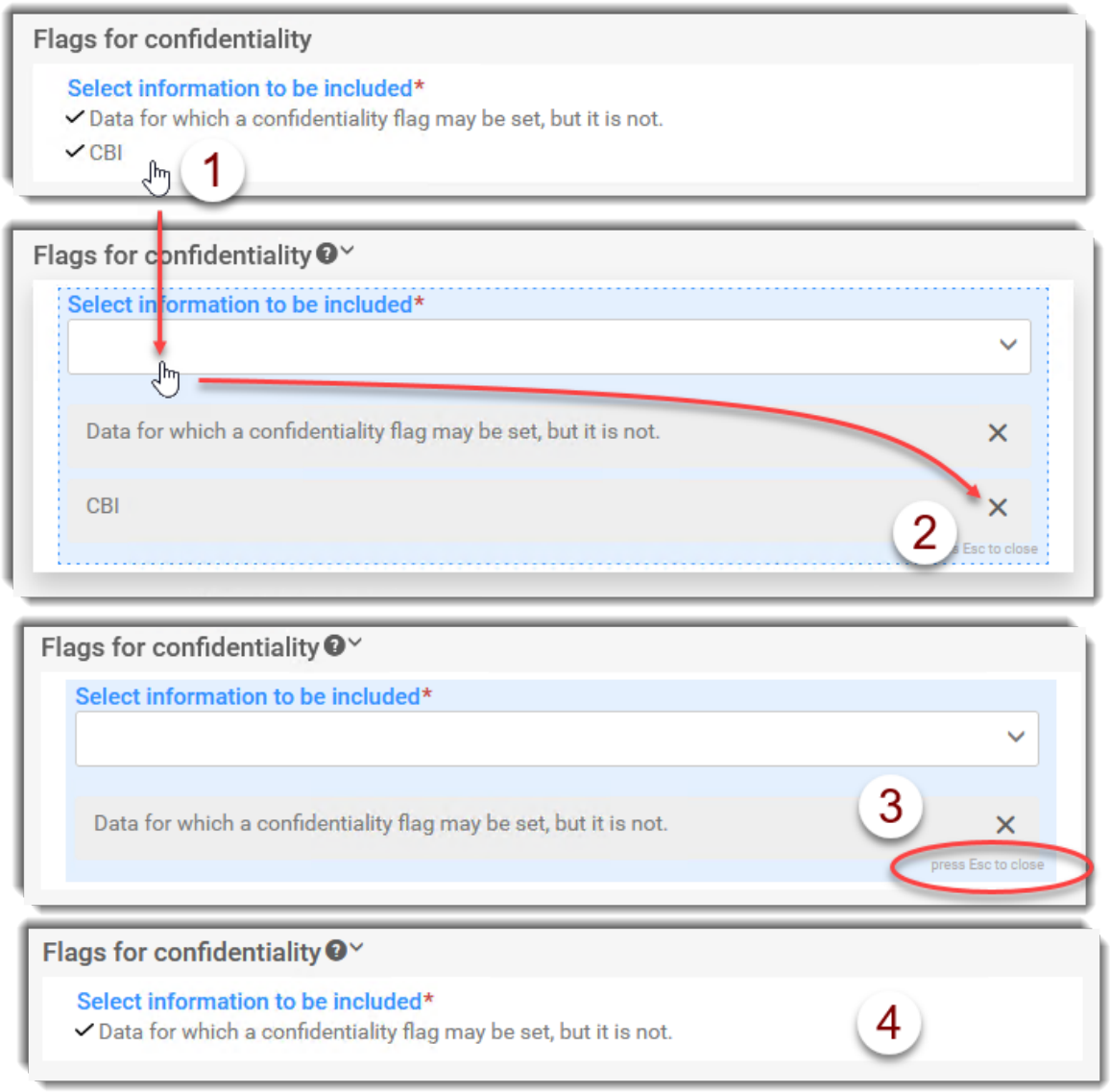
Figure 109: Example of a field marked as confidential but with no flag



6.2.1.3. Flags for confidentiality

Flags for confidentiality relates to flags, which are described in section *1.7.7 Flag*. By default, all the flagged data is included, except obsolete flags. Data that has an obsolete flag cannot be included. Inclusion is indicated by the presence of the type of field or flag with a tick on the left. To exclude data by type of field or flag, enter edit mode, and then remove the corresponding grey box by ticking on the cross icon on its right. Removed options can be re-instated from a menu in edit mode. An example is shown below, in which data flagged as being confidential business data (CBI) will be excluded from the *Dossier*.

Figure 110: Example of excluding data flagged as confidential business information (CBI) from a Dossier



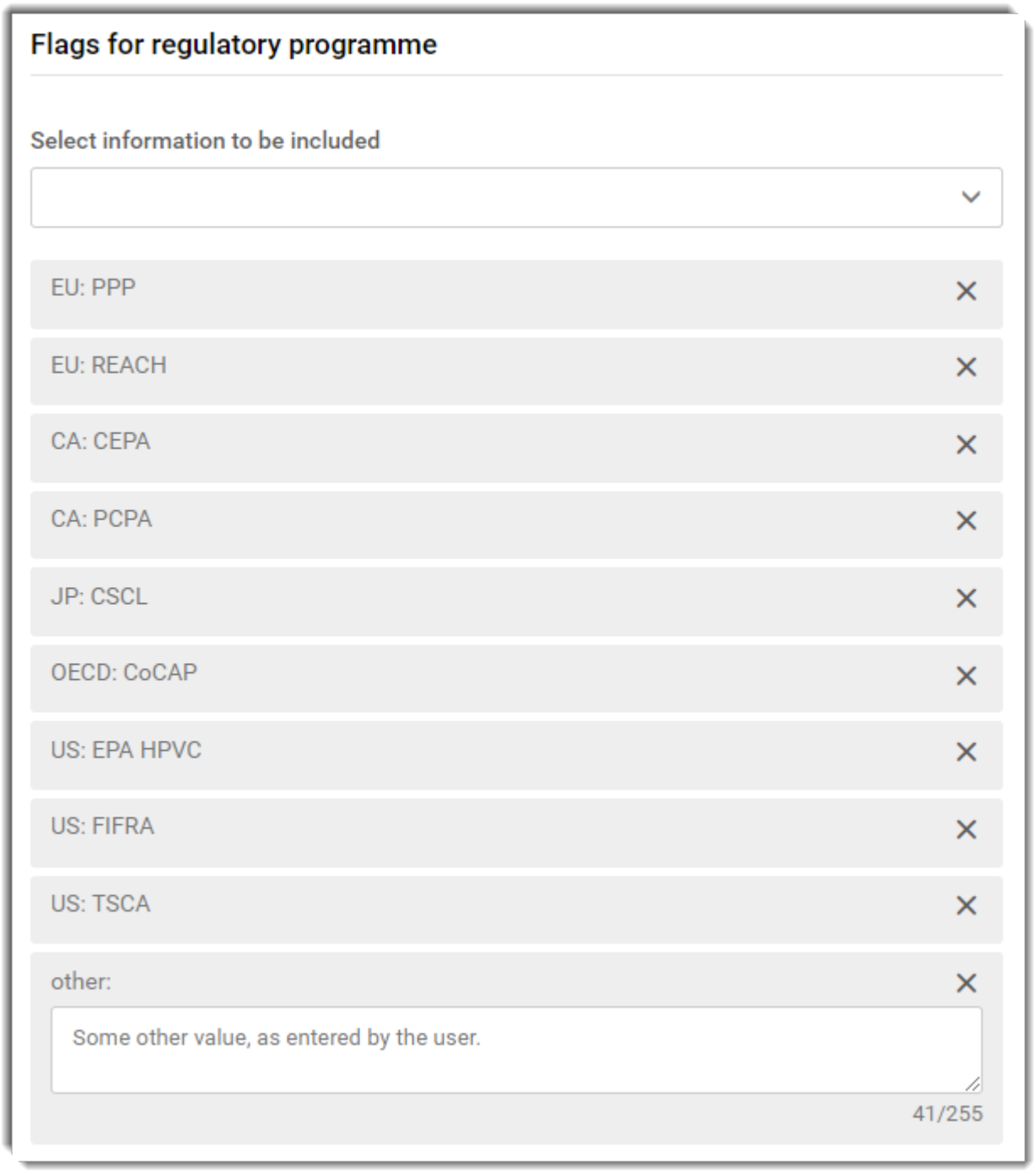
Legend for Figure 110

1. Click in the white box to enter edit mode;
2. In the box labelled CBI, click on the cross;
3. Exit edit mode by clicking in a different field, or by pressing the escape key (Esc) on your keyboard;
4. The ticked line for confidential business information (CBI) is no longer shown.

6.2.1.4. Flags for regulatory programme

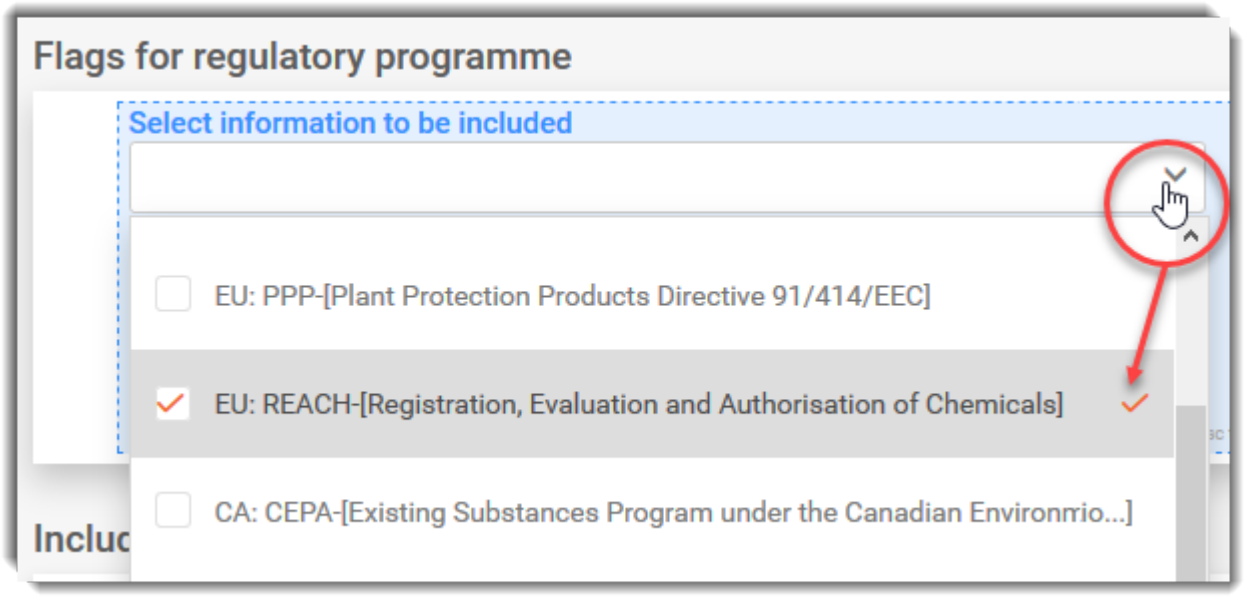
Flags for regulatory programme relates to flags, which are described in section *1.7.7 Flag*. By default, all the flagged data are included. Inclusion is indicated by the presence of a grey box that contains the name of the type of the flag. To exclude data that have a particular type of flag, remove its box by ticking the cross icon on its right. The options for regulatory programme are shown below. The field *other* is a free-text field.

Figure 111: Flags for regulatory programme



To add an option that is not shown on the list, open the drop-down menu, and then click on the item, as shown in the example below.

Figure 112: Include or exclude data from a Dossier according to regulatory programme flags

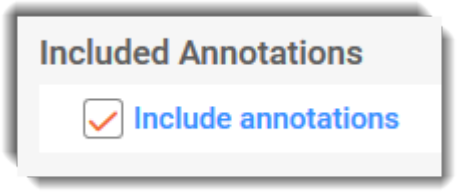


To save the change, exit edit mode by clicking in a different field, or by pressing the escape key (Esc) on your keyboard.

6.2.1.5. *Included Annotations*

This option allows *Annotation* entities to be excluded. The default is to include them all.

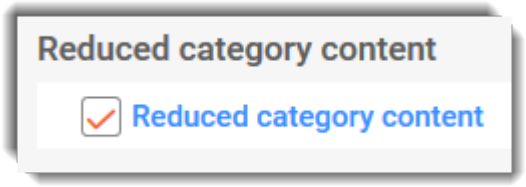
Figure 113: Exclusion of Annotation entities



6.2.1.6. *Reduced category content*

Reduced category content limits the size of a *Dossier* by omitting sections in the *Table contents* from other members of a *Category* to which the subject of the *Dossier* belongs.

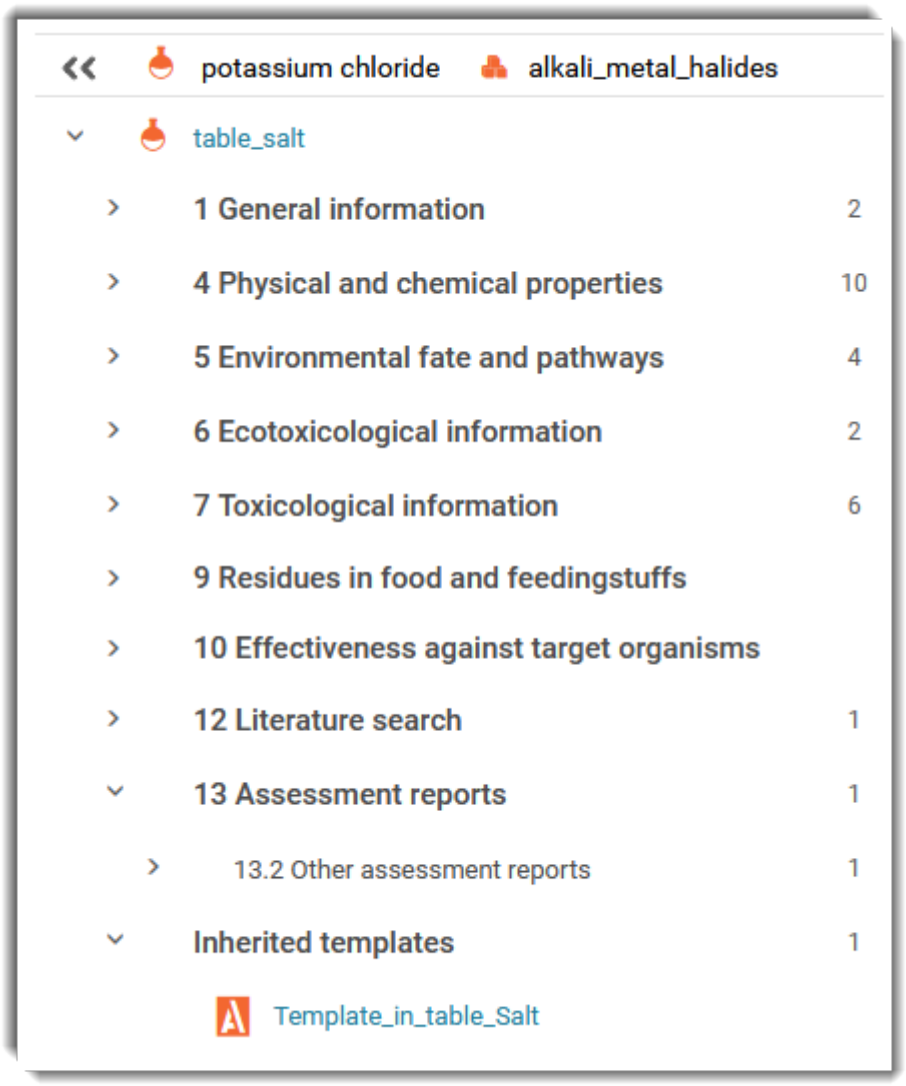
Figure 114: Reduced category content



By default, it is switched off. The feature applies only for working contexts that apply to REACH registrations and Annex XV dossiers, substance evaluation, and CLH dossiers.

An example is given below of what remains by default under *Linked Categories* for a member of a *Category* that is a *Substance*. The working context is *REACH Registration 10 – 100 tonnes*. Note the removal of sections 1.3 to 1.10, 2, 3, 8, 11, 13.1 and 14.

Figure 115: Reduced category content for a Substance in a Dossier

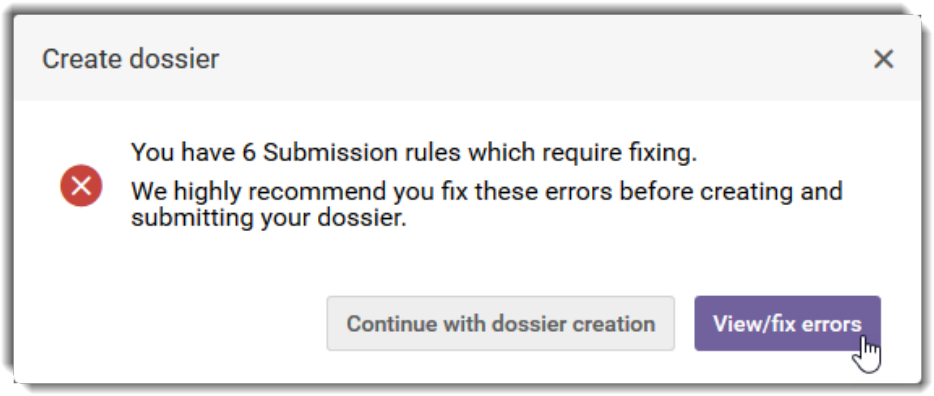


If you need to tailor this feature to your needs, contact the IUCLID Helpdesk for instructions.

6.2.2. Validation during creation of a Dossier

Next, the *Validation assistant* is run automatically in the background. If any *Submission checks* fail that would prevent the *Dossier* from being submitted to the relevant regulatory authority, an option is given to go straight into the *Validation assistant* to try to start fixing the problems in the dataset before actually creating a *Dossier*. It is also possible to ignore the warning and create a *Dossier*, but bear in mind it will not be possible to submit the *Dossier*.

Figure 116: Dossier creation – Option to use the Validation assistant

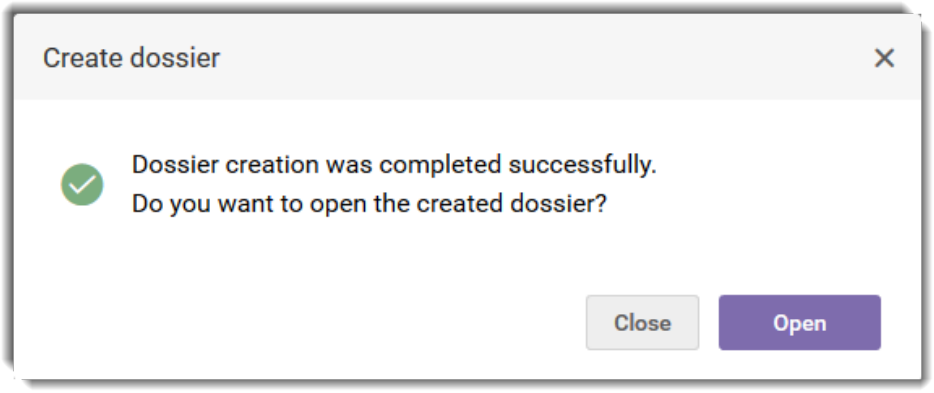


Clicking on *View/fix errors* opens the report of the *Validation assistant*, which is described in section *15 Validation assistant*.

6.2.3. Finishing the creation of a Dossier

If you click on *Continue with dossier creation*, or if the *Dossier* creation passes all the *Submission checks*, the *Dossier* is created, and the following message is shown.

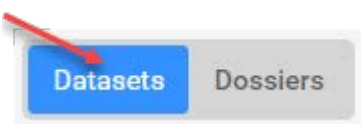
Figure 117: Successful Dossier creation



6.3. Viewing Dossiers and Substances or Mixture/Products

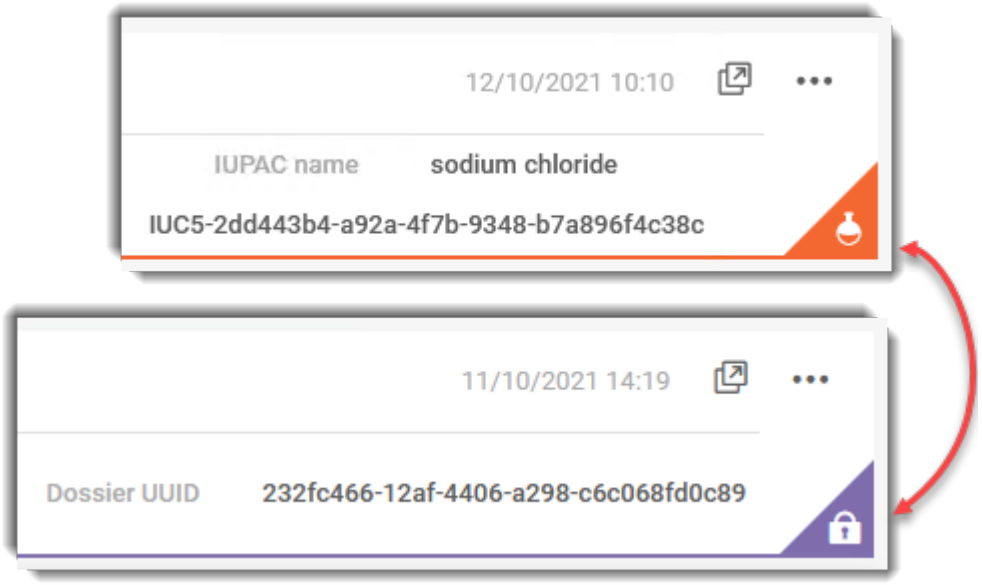
The icons for *Substance* and *Mixture/Product* lead to lists of entities. Access to *Dossiers* is merged with access to *Substances* or *Mixture/Products*. The windows for *Substances* and *Mixture/Products* can each display either datasets or dossiers. To switch between the two displays, click on the button shown in the example below:

Figure 118: Show a list of datasets



The type of entity in a record is indicated by an icon at the bottom right, as shown below.

Figure 119: Substance versus Dossier

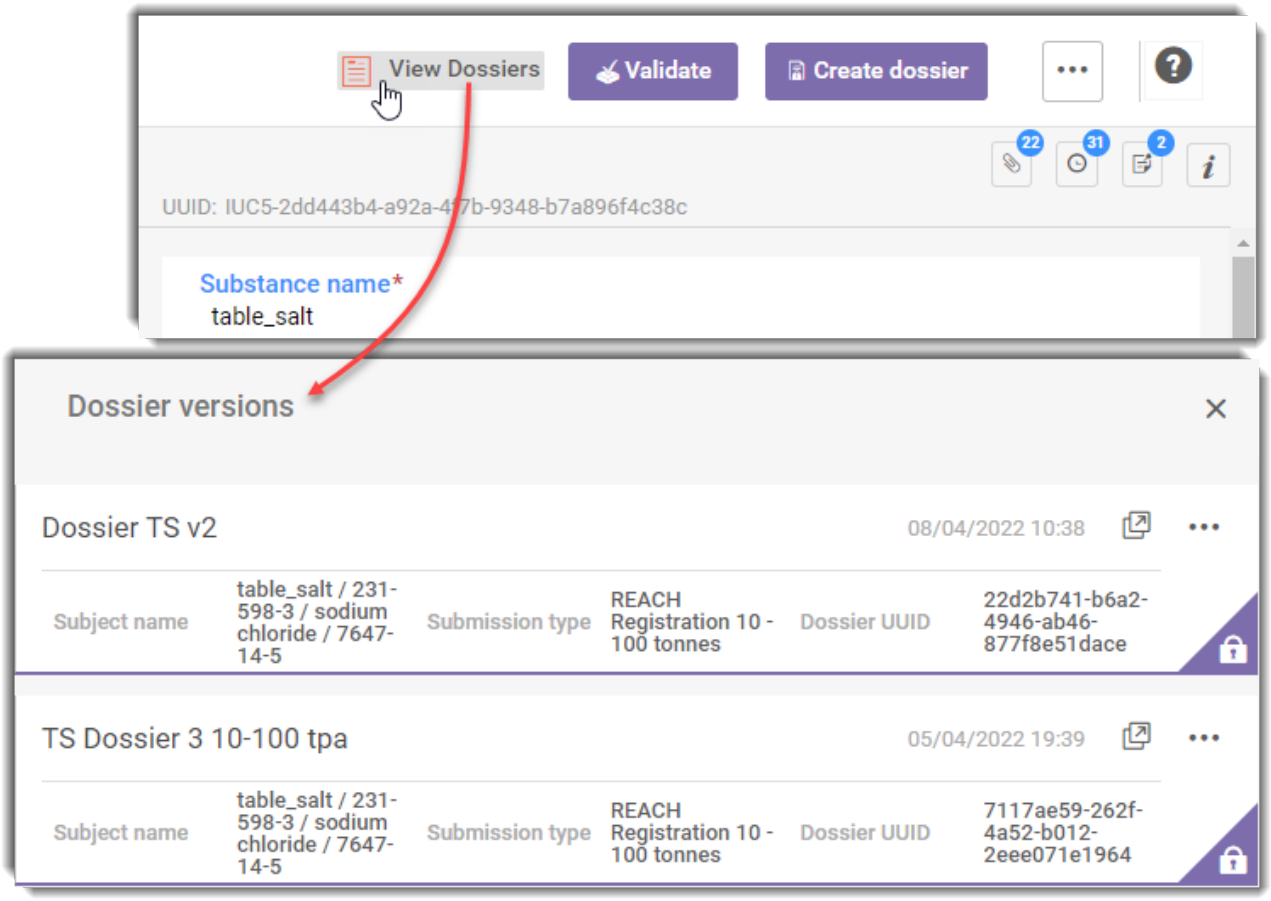


There is link from a *Dossier* to the *Substance* or a *Mixture/Product* from which it was created. There is also a list of links from each *Substance* or a *Mixture/Product* to the dossier(s) created from them.

Where multiple *Dossiers* have been created for a *Substance*, they can all be accessed via either the *Substance* or the *Dossier* record.

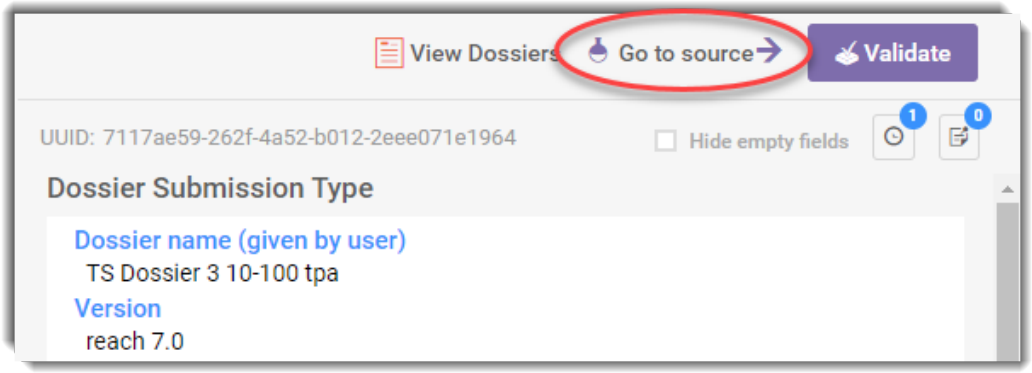
To get to a *Dossier* from a *Substance* dataset, click on the link *View Dossiers* at the top right of *Substance information*. This opens a list of all the *Dossiers* that refer to the *Substance*, as shown in the example below. To open a *Dossier*, click on its entry in the list.

Figure 120: View the Dossiers for a Substance



To go in the opposite direction, from a *Dossier* to a *Substance* dataset, click on the link *Go to source* that is at the top of the data window. An example is shown below.

Figure 121: View the Substance dataset for a Dossier

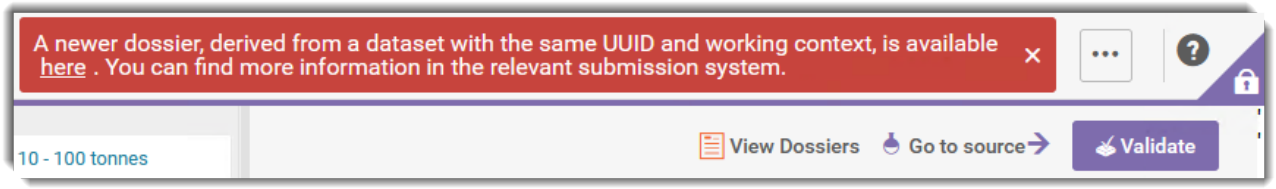


If *Go to source* is not visible, the source *Substance* dataset is not in the IUCLID database.

6.3.1. Warning message: “A newer dossier, derived from a dataset with the same UUID and working context, is available here.”

On opening a *Dossier*, you could see the warning message, “A newer dossier, derived from a dataset with the same UUID and working context, is available here. You can find more information in the relevant submission system.”. It indicates that there is a *Dossier* in the instance of IUCLID that is newer than the one that is being viewed, that was created from the same dataset. To view the newest *Dossier* created for the same dataset, click on the underlined link *here*. To view all the other *Dossiers* derived from the same dataset, click on *View Dossiers*, which is in the lower centre of the screenshot below. The complete set of *Dossiers* derived from a particular dataset can be viewed in a single list only from the raw dataset itself.

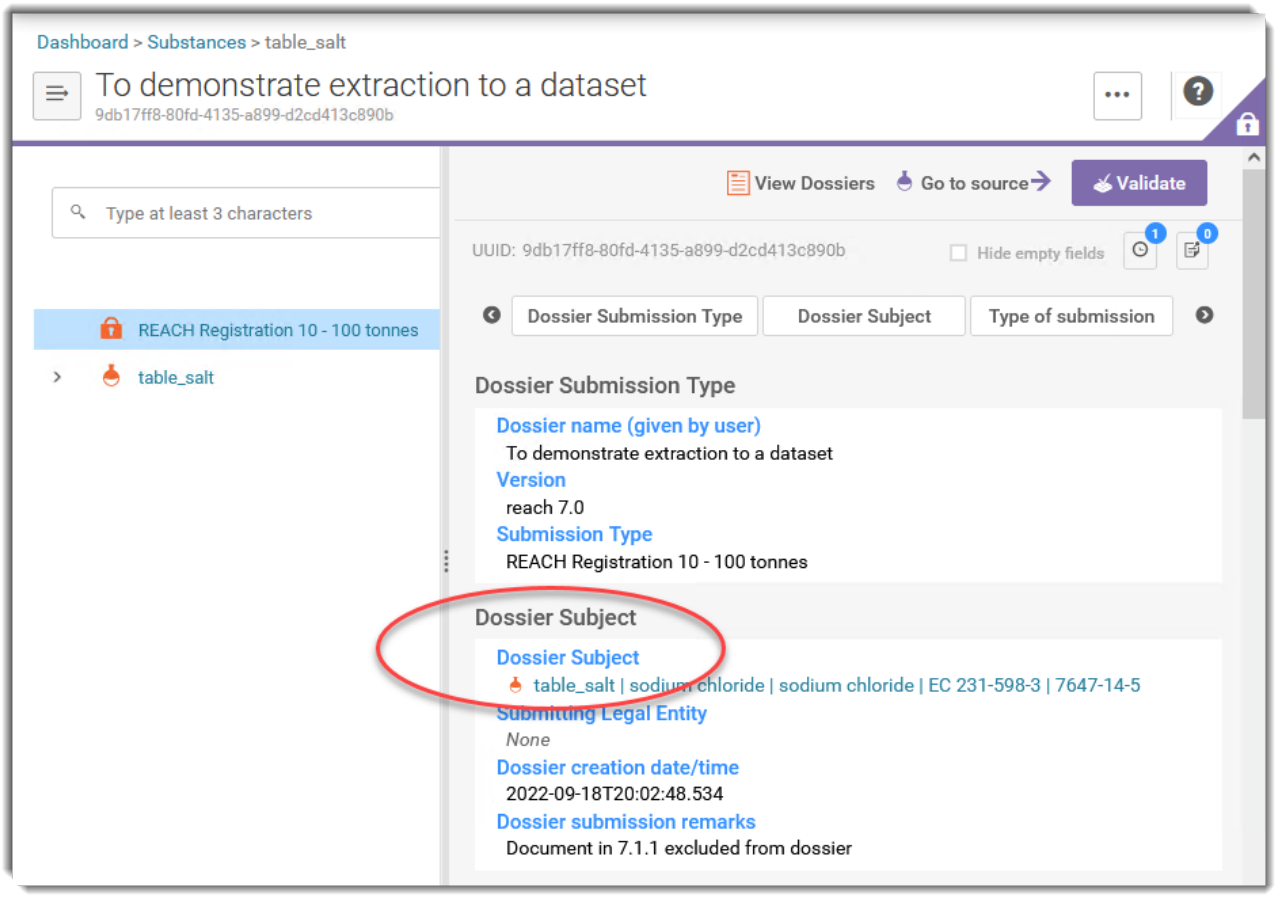
Figure 122: Waring message: “A newer dossier, derived from a dataset with the same UUID…”



6.4. Extract to Dataset

The raw dataset from which a Dossier was created is known as the *subject* of the Dossier. The Dossier contains a read-only copy of the raw dataset, which is its subject. An example is shown below where the *subject* is a *Substance dataset*.

Figure 123: The subject of a Dossier



Extract to Dataset is a two-step process. In the first step, it compares the data in the subject of the *Dossier* with any versions of the data that are present in the database in raw form. The result of the comparison is a view that provides control of how data will be over-written. The second step is to perform the actual extraction and writing of data. The second step is performed as a background task, as described in section *23 Background tasks*. The second step is started by clicking on the button *Extract*, at the foot of the comparison table on the right. Before clicking on the *Extract* button, if there are already any raw data relating to the dossier in the database, consider carefully the options to over-write, which are described below.

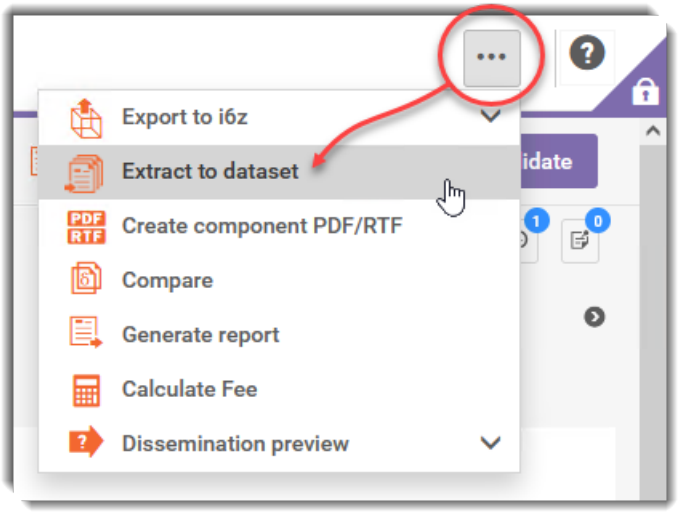
If the raw dataset is not present in the IUCLID database, an editable copy is created. The UUIDs of the entities and documents taken from the subject are not changed in the writing process. If the *Dossier* subject's raw dataset is in the IUCLID database, the entity of the subject must be overwritten because it has the same UUID. However, this does not apply to the entities and documents contained within or referred to by the subject entity. The user can include or exclude them from the extraction per entity or document. Also, the user can decide whether to over-write entities and documents that are already in the IUCLID database. The comparison of entities and

documents between the dossier subject and the raw dataset are done per UUID. For example, two documents can contain identical content, but they are treated separately because the UUIDs differ.

To extract to a dataset the IUCLID user must have a *Role* that permits the creation of the relevant type of dataset.

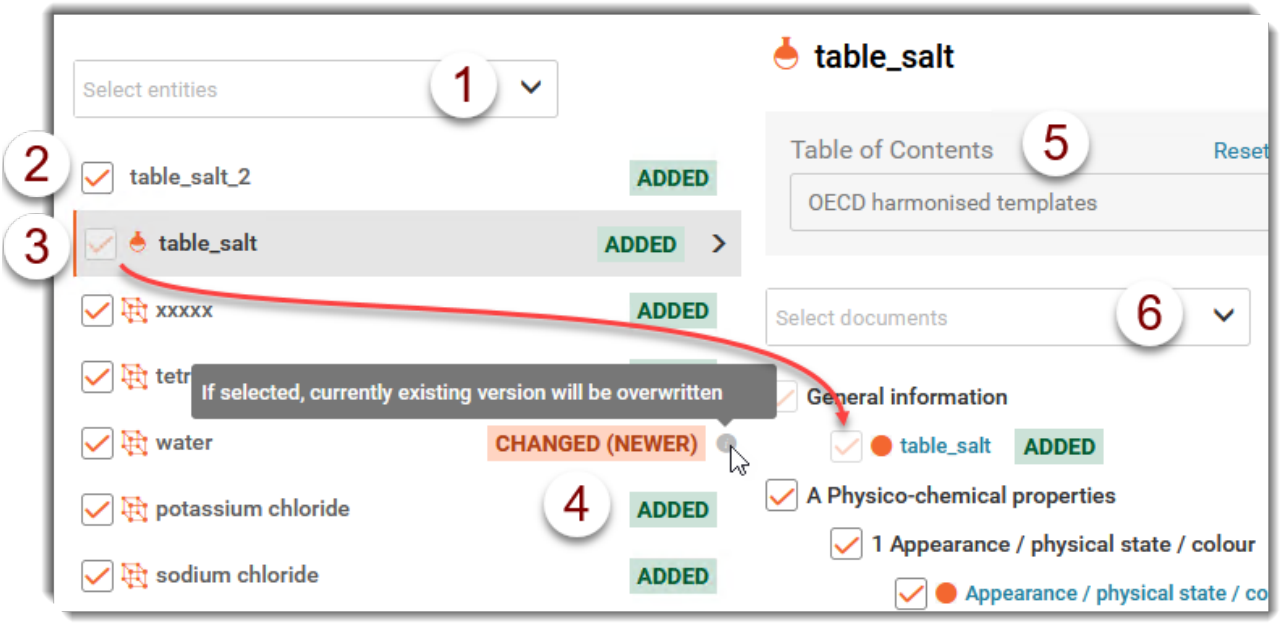
To extract data, start by viewing the record of the source *Dossier* and then select *Extract to dataset* from the upper menu labelled with three dots, as shown below.

Figure 124: Extract to dataset



When *Extract to dataset* is started, it compares the entities and documents in the Dossier with those in the IUCLID database that have the same UUIDs, and exist in their raw state outside of a Dossier. The result of the comparison is a preview menu of the extraction, from which entities and documents can be selected for extraction by ticking the box next to the name. Entities are shown on the left, and the documents they contain on the right. Each entity and document are classified from the reference point of the data in the Dossier. The classification is stated in a label on the right of the record. If there is no classification label, the entity or dossier to be extracted is identical to a copy in the raw data. An example is shown below in which a Dossier is to be extracted where neither its subject, nor any of the entities or documents it contains, have a version in the raw data.

Figure 125: Extract to dataset - Selection menu



Legend for Figure 125

1. Entities can be selected in bulk per classification, or all at once;
2. This represents the Dossier header and the information it contains. If it is selected, and a dataset is created, the dataset has the working context of the Dossier. If it is not selected, and a dataset is created, the dataset has no working context;
3. This represents the subject of the Dossier. It is essential to extract this, so it cannot be deselected. Likewise, the corresponding document on the right cannot be deselected;
4. These are classifications derived from the difference between the document or entity in the Dossier, and any raw data with the same UUID in the database. There are help texts under the grey icons. The classifications are described in the table below;
5. By default, the working context of the Dossier is selected. It can be changed here;
6. Documents can be selected in bulk per classification, or all at once;

Table 4: Extract to dataset - Classification

Classification	Description	Action if box is ticked
	The UUID is in the Dossier and the raw data. The entity or document is identical.	Entity or document in the raw data will not be touched.
ADDED	The UUID is in the Dossier, but it is not in the raw data.	Entity or document will be added to the raw data.
CHANGE(OLDER)	The UUID is in the Dossier and the raw data. The data is different. The value of *Last Modification Date* is older in the	Entity or document will be overwritten in the raw data by the older version from

	Dossier compared to the raw data in the database.	the dossier.
CHANGE(NEWER)	The UUID is in the Dossier and the raw data. The data is different. The value of *Last Modification Date* is more recent in the Dossier compared to the raw data in the database.	Entity or document will be overwritten in the raw data by the newer version from the dossier.
CHANGE	The UUID is in the Dossier and the raw data. The data is different. The value of *Last Modification Date* is the same in the Dossier as the raw data in the database.	Entity or document will be overwritten in the raw data.
REMOVED	The subject of the Dossier exists in the raw data. The UUID of the entity or document is in the raw data but is not in the Dossier.	Entity or document will be deleted from the raw data.

ADDED means that the UUID in the Dossier is **not** present as raw data in the IUCLID database. If the box is ticked, the data will be extracted, and the entity or document will be added to the raw data.

Where the UUID is in both the Dossier and the raw data, and the content differs, the classification is CHANGED. If the box is ticked, the entity or document in the raw data will be over-written by the data in the Dossier.

The OLDER and NEWER that can be stated after CHANGED refer to the value in the data of the property *Last Modification Date*. The value of *Last Modification Date* for an entity or document can be viewed in the data selection menu for *Advanced import*. For an example, see section *1.7.1.3 Import to* dataset.

A value of NEWER means that the value of *Last Modification Date* is more recent in the Dossier compared to the raw data in the database. Where the classification is CHANGED(NEWER), by default the data is selected because it is assumed that newer data in the Dossier is preferred. However, it can be de-selected, in which case after extraction the raw data will contain the older version.

Conversely, where the classification is CHANGED(OLDER), by default the data is not selected. It can be selected, in which case after extraction the raw data will contain the older version.

REMOVED can occur only when the raw dataset for the Dossier subject is present in the IUCLID database. REMOVED means that the document or entity exists in the raw dataset, but a read-only version with the same UUID cannot be found in the Dossier subject. If selected, these entries are deleted from the raw dataset.

The working context selected in the extraction preview affects what data are extracted. Data that are not shown in the table of contents for the working context are not extracted. If the subject of the Dossier exists as a raw dataset before the extraction, its working context is not affected by the working content selected in the extraction preview. If the subject of the Dossier does not exist as a

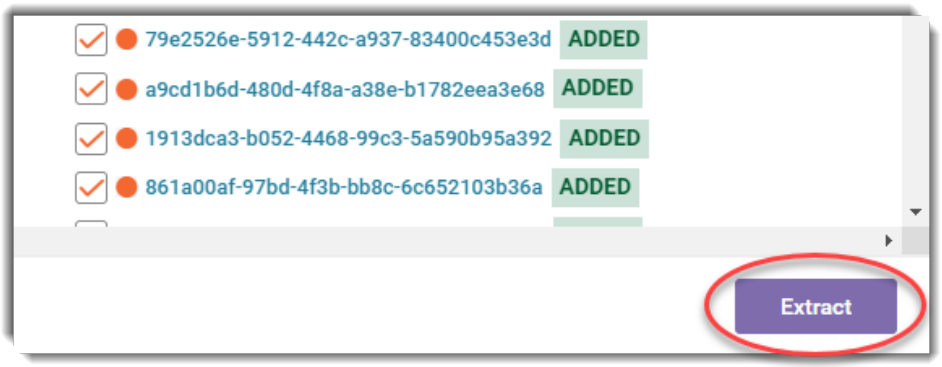
raw dataset before the extraction, the working context of the dataset created is the same as the Dossier.

For example, if a *Template* in a Dossier is not selected, the link within the raw dataset to the *Template* is removed. Raw data in the database for the *Template* is not touched.

If Instance Based Security (IBS) is active in the instance of IUCLID, the degree of access to the extracted data can be set in a menu at the foot of the interface. For more information see section *24.3.5.1 IBS management (IBS)*.

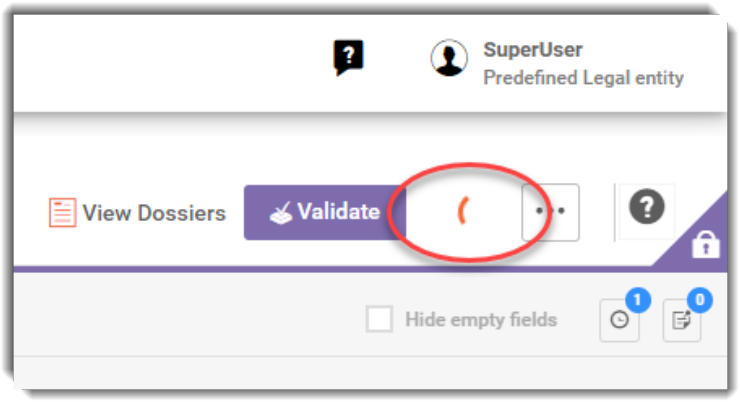
Where data is to be over-written or deleted, ensure that back-up copies are available. After ensuring that the selections of entities and documents are correct, click on the button labelled *Extract,* which is at the foot of the interface, on the right, as indicated below in an example.

Figure 126: The button to start the extraction and writing for Extract to dataset



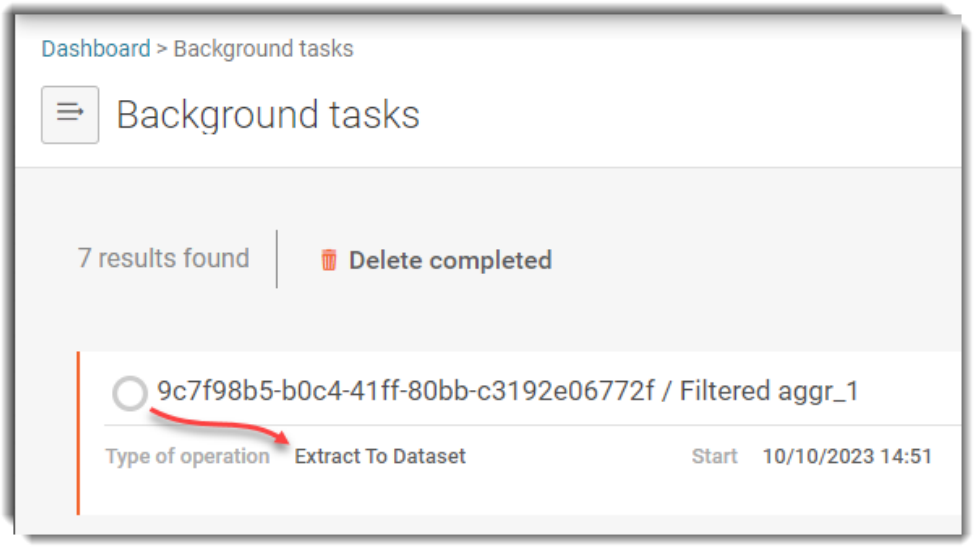
The extraction proceeds as a background task, and a rotating icon is shown in the application bar, as per the example below.

Figure 127: The rotating icon shown whilst a background task is running



Whilst the background task is running, you can either wait for it to finish, or continue working by navigating to other parts of the interface. For more information about background tasks see section *23 Background tasks*. The figure below presents an example of a background task for *Extract to dataset* that is still running.

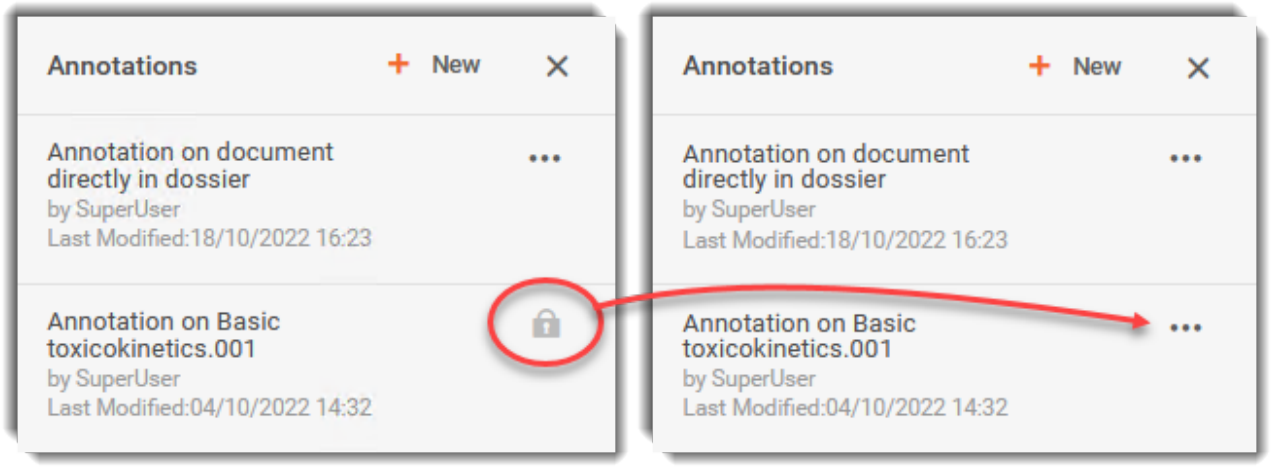
Figure 128: A background task for Extract to dataset



6.4.1. Extraction of Annotations

Extraction is possible for Annotations that have been added to the subject of the Dossier both before and after creation of the Dossier. Annotations added to the subject of the Dossier before creation of the Dossier, are read-only in the Dossier and are shown with a lock icon. After extraction they become editable, as is the case below.

Figure 129: Extraction of Annotations that were added after dossier creation (upper) and before (lower)



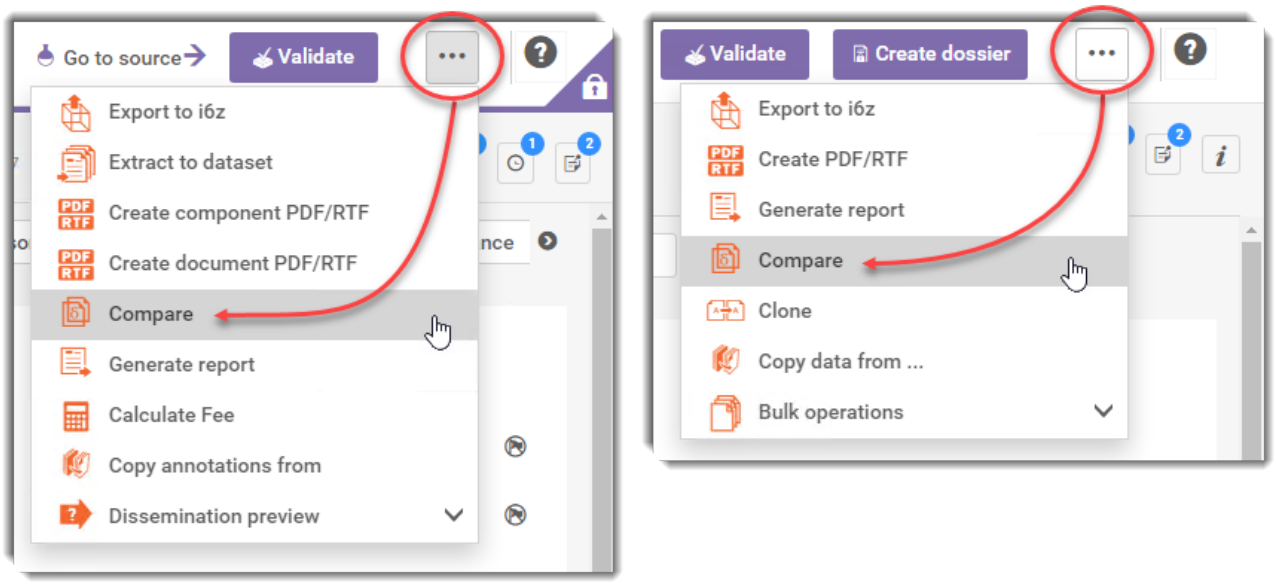
Annotations cannot be attached to the header of a raw dataset. Therefore, Annotations attached to the header of a Dossier are not extracted.

6.5. Compare

Compare produces a comparison of every value in any two *Dossiers*. or *datasets*. Dossiers cannot be compared with datasets, and vice versa. Note that it is also possible to compare only two individual documents, separately from the rest of the dataset or dossier, as described in section *1.7.13 Compare Document*.

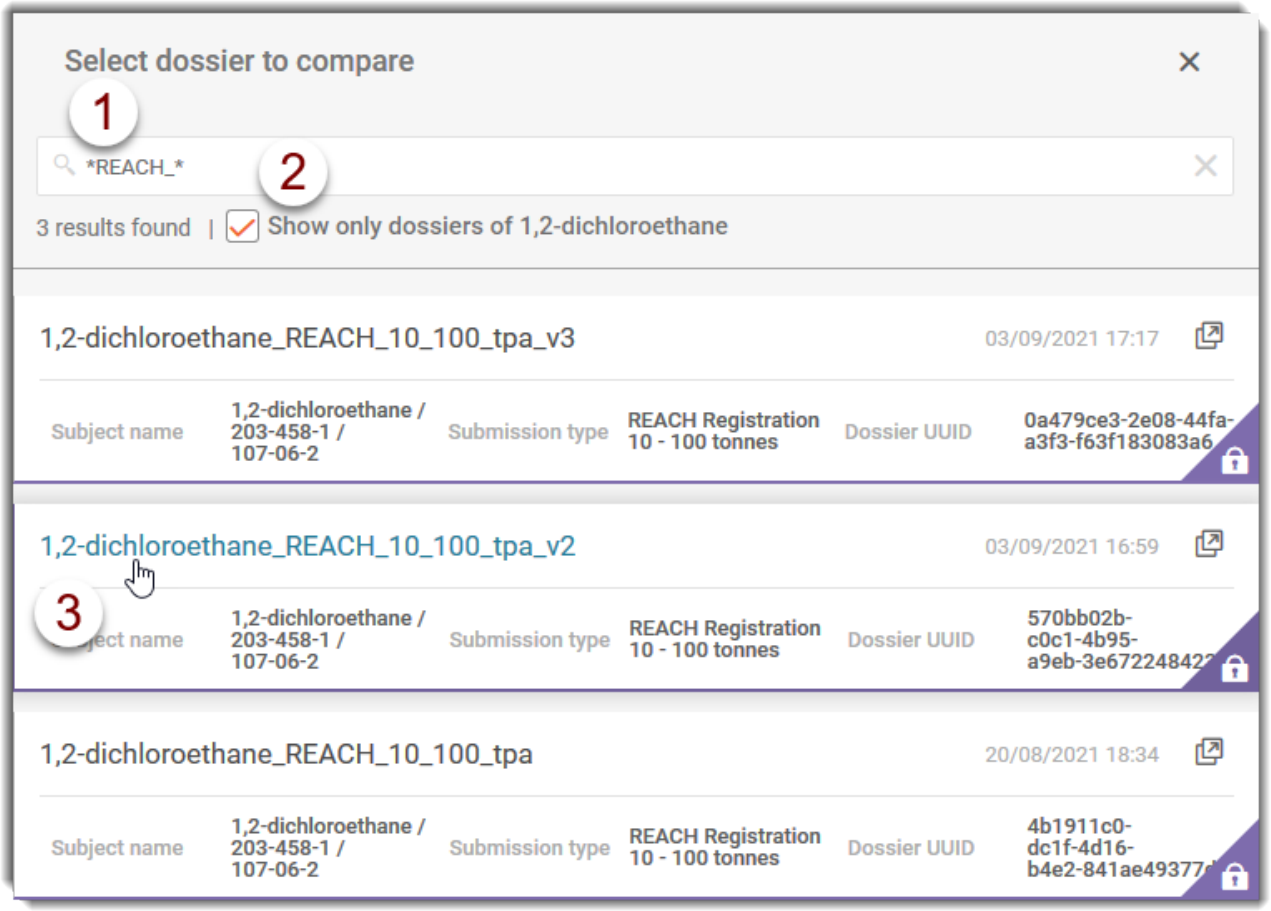
The output of *Compare* is an HTML file that can be viewed in a browser, for example by opening it in a tab alongside the user interface. To compare two *Dossiers* or datasets, start by viewing the record of the source against which the comparison will be made, and then select *Compare*, from the menu labelled with three dots, as shown below. The menu for *Dossiers* is on the left, and the menu for datasets is on the right.

Figure 130: Start the comparison of two Dossiers or two datasets



This opens a page from where the other, or target, *Dossier* or dataset will be selected. An example for a *Dossier* is described in the figure below. Note how only *Dossiers* are shown.

Figure 131: Select the target Dossier to be compared with the source



Legend for Figure 131

1. Search for a target *Dossier* by *Dossier* name, *Substance* name, and *Working context*, all at the same time;
2. This tick box limits the *Dossiers* shown to only those that were created from the same dataset as the source *Dossier*. If the *Dossiers* have different subjects, the comparison of documents is done differently than if they are the same. See below for more details;
3. Click on a target *Dossier* to generate the comparison report.

The comparison report is an HTML file with a name of the form:

`<name of source>_<name of target>_comparison.html`

Example: `DossierA_DossierB_comparison.html`

The structure of the comparison report is essentially the same for Dossiers and substance datasets. However, the dossier header in a substance dataset is referred to as a draft dossier header. The descriptions below focus on the comparison of Dossiers, but the same concepts apply for datasets.

The comparison report contains side by side comparisons divided into four sections which each represent a layer in the hierarchy of IUCLID. Where a difference is found, there is a hyperlink down the hierarchy to the point of difference.

Table 5: Sections in a Comparison Report for Dossiers

Dossiers	Identifiers of the source and target Dossiers
Dossier contents	The Dossiers' headers and the entities in the Dossiers
Section Document comparison	The documents in the Dossiers listed by name
Field-level content differences	The differences between the values of the fields. Only fields that contain a difference are included. The field paths are viewable under the info icon.

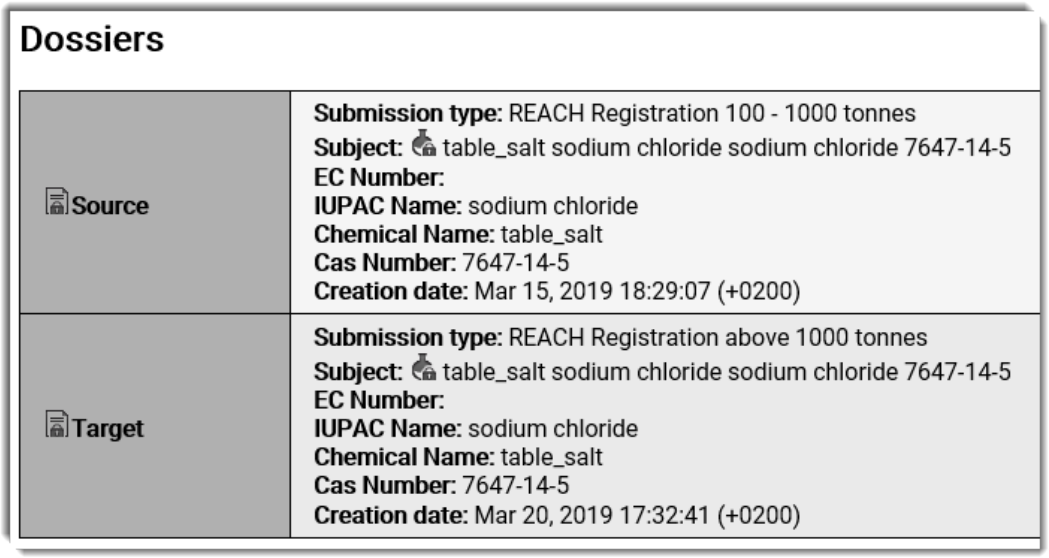
At the top of the comparison report there is a filter, *Show only differences*. This hides or reveals the entries for data that are identical in the source and target.

Figure 132: Show only differences in a comparison report

6.5.1. Comparison Report - Section 1: Dossiers

The first section of the comparison report, *Dossiers*, contains some basic information about the content of the source and the target *Dossiers*, as shown in the example below:

Figure 133: Comparison report – First section: Dossiers



6.5.2. Comparison Report - Section 2: Dossier contents

The second section of the comparison report, *Dossier contents*, contains a side-by-side comparison of the *Dossier* header and the entities, grouped by type of entity, for example *Substance*, as shown below.

Figure 134: Comparison report – Second section: Dossier contents

Dossier contents

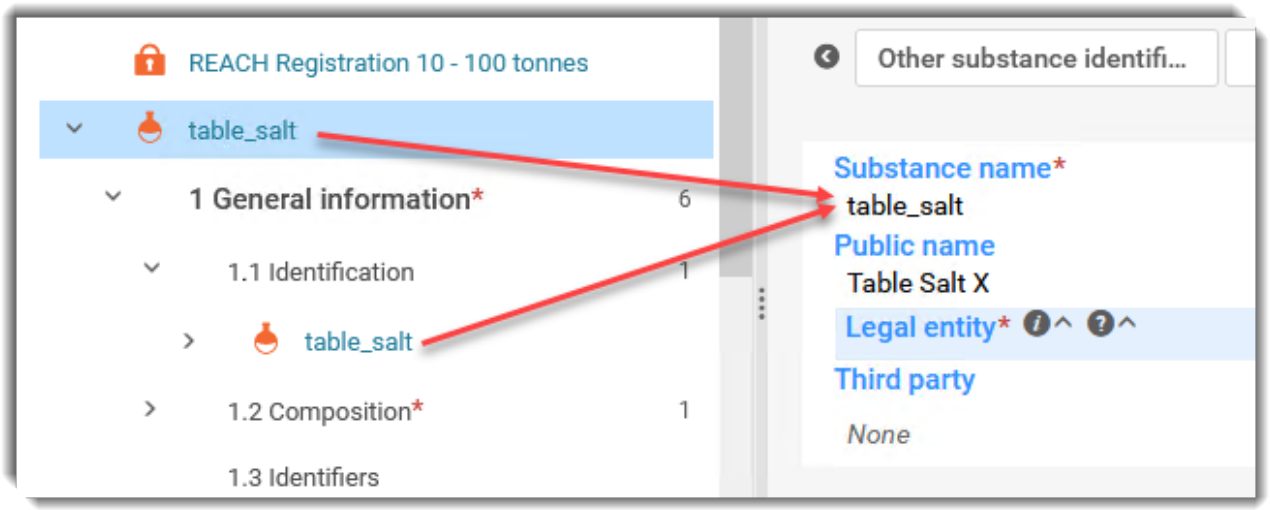
Source	Comparison	Target
Dossier headers		
R_10-100 / subject: table_salt sodium chloride sodium chloride 7647-14-5	Different	R_10-100 / subject: table_salt sodium chloride sodium chloride 7647-14-5
Substances		
table_salt sodium chloride sodium chloride 7647-14-5	Different	table_salt sodium chloride sodium chloride 7647-14-5

At the second level, the entity level, where the column *Comparison* contains the value *Different*, there is an internal hyperlink down to the corresponding entry at the third level, *Section Document comparison*, which is described below.

6.5.3. Comparison Report - Section 3: Section Document comparison

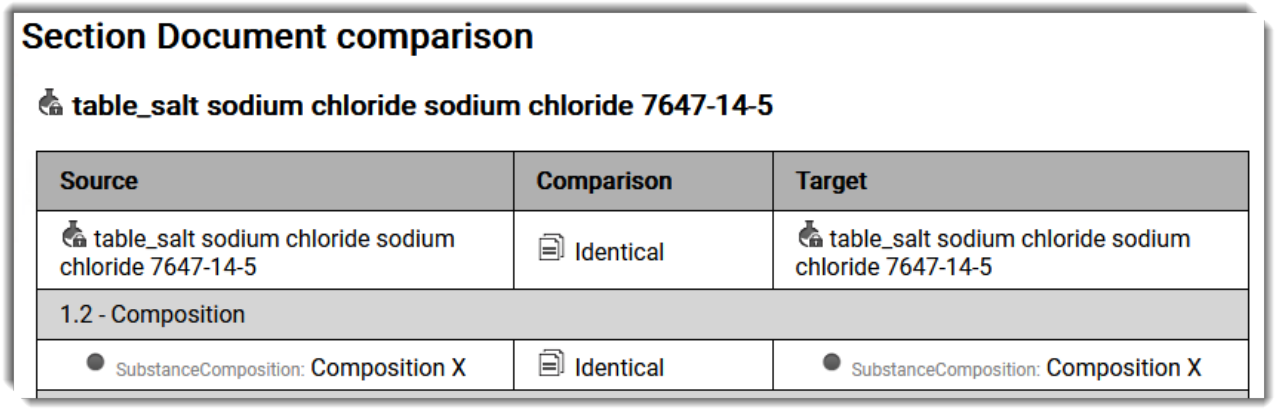
The third section of the comparison report, *Section Document comparison*, contains a side-by-side comparison of the documents in the *Dossiers*. However, the first row shows a comparison of the subject entities of the *Dossiers*. This is a comparison of only the values at the top level of the entities, which are viewed in the data window when the subject is selected. An example is given below for a working context under the REACH regulation.

Table 6: Values defined in the entity of the Dossier subject



An example is shown below of the start of *Section Document comparison*.

Figure 135: Comparison report – Third Section: Section document comparison



Section Document comparison

table_salt sodium chloride sodium chloride 7647-14-5

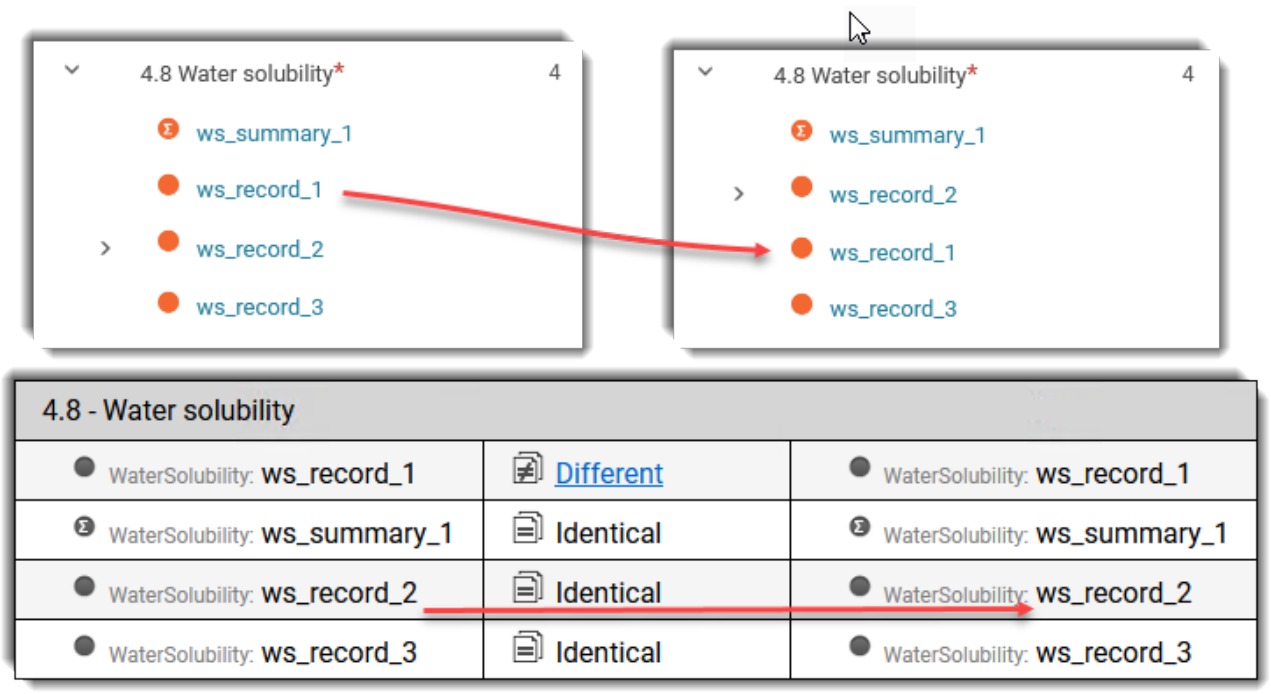
Source	Comparison	Target
table_salt sodium chloride sodium chloride 7647-14-5	Identical	table_salt sodium chloride sodium chloride 7647-14-5
1.2 - Composition		
SubstanceComposition: Composition X	Identical	SubstanceComposition: Composition X

Section Document comparison is arranged and numbered as per the table of contents (TOC) for the *Working context* of the source *Dossier*. Therefore, choose as the source *Dossier* the one with the numbering and structure that you prefer to see in the comparison report. An example is the difference between a REACH *Dossier*, and one for *OECD harmonised templates*.

The *Dossiers* being compared are considered to have the same subject if the subject entities have the same UUIDs. Other values do not matter. If the *Dossiers* have the same subject, the comparison is made between documents that have the same UUID. The order in which the documents are shown in the table of contents within a particular section does not matter. If the subjects of the two dossiers being compared are not the same, documents are compared in the order in which they are shown in the table of contents in that section. UUIDs of the documents are not taken into consideration. This can lead to different results in the comparison, as illustrated by the following example.

In the figure below a comparison is made between *Dossiers* that have the same subject, for example, a *Substance*. In the second *Dossier*, documents **ws_record_1** and **ws_record_2** have been swapped around in the table of contents, and data has been changed in **ws_record_1**.

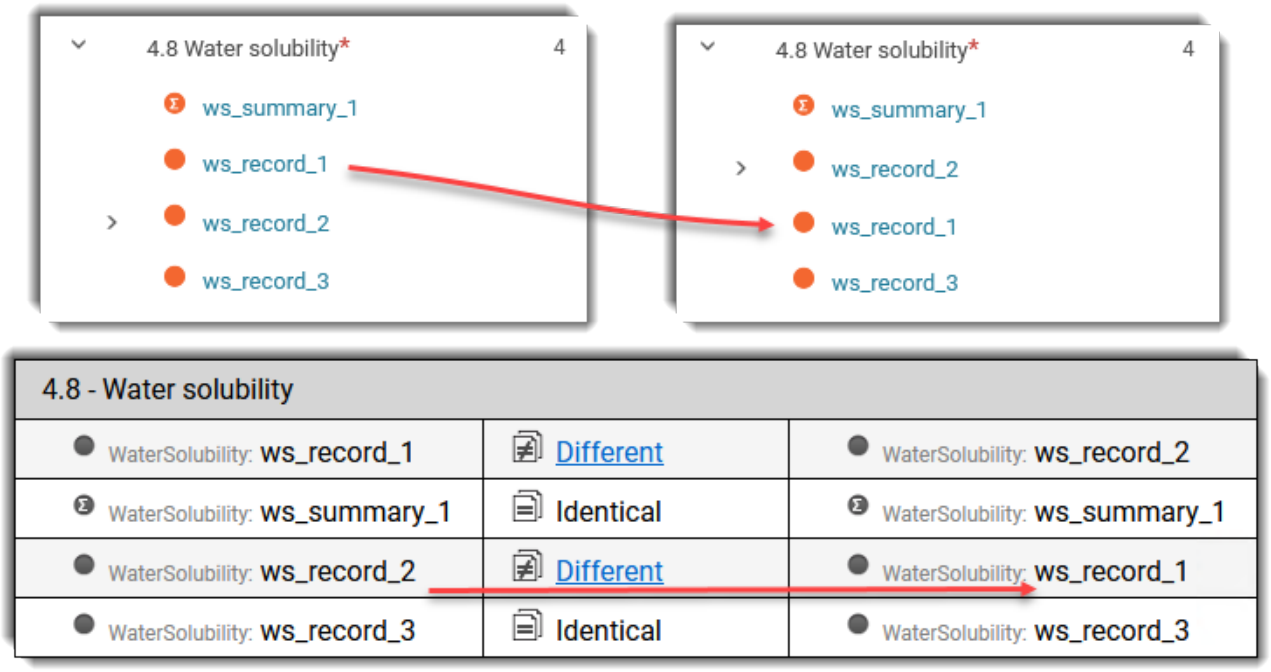
Figure 136: Compare dossiers that have the same subject



The document **ws_record_2** is shown as identical, even though its ranking in the table of contents has changed from third to second. This is because it has the same UUID.

The same scenario is shown below for *Dossiers* that have different subjects.

Figure 137: Compare dossiers that have different subjects



The document **ws_record_2** is compared with **ws_record_1** and is found to be different. The presence of a pair of identical documents in the section is masked by their different order in the table of contents.

A change in the name of the document is counted as a difference.

The possible values of the column *Comparison* on levels two and three are described in the table below.

Table 7: Key for the icons in the Dossier comparison report

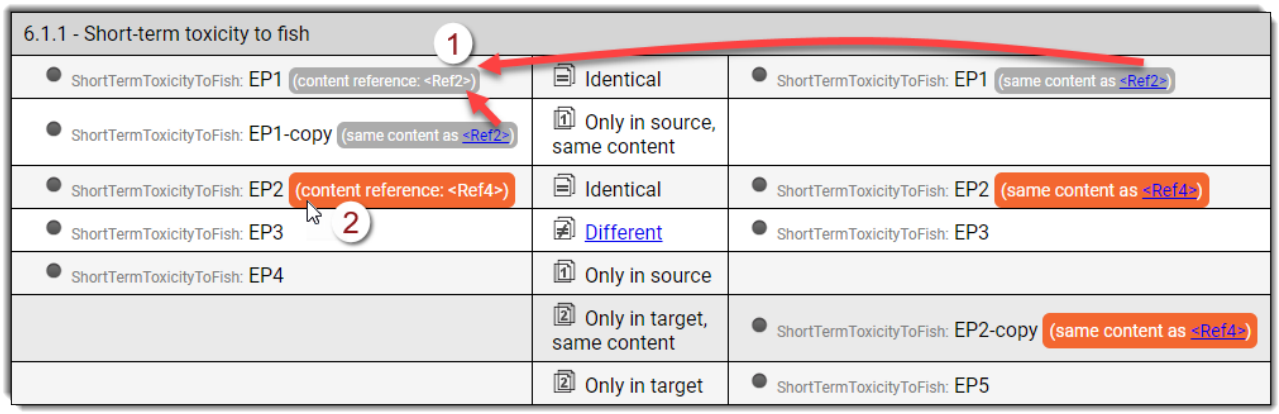
Icon	Label in interface	Description
		The descriptions below are for when the *Dossiers* have the same *Dossier* subject, as judged by the UUIDs of the subject entities. Where the subject entities differ, the comparison is done according to the order of the document in the table of contents, with no consideration of document UUID.
	Identical	The entity or document is exactly the same in both *Dossiers*. This is based on UUID and content.
	Different	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. The word *Different* is a hyperlink to the fourth level of the comparison report, where the differing field(s) and their values are shown.
	Only in source	The entity or document is in the source *Dossier*, but not the target *Dossier*. This is based on UUID.
	Only in target	The entity or document is in the target *Dossier*, but not the source *Dossier*. This is based on UUID.
	Only in source, same content	The entity or document is in the source *Dossier*, but not the target *Dossier*. This is based on UUID. There is another document in the source *Dossier* with the same content.
	Only in target, same content	The entity or document is in the target *Dossier*, but not the source *Dossier*. This is based on UUID. There is another document in the target *Dossier* with the same content.

At the third level, the document level, where the column *Comparison* contains the value *Different*, there is an internal hyperlink down to the corresponding entry at the lowest level in the report, which is *Field-level content differences*, as described in the next section on this level.

6.5.3.1. References in the comparison report

Where the same content is found in a different document, a link is created to the first instance of the content. The first instance is shown with a label *(content reference: <RefN>)* where N is its sequence number throughout the whole comparison. Links can be across the two *Dossiers* compared, or inside the same *Dossier*. Hovering over a link or its anchor, highlights the anchor and the reference(s) to it. An example is shown below in which there are two reference anchors, Ref2 and Ref4. Ref3 is in a difference section, and so cannot be seen in this view.

Figure 138: Links to duplicate content in the comparison report



Legend for Figure 138

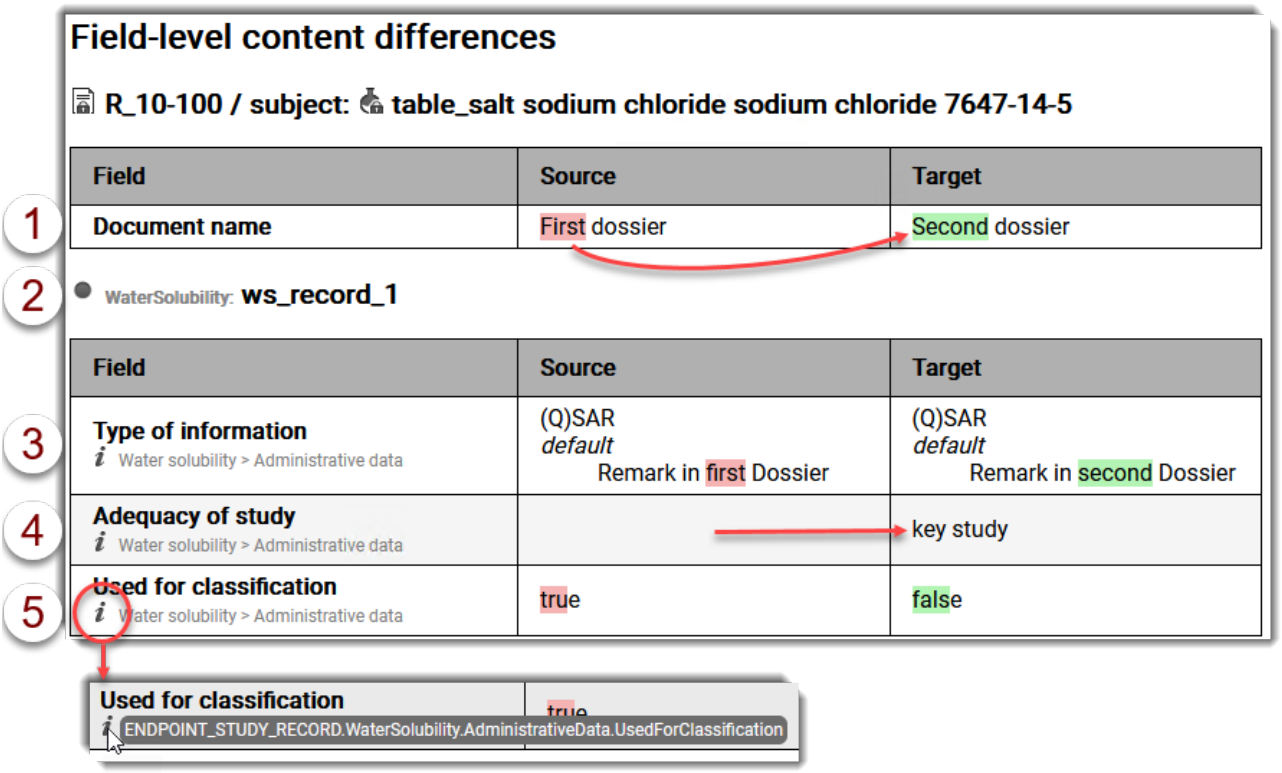
1. The source dossier is on the right. The target is on the left. The direction of the links to Ref2, in white on the left, are shown as red arrows. One link to Ref2 is in the source *Dossier*, and one is in the target *Dossier*. EP1 and EP1-copy in the source *Dossier* have identical content. Their UUIDs are different otherwise they could not exist in the same dataset;
2. The cursor is hovering over the content reference Ref4, causing it and its links to be highlighted. EP2 is in both the source *Dossier* and the target *Dossier*. There is also a copy of it in the target *Dossier*, hence the two links.

6.5.4. Comparison Report - Section 4: Field-level content differences

In the fourth section of the comparison report, *Field-level content differences*, there is a row for each field in which a difference was found. The field name and the values for the field are given. The values in the dossier from where the *Comparison tool* was launched are highlighted in green. The values from the dossier that was subsequently selected for comparison are highlighted in red.

An example is shown below for dossiers named *First dossier* and *Second dossier*. The difference in name is highlighted. Some values have been changed in a document that is an endpoint study record of type *Water solubility*.

Figure 139: Comparison report – Fourth section: Field-level content differences

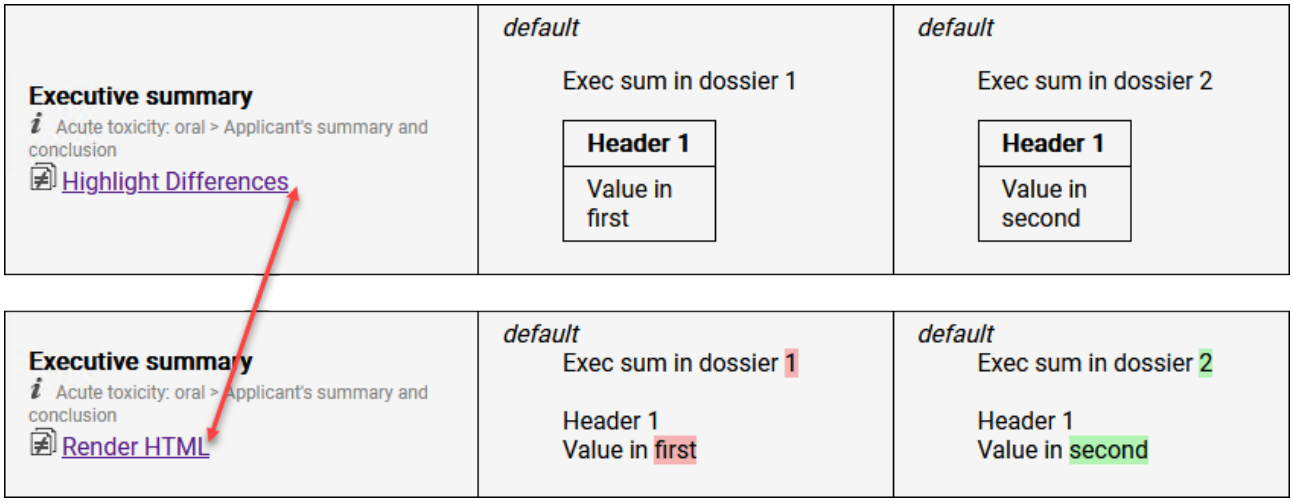


Legend for Figure 139

1. The names of the Dossiers. A change is indicated going from red to green;
2. The name of the document;
3. The name of a field within the document. A change is indicated going from red to green,
4. A previously empty field has had a value entered;
5. The path of the field in IUCLID can be viewed by hovering over the info icon.

Where the text is in a rich text field, there is an option to either highlight the differences, or show the HTML rendered. In the example below, the upper screenshot shows the HTML rendered, which reveals that the header of the table is formatted in bold.

Figure 140: Highlight the differences in a rich text field or render the HTML



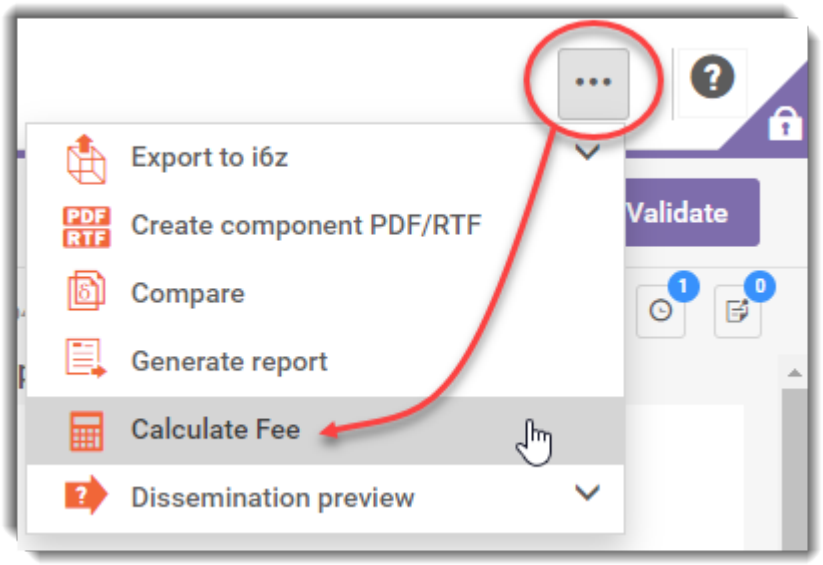
6.6. Calculate Fee

The *Fee calculator* assists users in calculating the fees for submission of data according to the REACH Fee Regulation (No 340/2008 of 16 April 2008, and subsequent amendments). The *Fee calculator* takes a *Dossier* as its input, and outputs a list of the expected fees. It works for all types of *Dossier* that industry users can submit to the European Chemicals Agency (ECHA) under the REACH regulation.

6.6.1. Running the Fee calculator

The *Fee calculator* is run from the top level of the record for a *Dossier*. Click on the button labelled with three dots, and then select *Fee calculator*, as shown ringed in red in the example below.

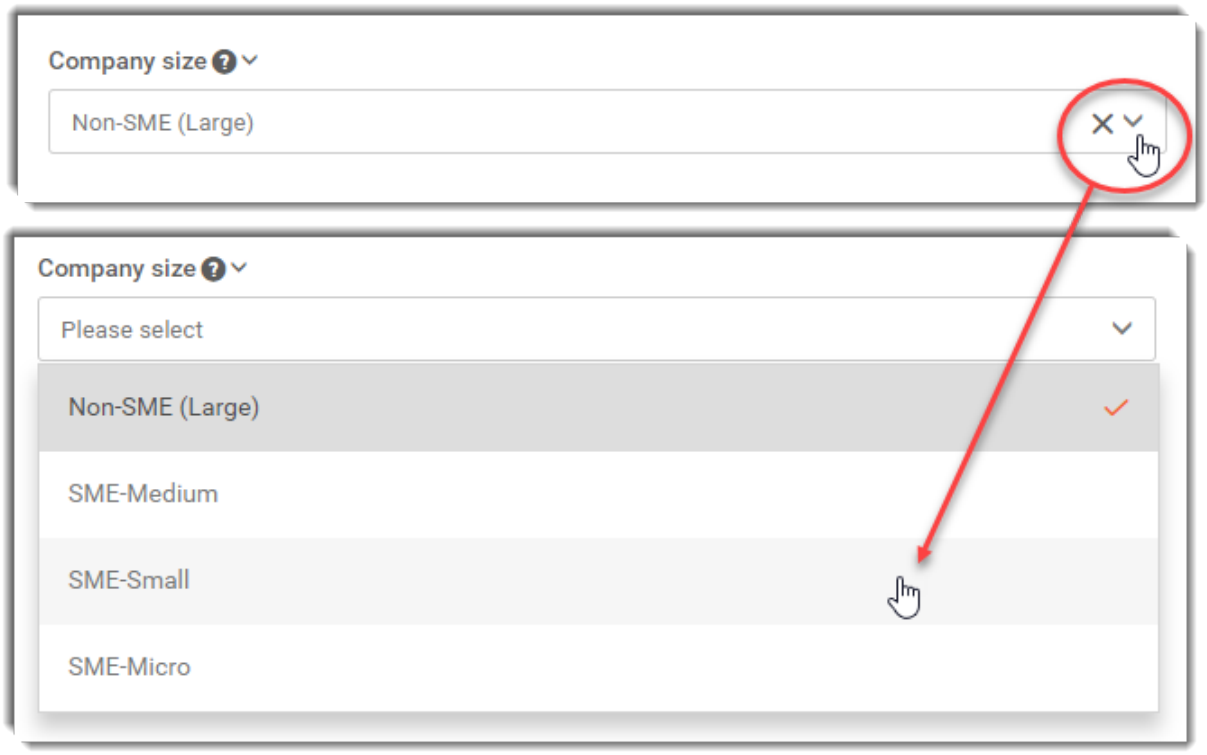
Figure 141: Run the Fee calculator



6.6.2. Selecting the company size

First, select the size of the company from the drop-down menu, as shown in the example below.

Figure 142: Selecting the company size: example for SME-Small



6.6.3. 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 set in the *Dossier*, the indicators will not appear.

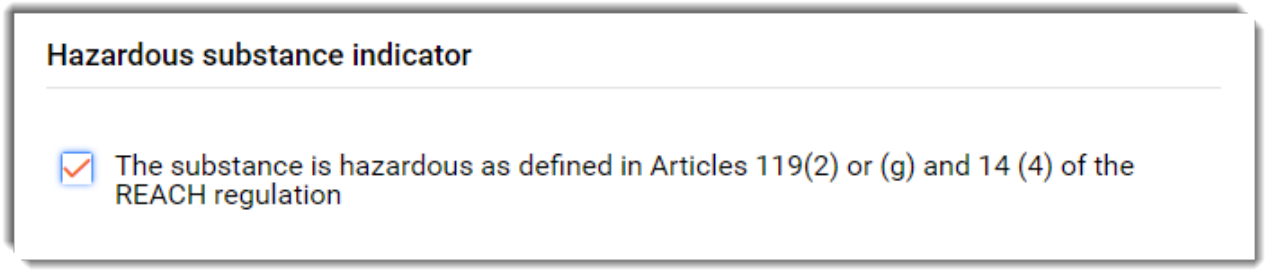
For calculating the fees of *Dossiers* with tonnage band 1 – 10 tonnes/year where the fee waiver has been claimed, you will need to indicate whether the substance fulfils the Annex III criteria.

6.6.3.1. 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 143: Hazardous substance indicator



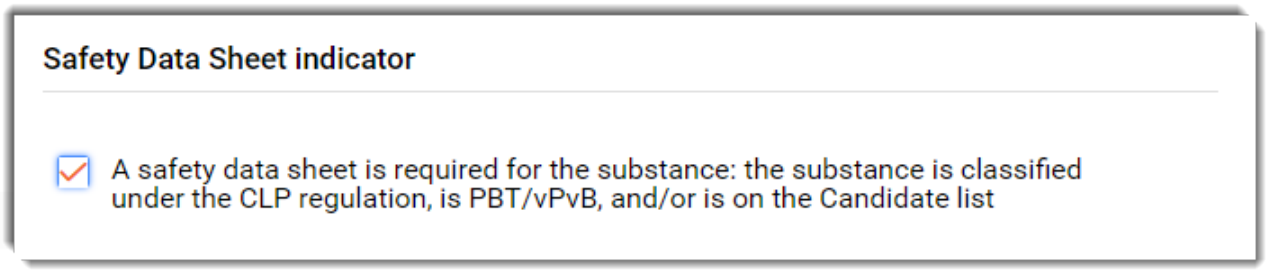
For more information, check the manual *Dissemination and confidentiality under the REACH Regulation*: https://echa.europa.eu/manuals.

6.6.3.2. Safety Data Sheet indicator

If the safety data sheet is required for the substance according to Article 31 of the 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 144: Safety Data Sheet indicator



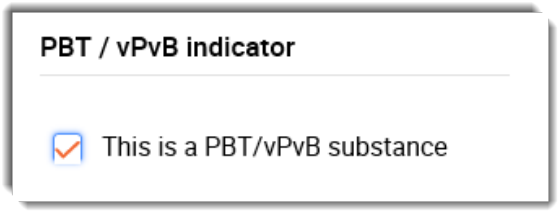
For more information, check the manual *Dissemination and confidentiality under the REACH Regulation*: https://echa.europa.eu/manuals.

6.6.3.3. PBT/vPvB indicator

If the substance is assessed to be PBT/vPvB according to Annex XIII of REACH Regulation, tick the box next to the text *PBT / vPvB indicator*.

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

Figure 145: PBT/vPvB indicator



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

6.6.3.4. Annex III criteria indicator

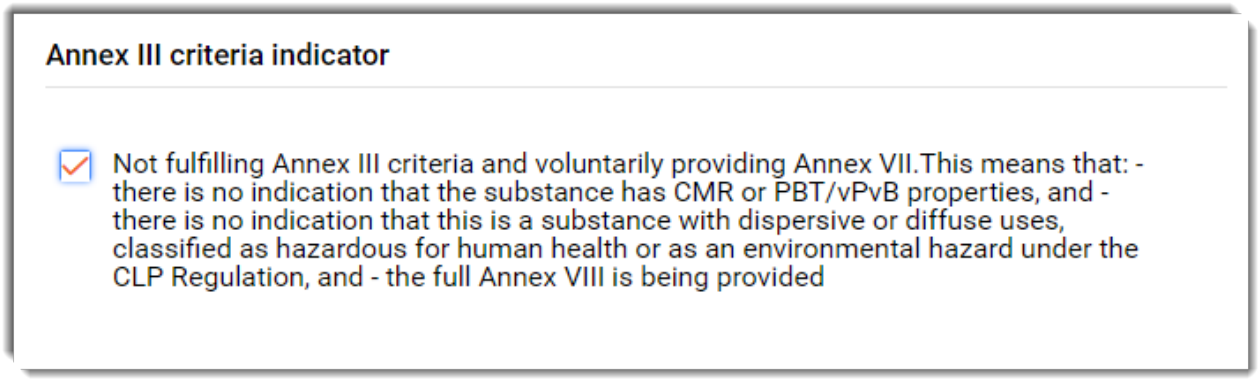
If the substance does not fulfil the Annex III criteria according to REACH Regulation, and the full Annex VII is voluntarily provided, tick the box next to the "Annex III criteria indicator".

The Annex III criteria is not fulfilled when:

3. 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
4. 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.

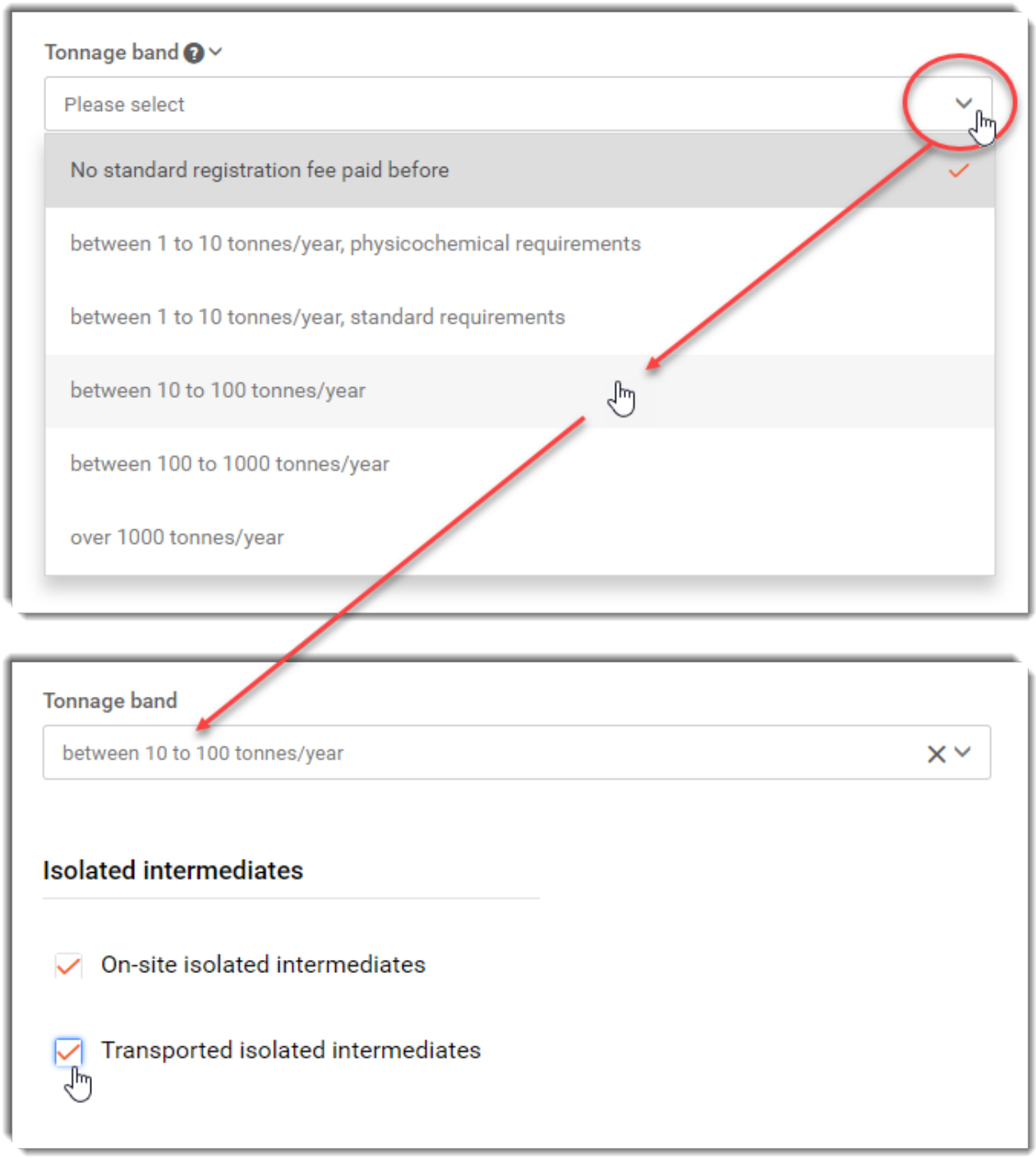
Figure 146: Annex III criteria indicator



6.6.4. Dossier is for an update to a previous submission

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

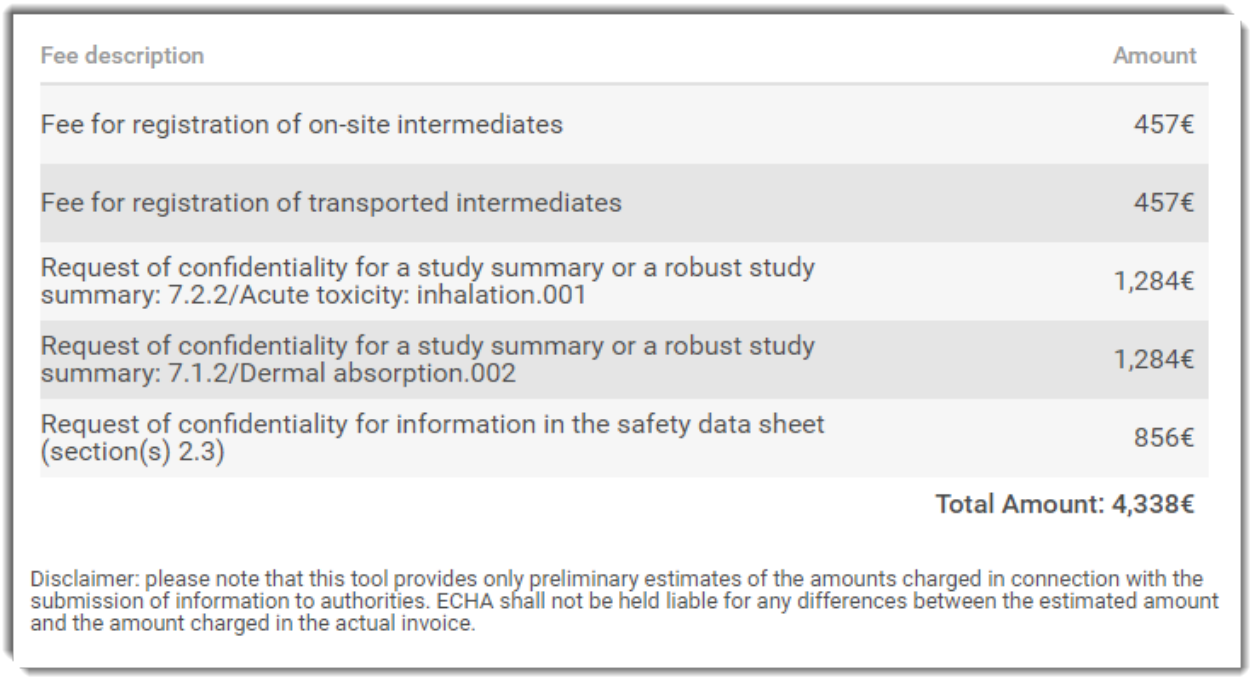
Figure 147: Select the tonnage band of the previous submission, and information on intermediates



6.6.5. Fee calculator results window

Clicking on the button labelled *Calculate* at the foot of the page generates an itemised list of the fees calculated according to the *Dossier* information, and the information inserted manually into the *Fee calculator*. An example is shown below.

Figure 148: Fee calculator results window – example showing intermediates and confidentiality claims



Fee description	Amount
Fee for registration of on-site intermediates	457€
Fee for registration of transported intermediates	457€
Request of confidentiality for a study summary or a robust study summary: 7.2.2/Acute toxicity: inhalation.001	1,284€
Request of confidentiality for a study summary or a robust study summary: 7.1.2/Dermal absorption.002	1,284€
Request of confidentiality for information in the safety data sheet (section(s) 2.3)	856€
	Total Amount: 4,338€

Disclaimer: please note that this tool provides only preliminary estimates of the amounts charged in connection with the submission of information to authorities. ECHA shall not be held liable for any differences between the estimated amount and the amount charged in the actual invoice.

6.6.6. Version of the Fee calculator

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 to an individual component. To be informed of changes, sign up to the general newsletter of IUCLID by logging in to the IUCLID website, opening *My account*, and then ticking the relevant box.

6.6.7. 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.

6.7. Dissemination preview

The *Dissemination preview* 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 output of the *Dissemination preview* is a file in the format of Microsoft Excel (XLSX).

The output contains an indication of the information which would be, if submitted to ECHA, be made publicly available over the internet.

The Filtering Process in the tool, that prescribes the output, 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 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 output 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); so, by default, it will remove information claimed confidential. 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 that indicated in the output of the *Dissemination preview*.

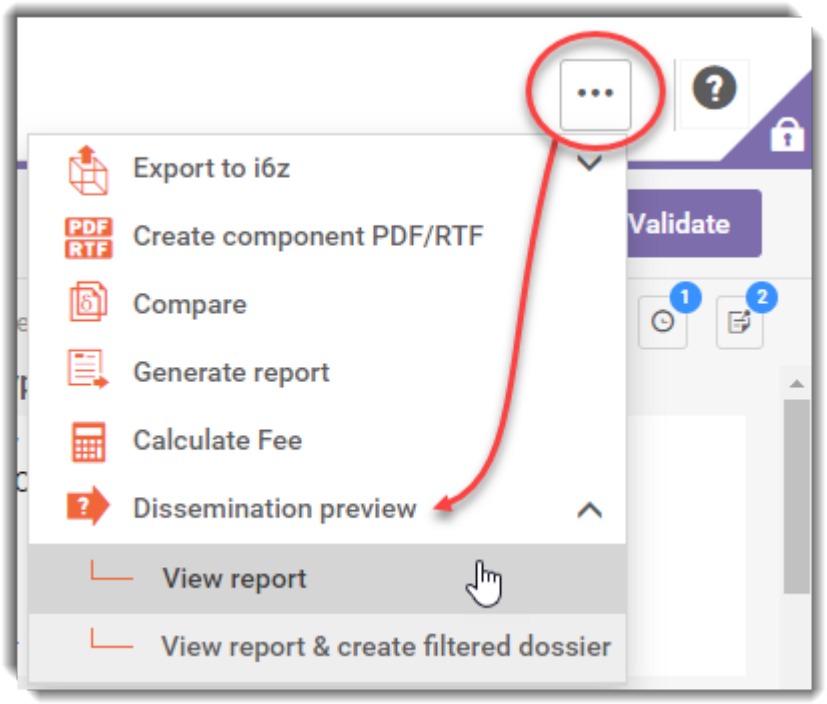
The following subsections describe how to run the *Dissemination preview*, and how to understand its output.

Note: It is recommended to always use the latest version of the *Dissemination preview*, which in practice means using the latest version of IUCLID.

6.7.1. Running the Dissemination preview

The *Dissemination preview* is run from the top level of the record for a *Dossier*. Click on the menu button labelled with three dots, and then select *Dissemination preview*, as shown ringed in red in the example below.

Figure 149: Run the Dissemination preview



6.7.2. Output of the Dissemination preview

The output is available in two forms: A *Report* in the format of Microsoft Excel (XLSX), a *Filtered dossier*, which is a IUCLID *Dossier* containing the information that can be made publicly available on the ECHA website.

In the report, there is a row per field that states the location of the data within IUCLID, and whether data in that field is published publicly on the ECHA website. The publication is indicated in the column named *Outcome*. If a field is empty, there is no row for it in the output of the *Dissemination preview*.

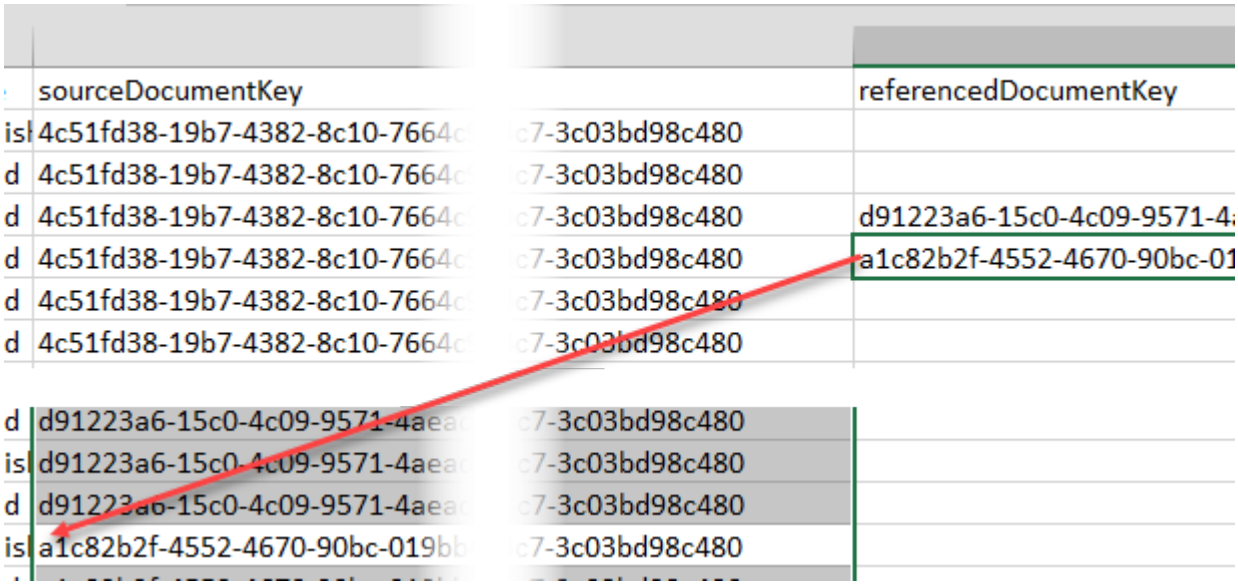
6.7.2.1. Report: Fields for which there is a reference within IUCLID

In IUCLID, an entity or a document can refer to another entity. The types of entity that can be referred to are: *Reference substance*, *Test material*, *Contact*, *Legal entity*, *Literature reference*, and *Category*. For example, a *Substance* can refer to a *Reference substance*.

Where data exists in cases such as this, there are rows in the output of the *Dissemination preview* for the fields at both ends of the reference. For example, the field in a *Substance* where it refers to a *Reference substance* has a row. Also, the fields in the *Reference substance* have their own rows. If the row in the *Substance* has an outcome of “Published” this does not necessarily mean that all the fields for the *Reference substance* are published.

Where a reference exists from the field in a row, the row contains a value in the column named *referencedDocumentKey*. This value is present in the column *sourceDocumentKey* for the rows to which the reference points. Thus, the values can be used to find the rows to which a reference points. An example is shown below.

Figure 150: The link between a referencing field and a referenced field in the Dissemination preview



The outcomes for referenced entities are at the bottom of the report, but they can be seen more clearly using the filter function of Excel, as described in the example below.

Example

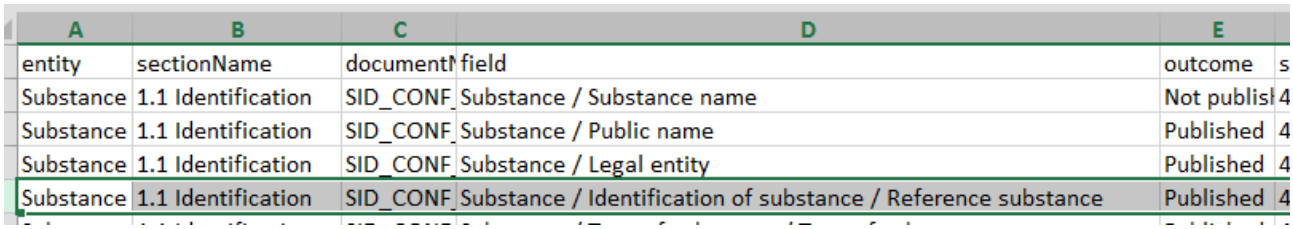
A substance contains a link in section *1.1 Identification* to a *Reference substance*.

Open the *Dissemination report* and then find the field required, using the column named *field*. In this example it is:

`Substance / Identification of substance / Reference substance`

From the screenshot below it can be seen that the *Reference substance* will be published, but what about the individual fields inside the *Reference substance*? Their values for *Outcome* can be viewed as follows.

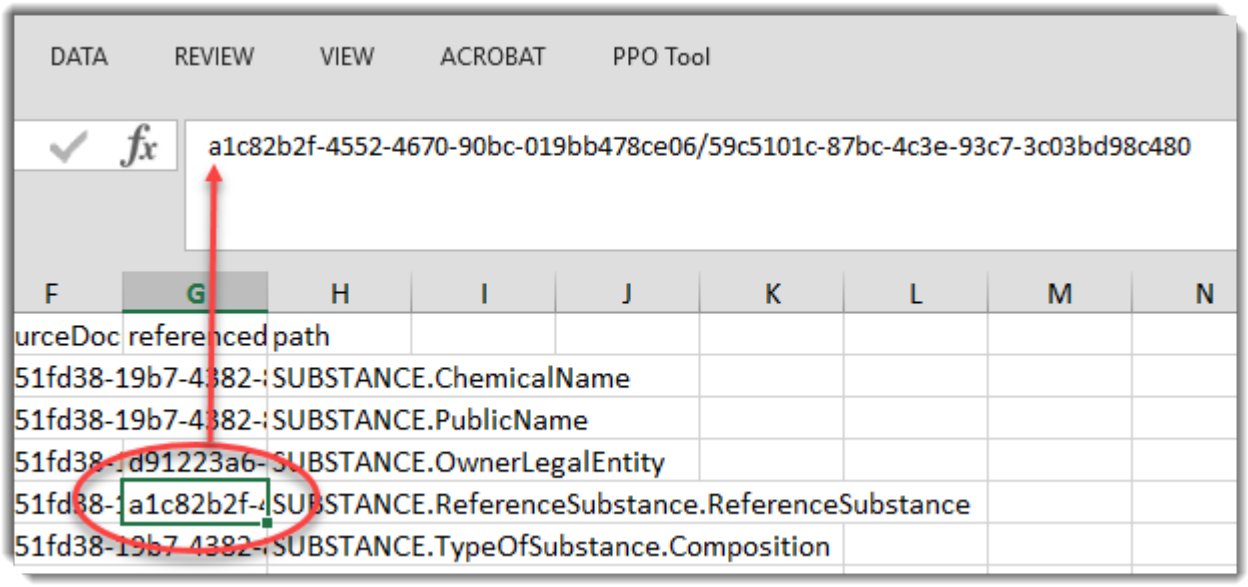
Figure 151: Example Dissemination report for a field in a Substance that links to a Reference substance



A	B	C	D	E
entity	sectionName	documentN	field	outcome
Substance	1.1 Identification	SID_CONF_	Substance / Substance name	Not publis
Substance	1.1 Identification	SID_CONF_	Substance / Public name	Published
Substance	1.1 Identification	SID_CONF_	Substance / Legal entity	Published
Substance	1.1 Identification	SID_CONF_	Substance / Identification of substance / Reference substance	Published

Copy the value of *referencedDocumentKey* (Column G) for the row to the clipboard, for example by selecting it, and then using right-click *Copy*. It is displayed by selecting the cell, as shown below.

Figure 152: The identifier of a Reference substance in *referencedDocumentKey* (Column G)

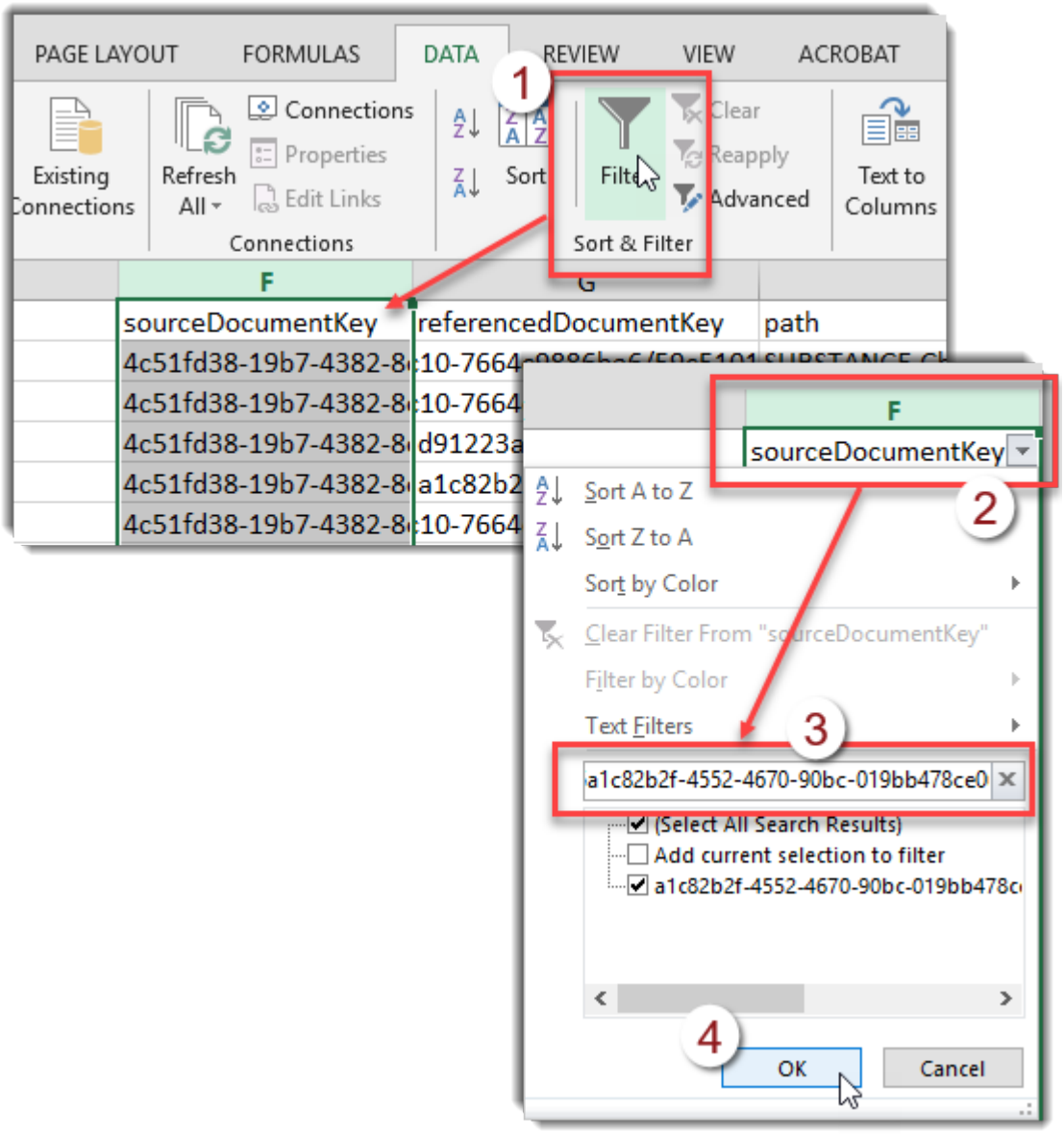


In this example the value is:

a1c82b2f-4552-4670-90bc-019bb478ce06/59c5101c-87bc-4c3e-93c7-3c03bd98c480

Apply a filter in MS Excel to the column *sourceDocumentKey* (F) as shown in the figure below.

Figure 153: Apply a filter to *sourceDocumentKey* in MS Excel

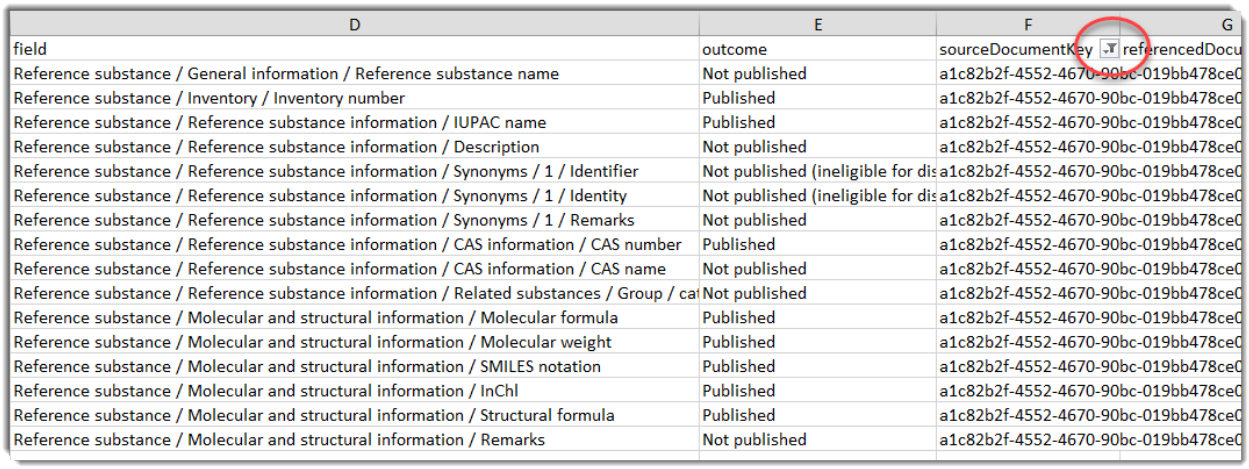


Legend for Figure 153

1. With the column *sourceDocumentKey* (F) selected, click on *DATA* > *Filter*;
2. Open the filter window;
3. Paste the value of *referencedDocumentKey* copied earlier, into the box *Text Filters*;
4. Click OK;

The result shows the predicted outcome for all the fields in the *Reference substance*, as shown below. Note that even though the outcome for the link to the *Reference substance* is “Published”, not all the fields in the *Reference substance* itself are published.

Figure 154: Output of the Dissemination preview filtered for a single reference to a Reference substance



D	E	F	G
field	outcome	sourceDocumentKey	referencedDocu
Reference substance / General information / Reference substance name	Not published	a1c82b2f-4552-4670-90bc-019bb478ce0	
Reference substance / Inventory / Inventory number	Published	a1c82b2f-4552-4670-90bc-019bb478ce0	
Reference substance / Reference substance information / IUPAC name	Published	a1c82b2f-4552-4670-90bc-019bb478ce0	
Reference substance / Reference substance information / Description	Not published	a1c82b2f-4552-4670-90bc-019bb478ce0	
Reference substance / Reference substance information / Synonyms / 1 / Identifier	Not published (ineligible for dis	a1c82b2f-4552-4670-90bc-019bb478ce0	
Reference substance / Reference substance information / Synonyms / 1 / Identity	Not published (ineligible for dis	a1c82b2f-4552-4670-90bc-019bb478ce0	
Reference substance / Reference substance information / Synonyms / 1 / Remarks	Not published	a1c82b2f-4552-4670-90bc-019bb478ce0	
Reference substance / Reference substance information / CAS information / CAS number	Published	a1c82b2f-4552-4670-90bc-019bb478ce0	
Reference substance / Reference substance information / CAS information / CAS name	Not published	a1c82b2f-4552-4670-90bc-019bb478ce0	
Reference substance / Reference substance information / Related substances / Group / ca	Not published	a1c82b2f-4552-4670-90bc-019bb478ce0	
Reference substance / Molecular and structural information / Molecular formula	Published	a1c82b2f-4552-4670-90bc-019bb478ce0	
Reference substance / Molecular and structural information / Molecular weight	Published	a1c82b2f-4552-4670-90bc-019bb478ce0	
Reference substance / Molecular and structural information / SMILES notation	Published	a1c82b2f-4552-4670-90bc-019bb478ce0	
Reference substance / Molecular and structural information / InChI	Published	a1c82b2f-4552-4670-90bc-019bb478ce0	
Reference substance / Molecular and structural information / Structural formula	Published	a1c82b2f-4552-4670-90bc-019bb478ce0	
Reference substance / Molecular and structural information / Remarks	Not published	a1c82b2f-4552-4670-90bc-019bb478ce0	

7. 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.

The creation and editing of a *Legal entity* can done either from the list page of entities, which is accessible from the main menu, or from the point where the *Legal entity* is referred to in a dataset.

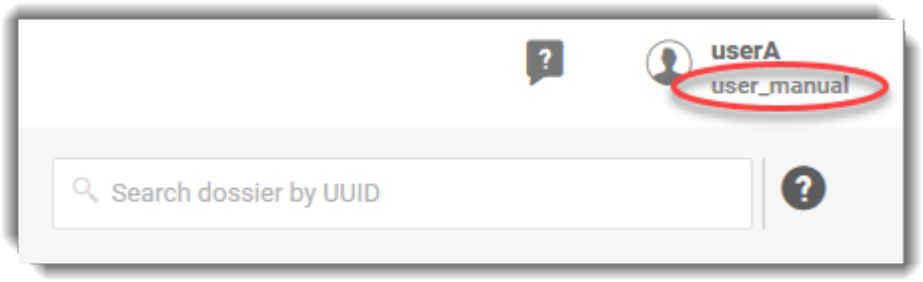
A *Legal entity* can be associated with various entities, such as *Substance*.

7.1. Working Legal entity

When a *User* creates an entity, for example a *Substance*, 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 current *working Legal entity*.

The *working Legal entity* is indicated at the top right of the interface, as shown below circled in red.

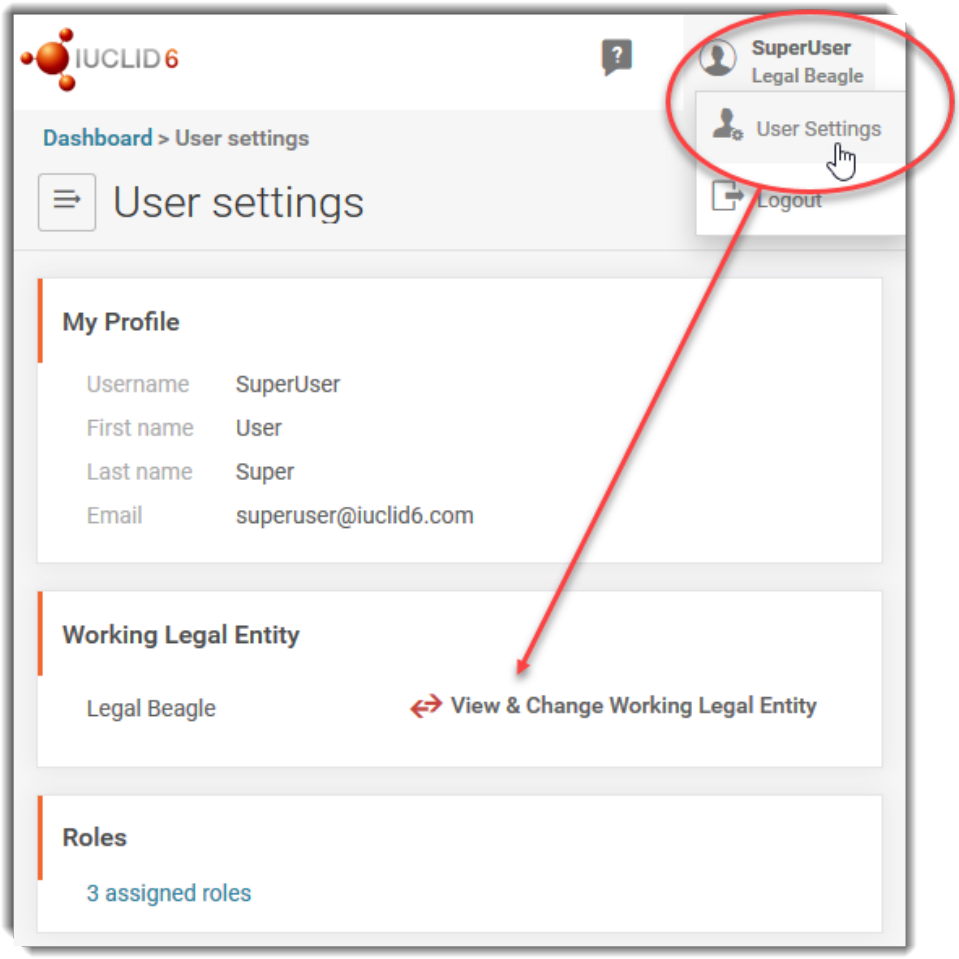
Figure 155: The working legal entity



A *User* can set the *working Legal entity* to be any *Legal entity* that has been assigned to the *User*. Assignment is not the same as having access to a *Legal entity* via the list page. The assignment can be done only by a *User manager*. However, in IUCLID 6 Desktop all actions are effectively carried out by the *SuperUser*, which can do the assignment. This means that in IUCLID 6 Desktop a *Legal entity* can be created and immediately set as the *working Legal entity*. That is not the case in IUCLID 6 Server, where the assignment must be done by a *User manager*, other than the *User* that created the *Legal entity*.

The *working Legal entity* is set from the *User Settings* menu accessed from the top right of the interface, as shown below.

Figure 156: View and change the working Legal entity in IUCLID 6 Desktop



7.2. General information

The name of the *Legal entity* must be entered, but the other fields are optional. The type of the *Legal entity* and other names are for information purposes.

7.3. 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 identifiers can be selected. For example, *Legal entity* has an option for DUNS.

7.4. Contact information

An address can be defined for a contact of the *Legal entity* and links can be made to one or more entities of type *Contact*.

8. Legal entity site

A *Legal entity site* is an entity that is used to associate a *Legal entity*, and therefore 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, a value in the field *Site* to indicate the physical location, and be associated with a *Legal entity*. The creation and editing of a *Legal entity site* are done from the point where the *Legal entity site* is referred to in a dataset.

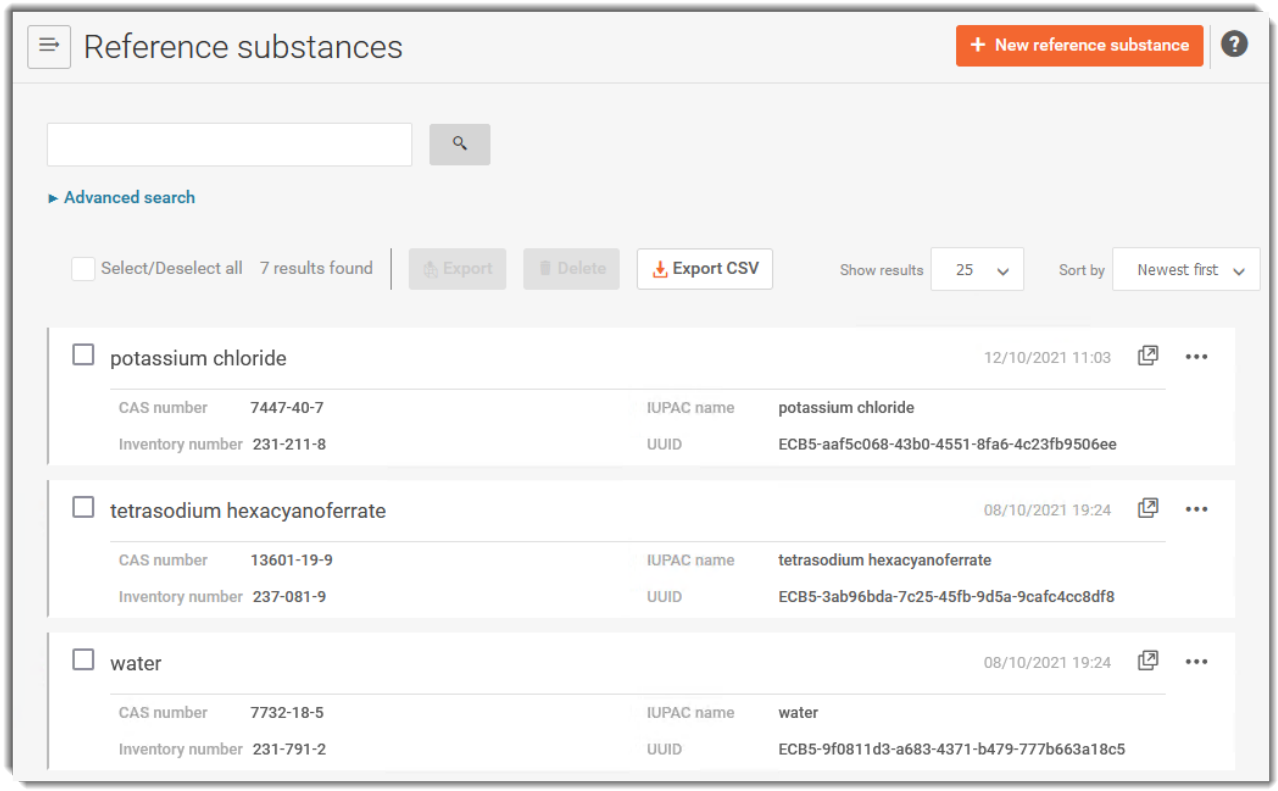
9. Reference substance

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*.

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 is available to download free of charge from the IUCLID website under the section *Support / Get Reference Substances*. If the required *Reference substance* is not available on the website, or if you otherwise prefer, it is possible to create a *Reference substance* within IUCLID. This can be done from the point where the *Reference substance* is referred to in a dataset, or from the list page of *Reference substances*, from where deletion and editing are also available. The list page is opened from the main menu.

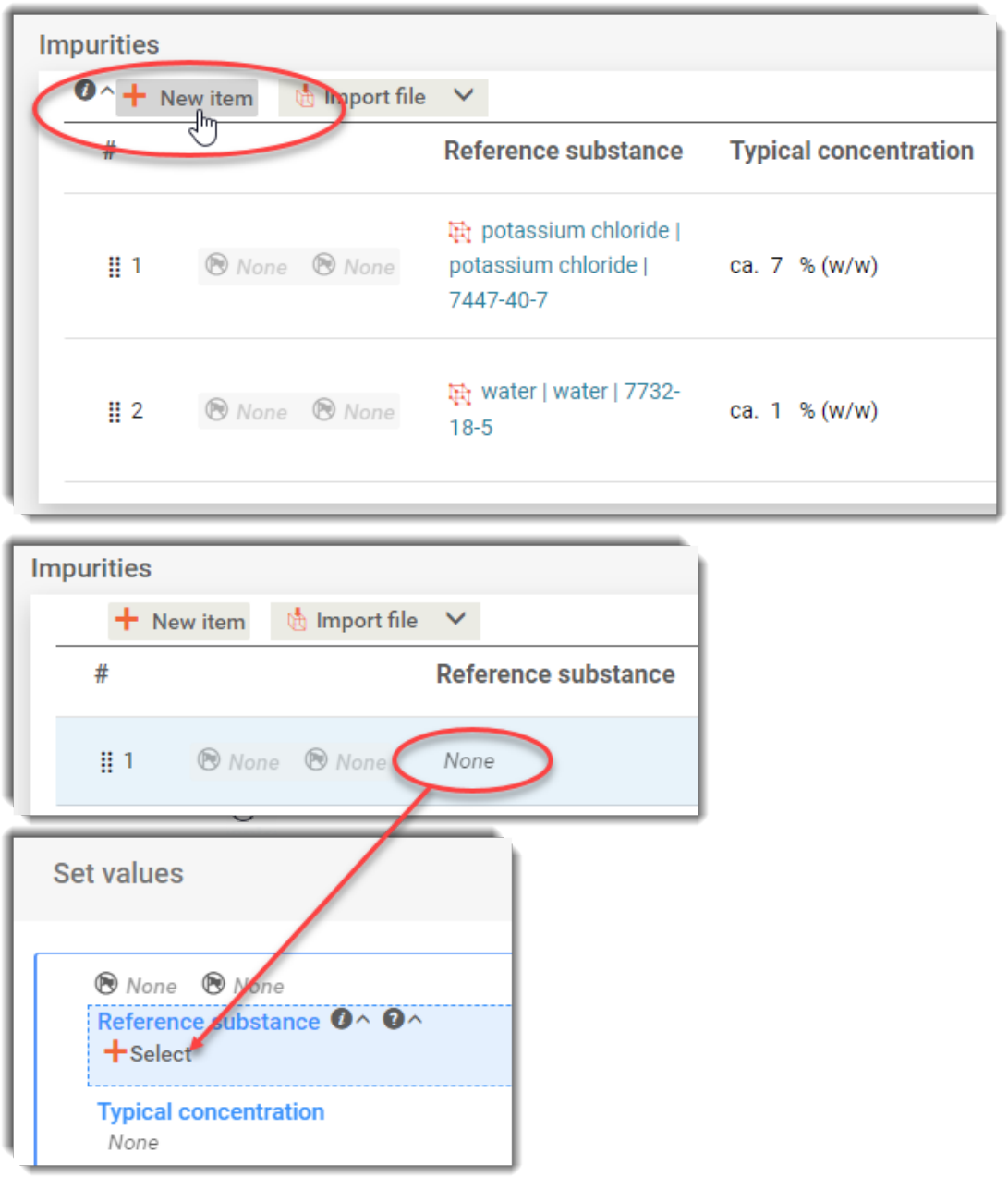
The list page for *Reference substance* is shown below. It has the same navigation and search features as the list pages for *Substance* and *Mixture/Product*. *Delete* is under the button, with the three dots that is on the right of an entry in the list.

Figure 157: The list page for Reference substances



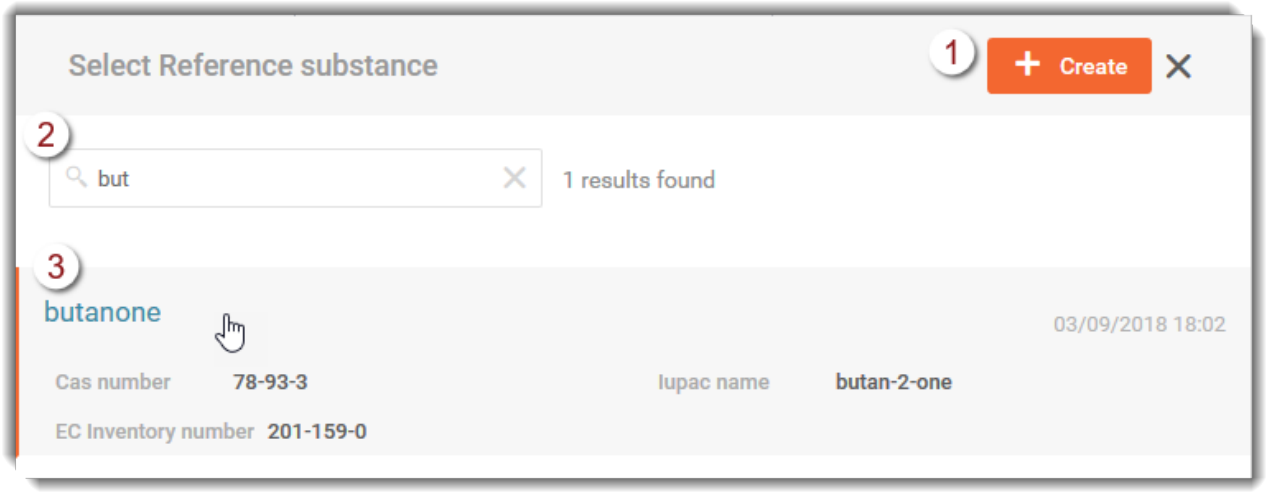
An example of how to refer to a *Reference substance* is given below for the section *Identification of substance / Impurities*. To add an impurity, create a new row, click in the new row to open it for editing, and then in the *Reference substance* field, click on *Select*, as shown below.

Figure 158: Enter a Reference substance into the field Impurities for a Substance



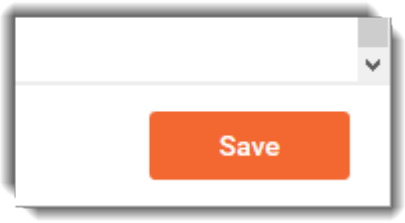
A window opens that allows a *Reference substance* to either be created (1), or selected from those already in the database (2, 3), as shown below.

Figure 159: Create a Reference substance, or select one from the IUCLID database



Clicking on *Create*, opens a window into which the values are entered for the *Reference substance*, as described in the subsections that follow. To record the values entered below, remember to click on the *Save* button at the lower right of the window.

Figure 160: Save



9.1. Reference substance name

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.

9.2. IUPAC name

Use this field to enter the name according to the *International Union of Pure and Applied Chemistry (IUPAC)*.

9.3. Description

This is free-text field to contain a description of the *Reference substance* and the data provided within it.

9.4. Inventory

The group of fields under *Inventory* allows substance identity information to be recorded that relate to chemical inventories.

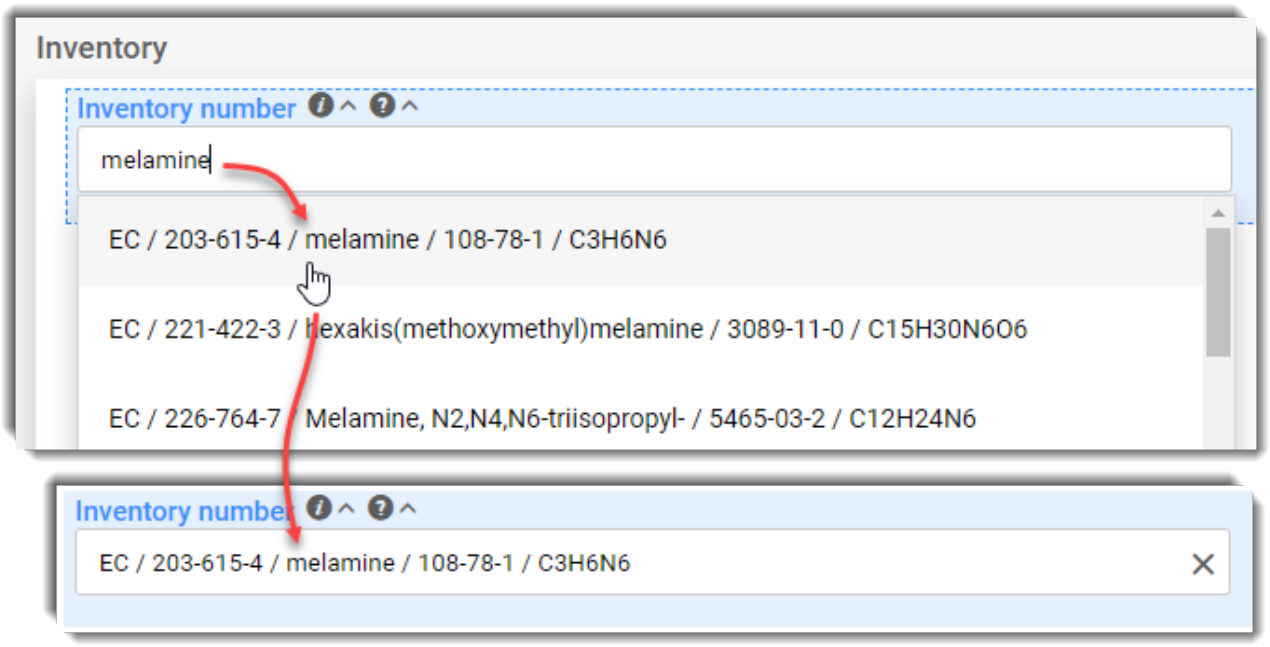
9.4.1. Inventory number

Inventory number is an identifier that is stored as a text value. It provides a function that searches the inventories that are available within the installation of IUCLID. The *EC Inventory* is supplied with IUCLID 6 Desktop and the default IUCLID 6 Server. This is the same *EC Inventory* that is available to download as an archive on the IUCLID website. If the instance of IUCLID does not contain the *EC Inventory* it can be downloaded from the IUCLID website and then imported in the same way as for other IUCLID data, as described in section *1.7.1 Import*. In addition, custom inventories can be created and imported into IUCLID, after which they become available in this field.

The field contains a dynamic search feature that tries to find a match between the value entered, and the inventory values available in the installation of IUCLID. The matches are offered as selectable options.

An example is shown below where the *EC Inventory* is present in the installation of IUCLID. The text “melamine” has been entered, and then the highlighted search hit has been selected. Note that the inventory contains various chemical identifiers, not just the *EC Number*.

Figure 161: Automatic searching of inventories for inclusion in a Reference substance

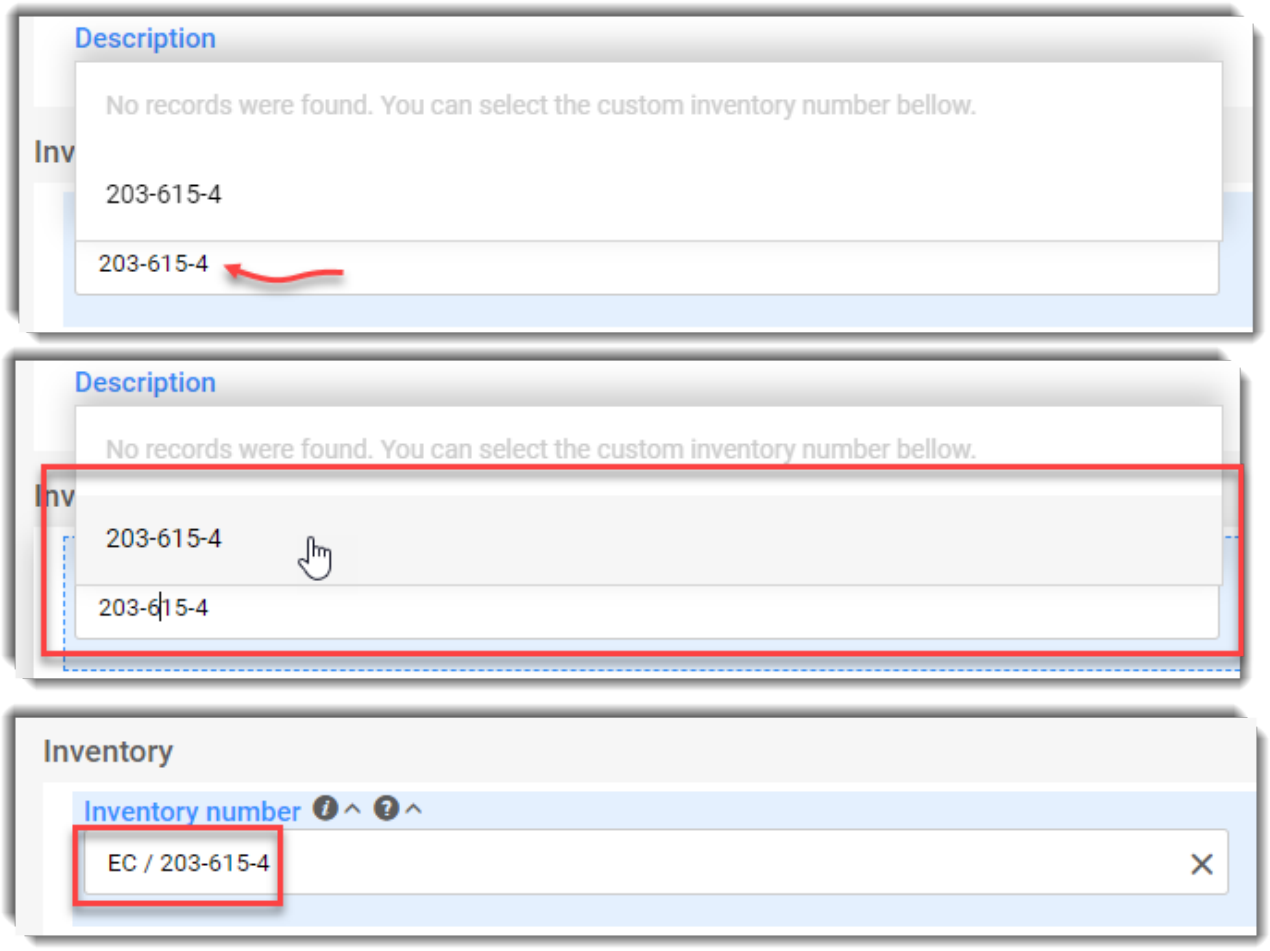


If an *EC Inventory* number is required that is **not** in the instance of IUCLID, instead of creating a custom inventory file to import, a single *EC number* can be entered manually into the field *Inventory number*. In that case, enter the *EC Number* as text, select the whole value by clicking in it, and then click on the *Save* button. The value appears in the field with the label “*EC /* “ prepended to indicate that it is an *EC Number*. The value can contain up to ten characters. If you get an error message, try again making sure that the text value you entered is selected in the menu before clicking *Save*.

An example is shown below where the *EC Inventory* is **not** present in the installation of IUCLID. The required EC Number has been entered as text “203-615-4”, but there are no hits. Next, the *EC*

number has been entered, selected by clicking in it, and then saved. Note that “EC / “ has been prepended to the value entered.

Figure 162: Enter an EC Number manually into a Reference substance



9.4.2. No inventory information available - Justification

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

9.4.3. CAS number

This field is for a number as assigned by the *Chemical Abstracts Service (CAS)*.

9.4.4. CAS name

This field is for a name as assigned by the *Chemical Abstracts Service (CAS)*.

9.5. Synonyms

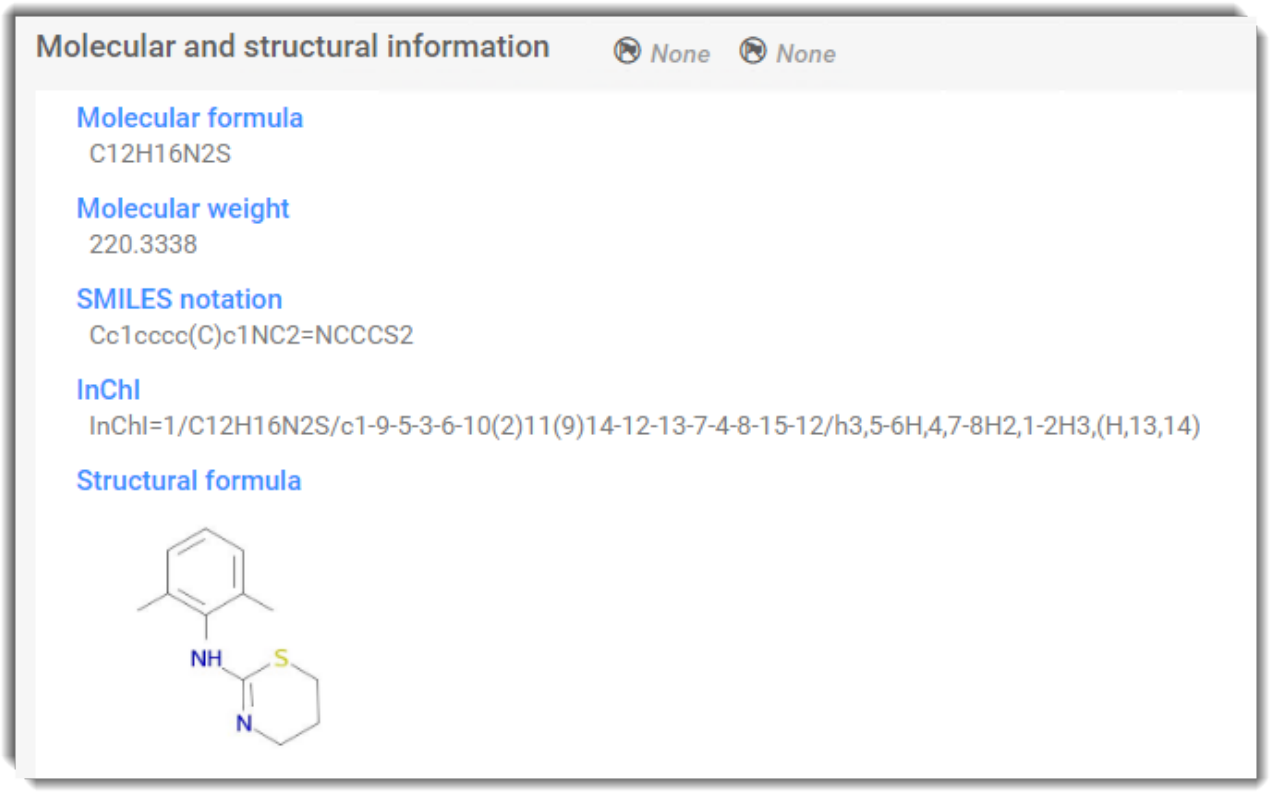
This is a repeatable list where alternative IDs can be added. There are predefined types of IDs, such as *BAS Number* and *ChemSpider ID*.

9.6. Molecular and structural information

In *Molecular and structural information*, enter the molecular formula, the molecular weight, and upload an image of the structural formula in either the format: JPEG, GIF, or PNG. The field *Molecular formula* accepts text but no characters in subscript, so for example ethene would be C2H4. There are also fields for identifiers of type *SMILES* and *InchI*.

A single flag can be applied to all the data in *Molecular and structural information*. See the example below.

Figure 163: Molecular and structural information - example



9.7. Related substances

This is a repeatable list where relationships between substances can be recorded. There are predefined relationships such as: anhydrate, monomer, polymer. There is a single field where the group or category of a *Reference substance* can be recorded.

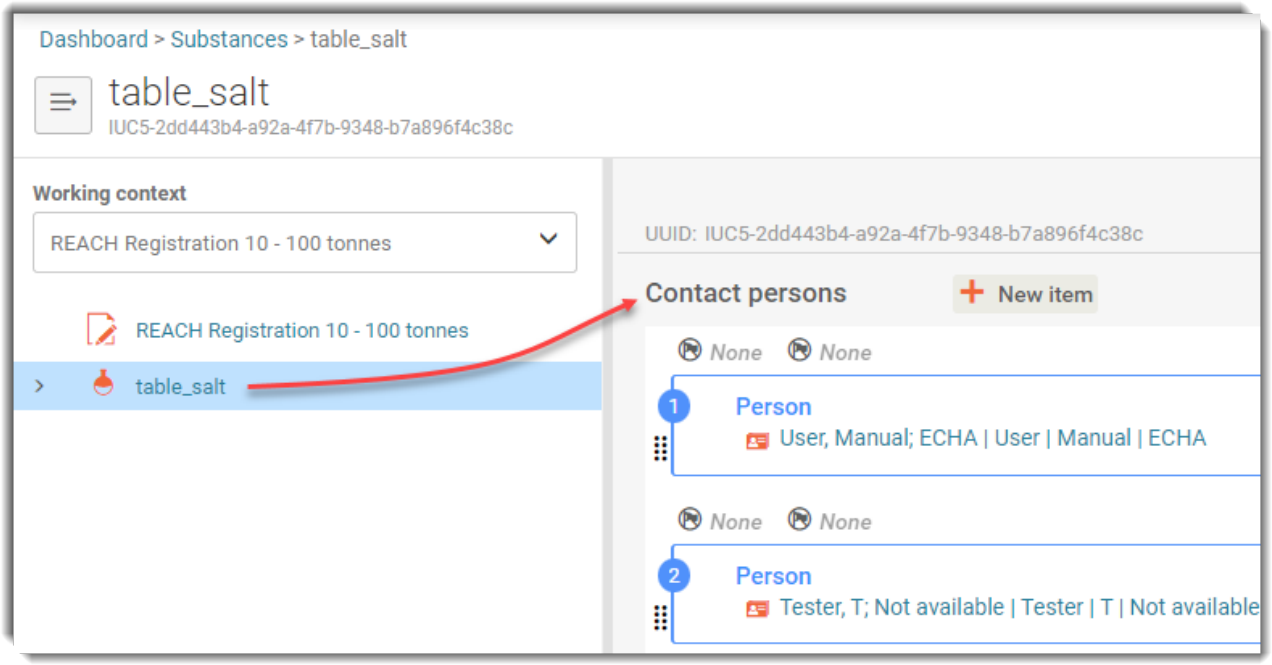
10. Contacts

A *Contact* is an entity that is used to record 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*, *toxicologist* and *other*.

A *Contact* can be either edited or created from the place within a document or entity that links to it. Typically, a link can be made to more than one *Contact* from the same place. An example of a field that refers to two *Contacts* is given below for *General information* > *Identification of substance* > *Contact persons*, which is section 1.1 under REACH. Note that the cursor is hovering over the first contact, causing a highlighted box to be displayed.

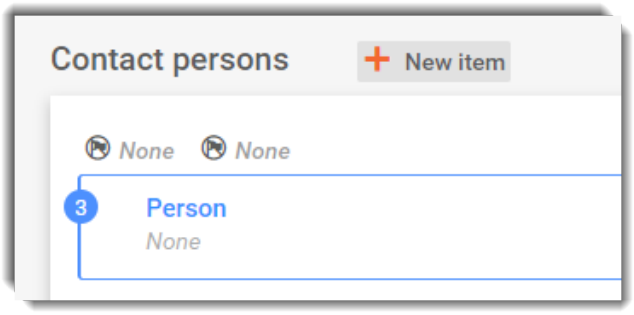
Figure 164: Contacts in the identification of a substance dataset



A *Contact* in a field is actually a link to a *Contact*, not the *Contact* itself. A link can be removed by clicking on the red delete icon ✕. This does not delete the *Contact*. Clicking on the highlighted blue box for a link to a *Contact* opens the linked *Contact* for editing.

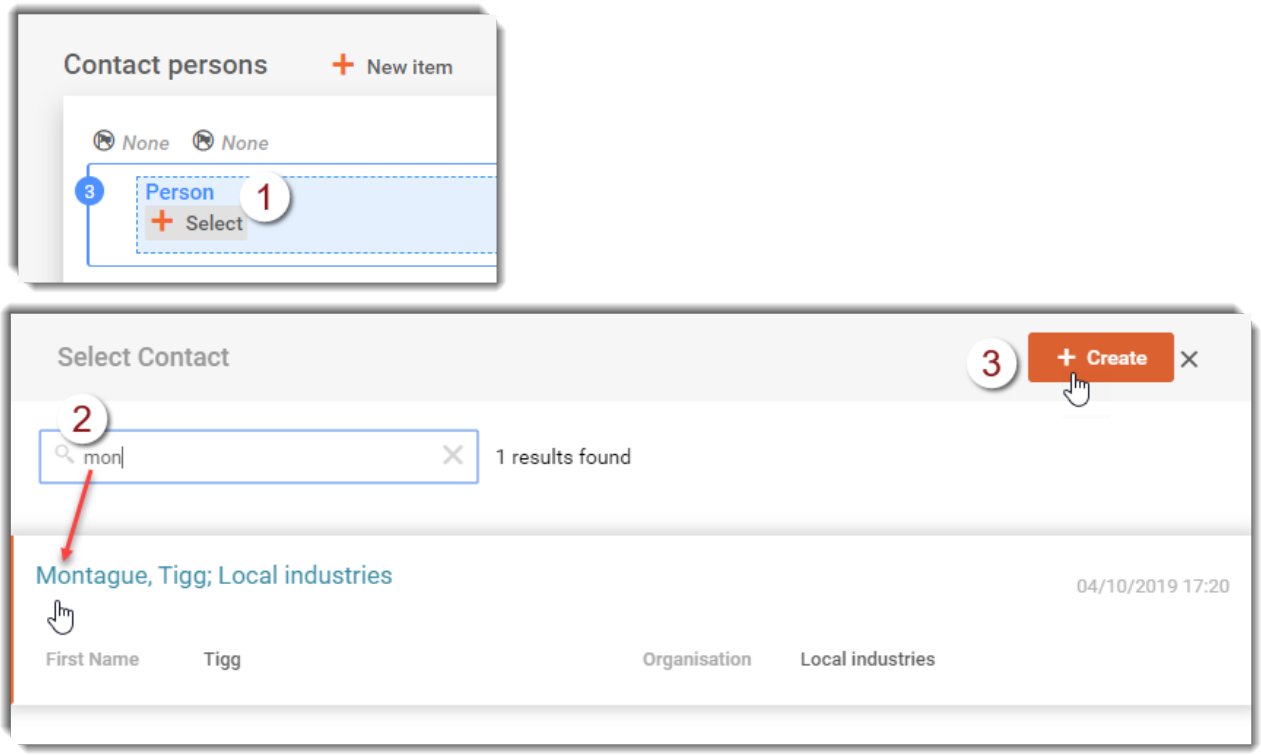
A link can be created by clicking on + *New item*. A newly created link contains no *Contact*, as shown below:

Figure 165: A newly created link to a Contact



To place a *Contact* in a new link, edit the link by clicking on the blue highlighted box. Either link to an existing *Contact*, or create one, as shown below.

Figure 166: Place a Contact in an empty link

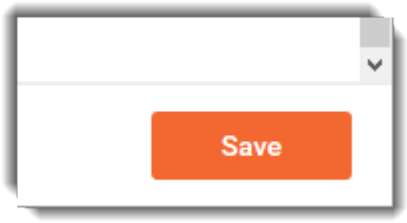


Legend for Figure 166

1. To place a *Contact* in a newly created empty link, first click on *Select item* within the link;
2. To place an existing *Contact* in the link, first search for it by entering a search term to match the name or organisation, then click on its entry in the search results;
3. To create a *Contact* and place it in the link, click *Create*.

After editing or creating a link to a *Contact*, click on the *Save* button at the bottom right of the interface.

Figure 167: Save



11. 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.

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 creation and editing of a *Test material* are done from the point where the *Test material* is referred to in a dataset.

The composition can have components of type *constituent*, *impurity* or *additive*. Each component should be linked to a *Reference substance* and given a concentration range. 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…* . Next, edit the text in square brackets, as required.

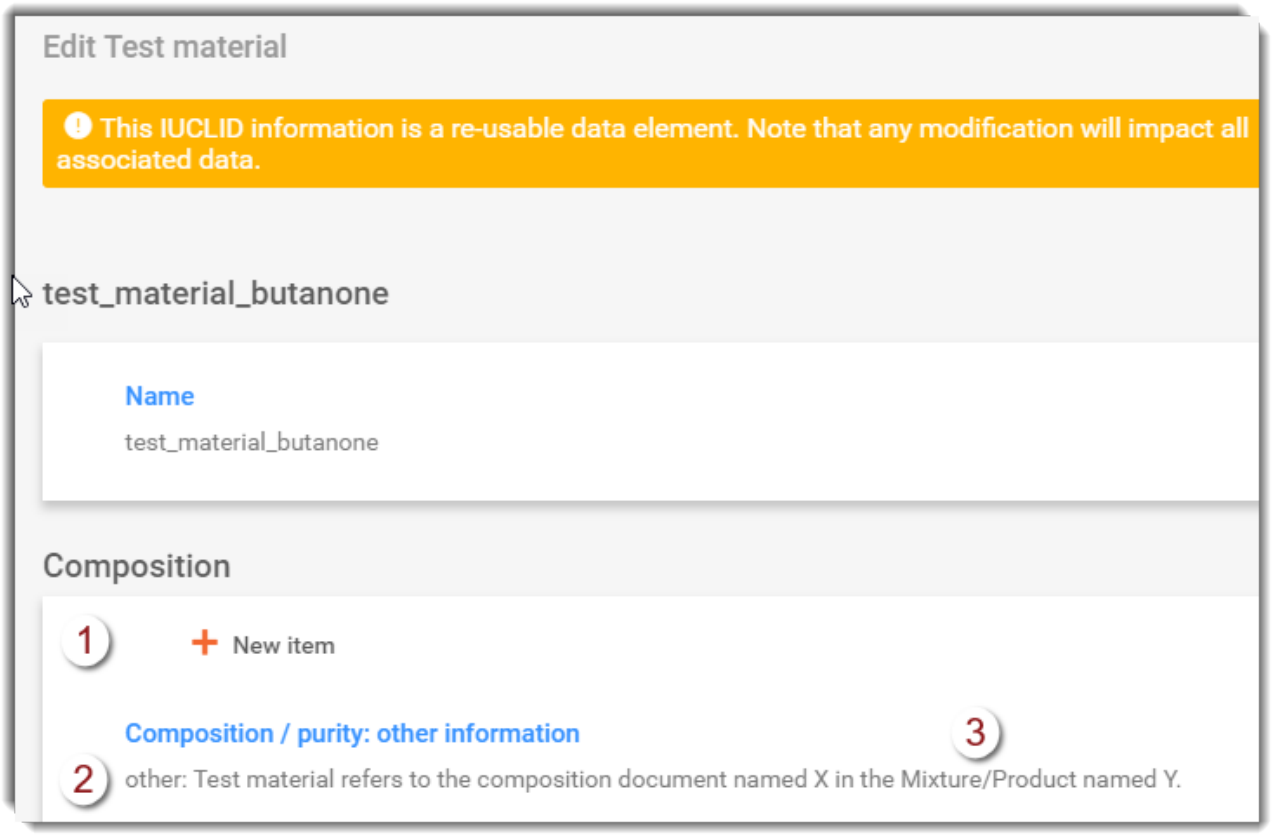
The value of the field *Confidential details on test material* can be excluded during *Dossier* creation, and during *Export* of data that is outside a *Dossier*. A value that has been included in a *Dossier* cannot be excluded during *Export* of the *Dossier*.

11.1. Test material for a Mixture/Product

A *Test material* can be created for a *Mixture/Product*. In that case, there is no need to enter values for the fields *Type*, *Reference substance*, *Concentration* and *Remarks*, because in this context those values are relevant only for a *Substance*. Instead, the composition is indicated by referring to a composition in a *Mixture/Product* dataset. Usually this is the composition of the *Mixture/Product* in which the *Test material* is located, which for example in BPR is in section 2.3.

To make the reference to the composition, first set the field *Composition/purity* to ‘other:’. This causes a text field to appear. Then, enter the name of the composition and the name of its dataset. An example is shown below.

Figure 168: Test material in a Mixture/Product – example where the Test material refers to the composition of the Mixture/product



Legend for Figure 168

1. No value is required here;
2. Select '*other:*';
3. State to which composition document the *Text material* refers.

Any information about the batch number, expiry date, and other information should be entered into the fields *Details on test material*, and/or *Confidential details on test material*.

12. Category

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

12.1. 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.

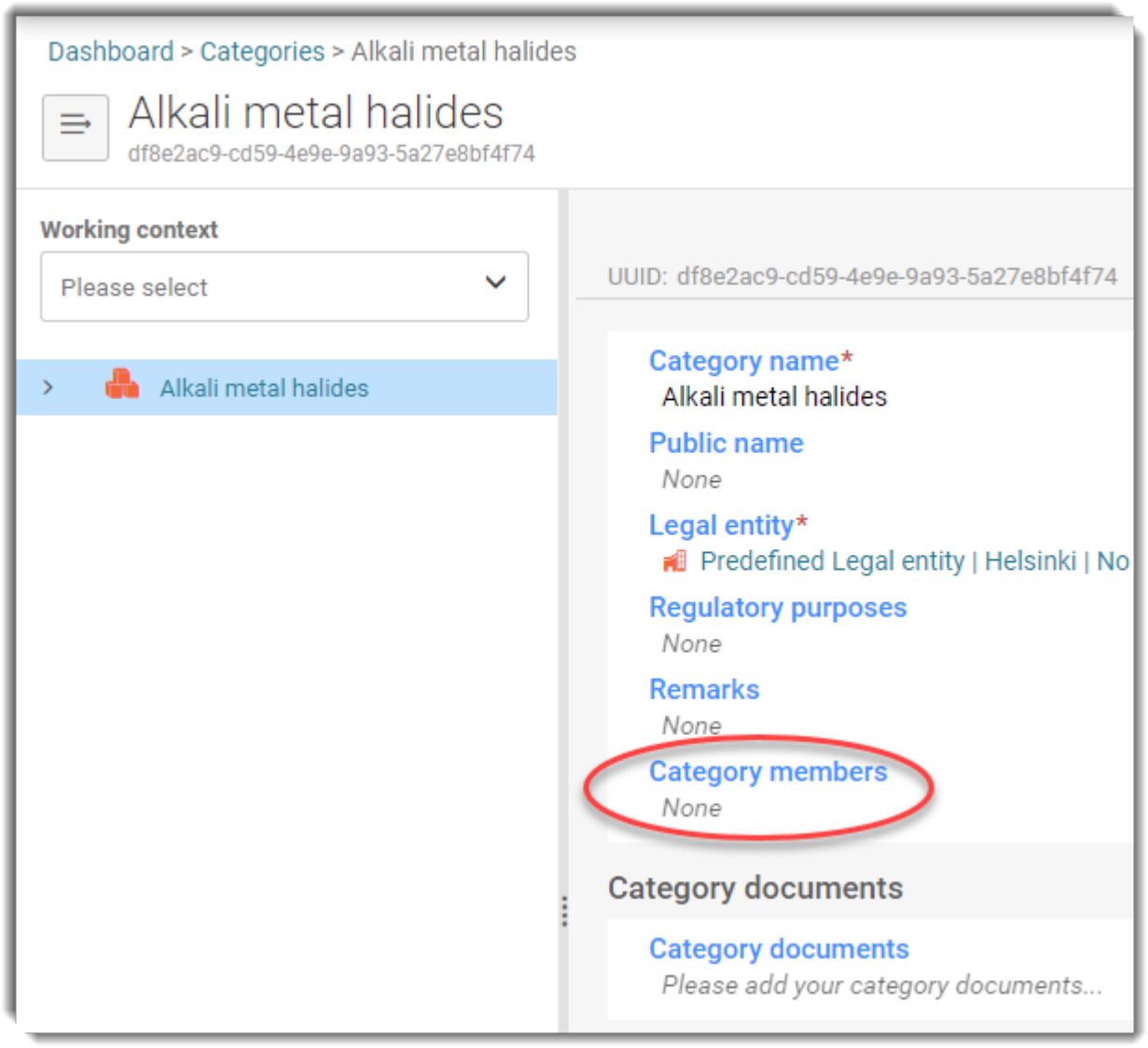
Data gaps in a chemical category can be filled by using various approaches, including simple read-across, trend analysis (interpolation and extrapolation) and computational methods based on SARs, QSARs or QAARs.

12.2. 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*. When a *Category* is created, by default it is associated with the working *Legal entity* of the user. The *Legal entity* can be changed later if required. There is an option to indicate the regulatory purpose of the category. A newly created *Category* has no members, as shown below.

Figure 169: A newly created Category



To add a member, first click within the field *Category members* to make it editable. An option *Select* appears. Clicking on *Select* gives an option of whether to add a *Substance*, or *Mixture/Product*, as shown below.

Figure 170: Select whether the new member of a Category is to be a Substance or a Mixture/Product

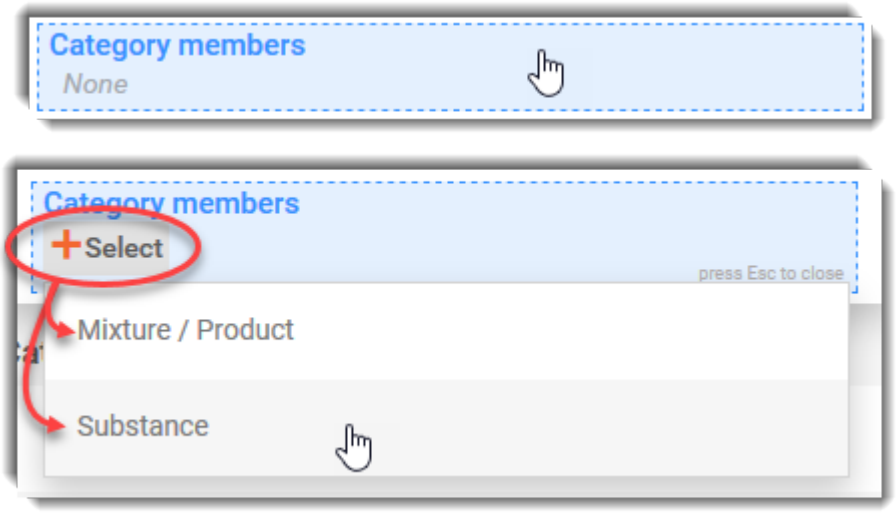
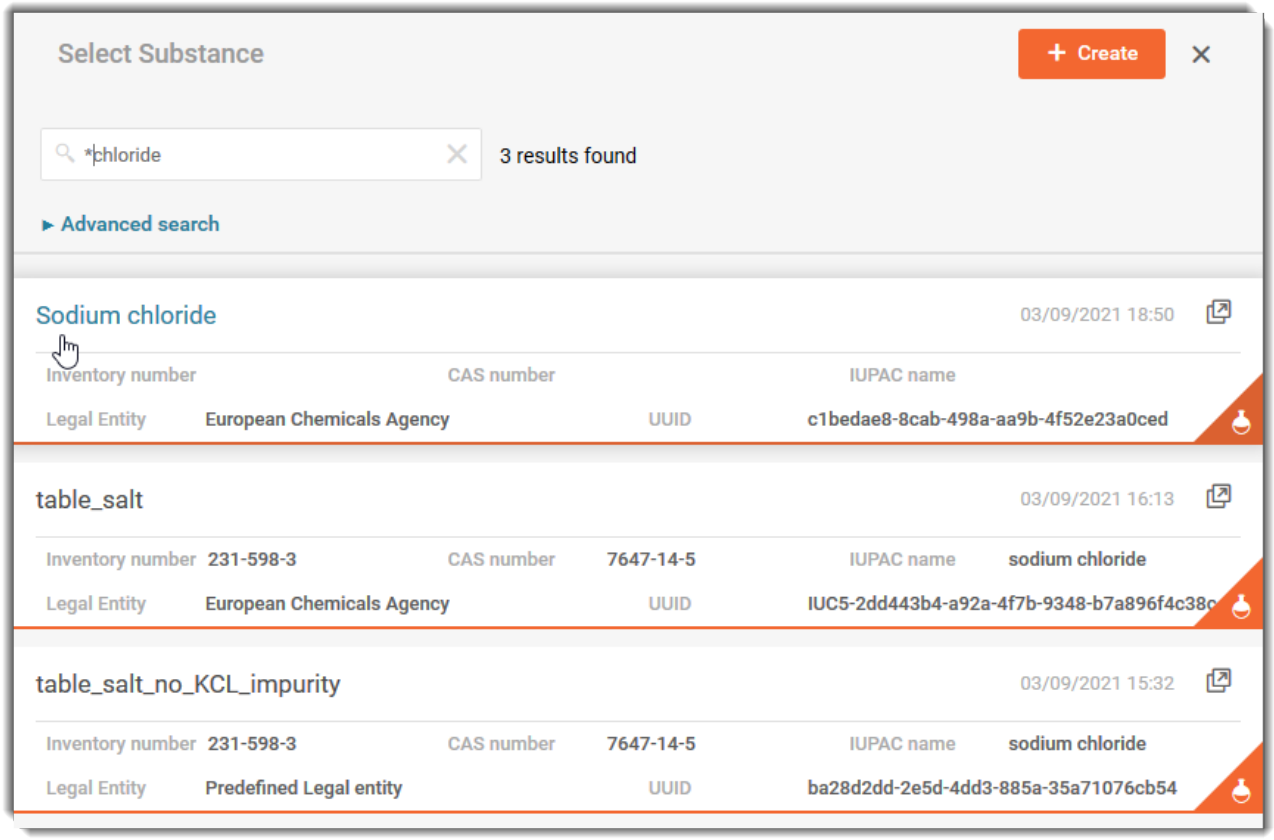
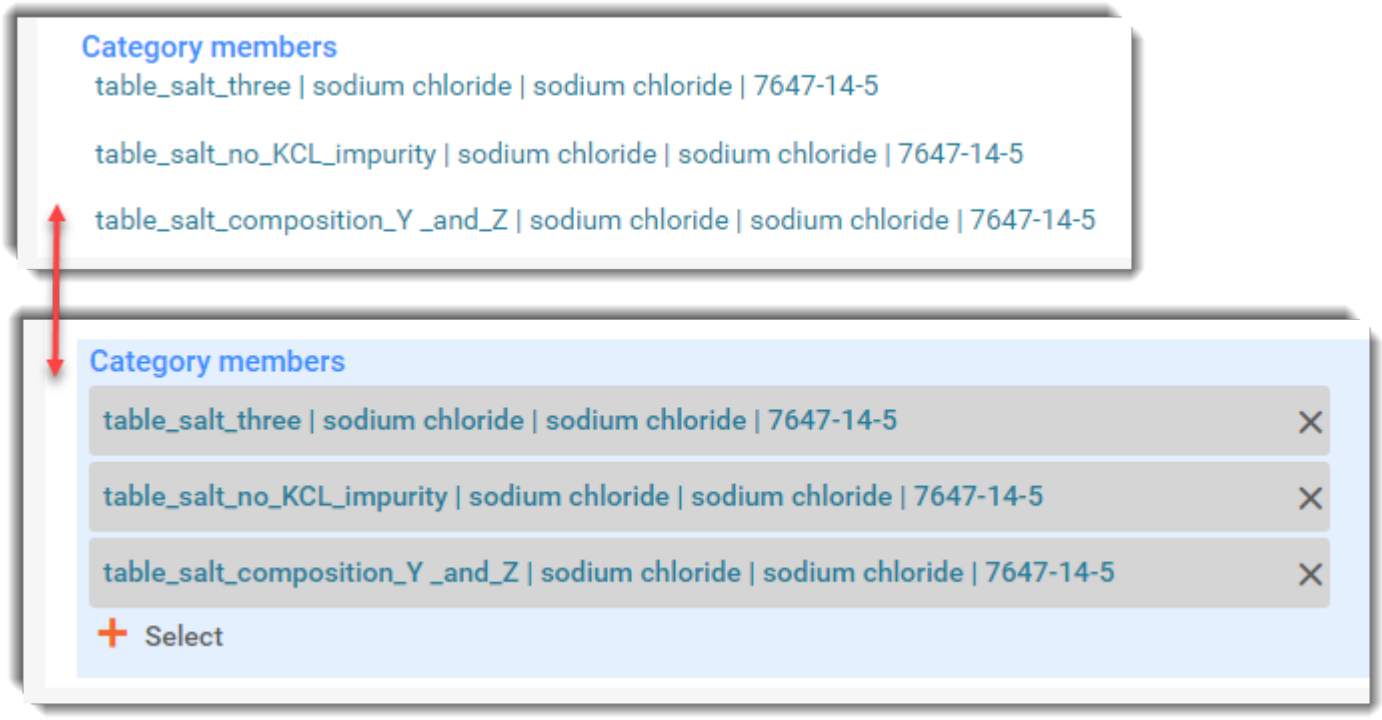


Figure 171: Add a member to a Category



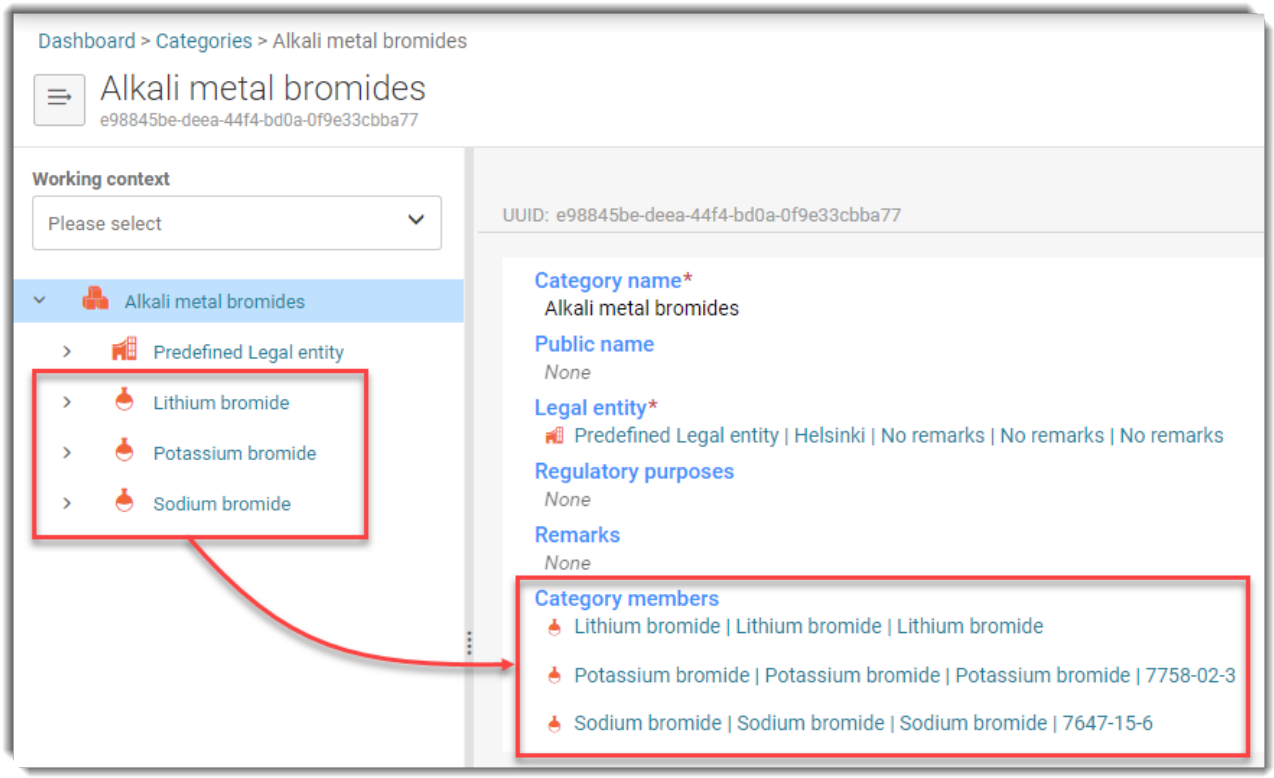
In the example shown below, three members have been added. These can be edited by clicking in the field *Category members*.

Figure 172: Toggle the edit mode for the members of a Category

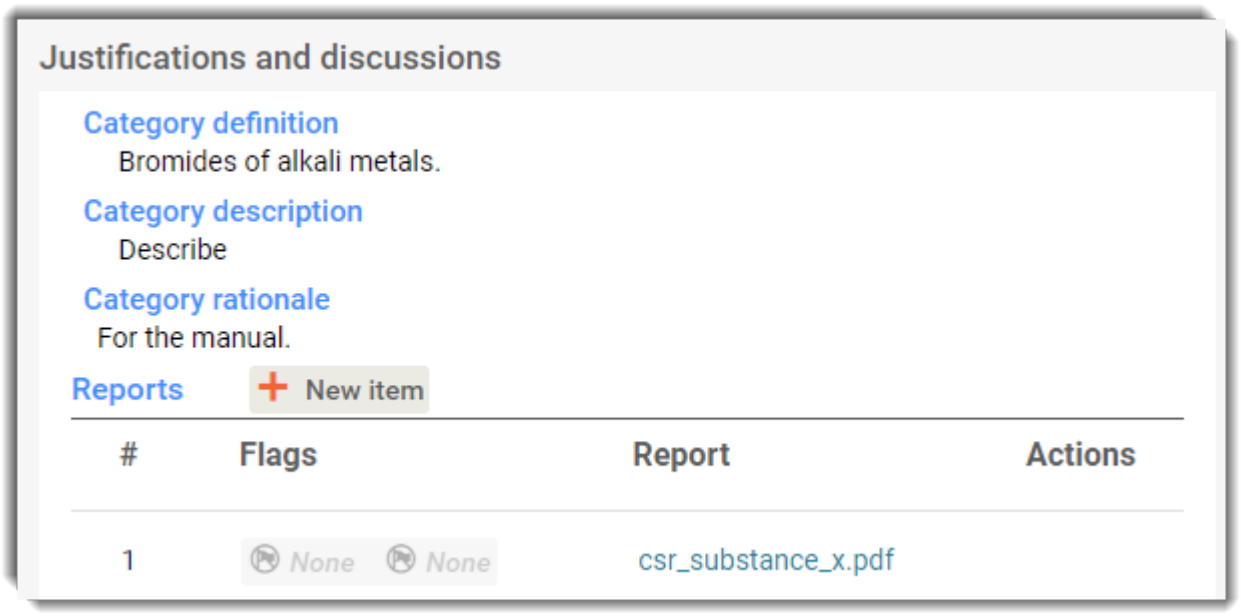


The members are shown in the record of the *Category*, and in table of contents on the left, where their own table of contents can be expanded.

Figure 173: Members of a Category in the table of contents



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



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

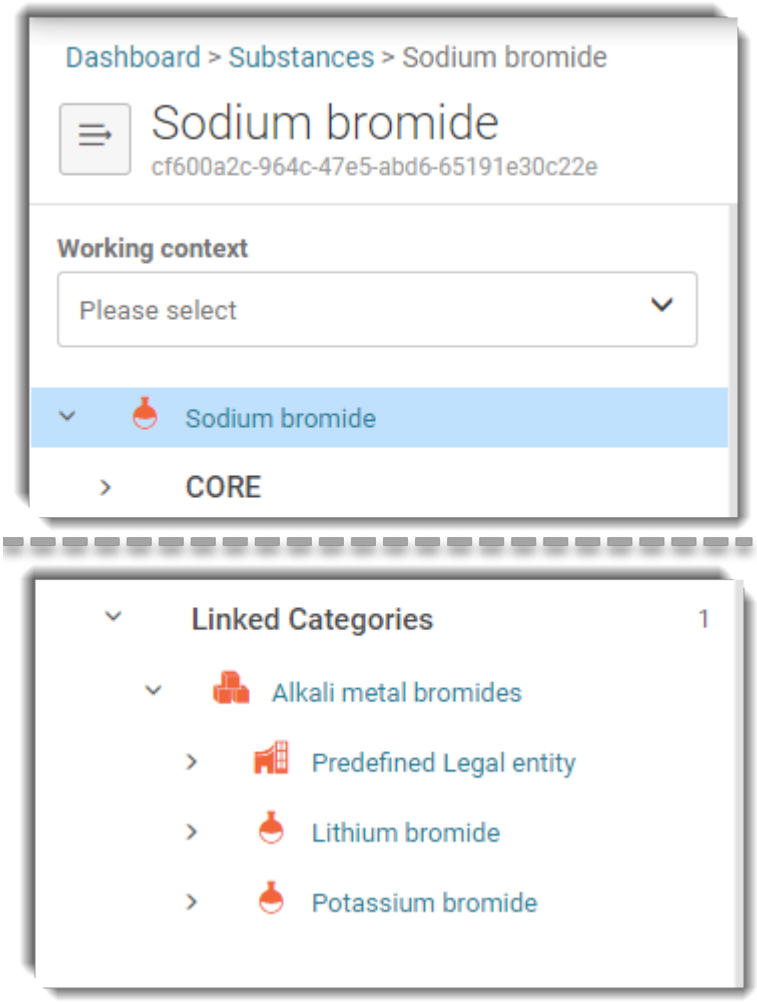
In the field *Category order description*, describe the order of the substances grouped in the category including a brief explanation, if the properties of the category members follow a certain pattern.

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.

Datasets that are a member of a *Category* have a link to the *Category* at the foot of their *Table of contents*, as shown below. The other datasets in the *Category* or *Categories* are listed.

Figure 174: Membership of a Category indicated in the Table of contents of a dataset



13. Article

Article is a type of IUCLID entity that relates to the SCIP database. It has one working context, *SCIP notification*. See the ECHA website for more information here. A quote from that web page is provided below.

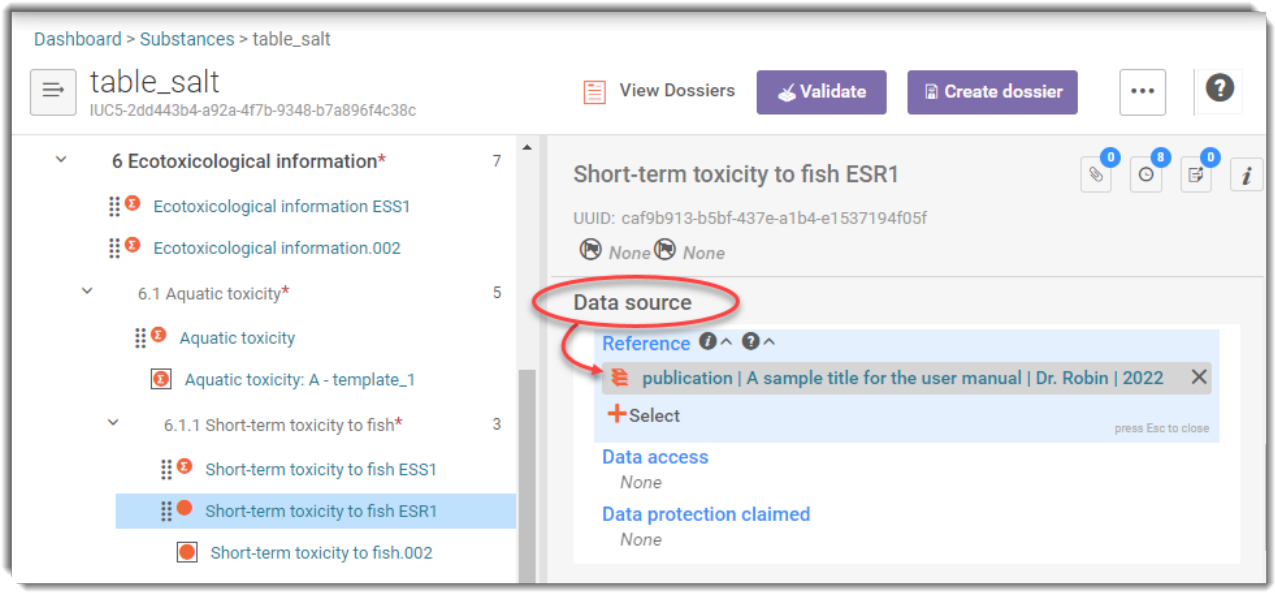
"SCIP is the database for information on Substances of Concern In articles as such or in complex objects (Products) established under the Waste Framework Directive (WFD).

Companies supplying articles containing substances of very high concern (SVHCs) on the Candidate List in a concentration above 0.1% weight by weight (w/w) on the EU market have to submit information on these articles to ECHA, as from 5 January 2021. The SCIP database ensures that the information on articles containing Candidate List substances is available throughout the whole lifecycle of products and materials, including at the waste stage. The information in the database is then made available to waste operators and consumers."

14. Literature reference

A *Literature reference* is an entity that identifies a particular document that contains information on a *Substance* or a *Mixture/Product*. The creation and editing of a *Literature reference* are done from the point where the *Literature reference* is referred to in a dataset. 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 *Reference*. An example is shown below.

Figure 175: Literature references in the field Data source



15. Validation assistant

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 *Substance* 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 working contexts 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*, and how it is used.

15.1. Structure

The *Validation assistant* is based on the following components:

1. *Scenarios*. A scenario refers to a specific working context. For simple working contexts, a scenario equals a dossier template, but for more complex types, additional parameters are calculated.
2. *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.
3. *Rule sets*. The rule sets are used to configure which rules should be run for each scenario.
4. *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 IUCLID user, it is not necessary to understand this structure I detail. However, it may be useful if in doubt about the outcome of the validation, to verify that the validation scenario was the intended one.

15.2. Supported validations

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

1. The *completeness check* on the technical dossier (TCC), for REACH registrations and PPORD notifications;
2. 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;
3. 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.

15.2.1. 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 closely 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

15.2.2. 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

15.2.3. Quality checks

The quality check feature enables users to check their IUCLID 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 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 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.

15.3. Run the Validation assistant on a Substance or Mixture/Product

The *Validation assistant* is run from the top level of the record for a *Substance* or *Mixture/Product*. This can be displayed either from the list of *Substance* or *Mixture/Product*, or by clicking on the

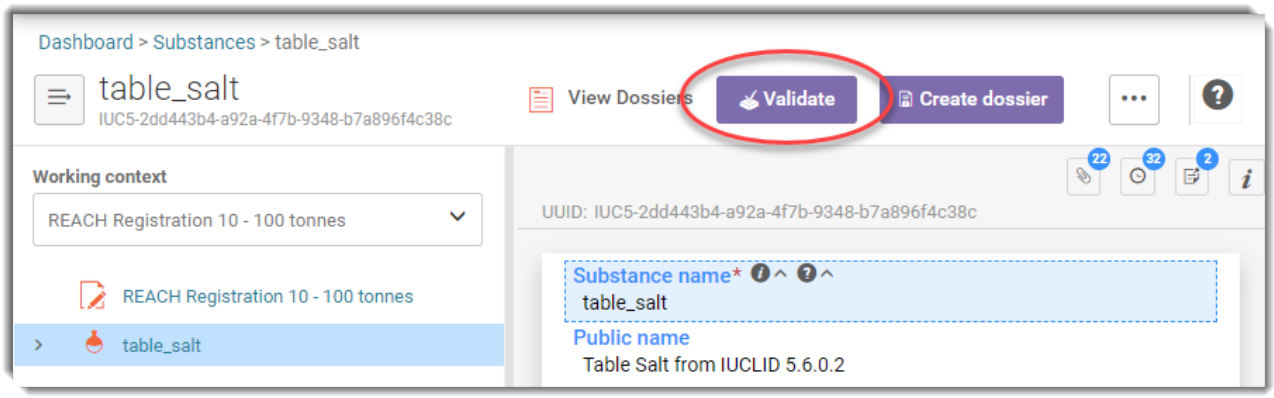
name of the entity in the breadcrumbs. The latter approach is useful if you have just edited a document, and you want to see the effect the edit has had on the validation.

Before running the *Validation assistant* on a dataset, a *Working context* must be selected. This allows the IUCLID interface to present to the user, either a pre-filled or blank *Dossier* header of the correct type, before carrying out the actual validation. The *Dossier* header provides the information that allow the checks applied to fit the regulatory context in which the data will be submitted to an authority.

The *Validation assistant* is run by clicking on the button labelled *Validate*, which is shown at the upper right of the record of a dataset. If the button is dimmed and cannot be clicked on, select a *Working context*.

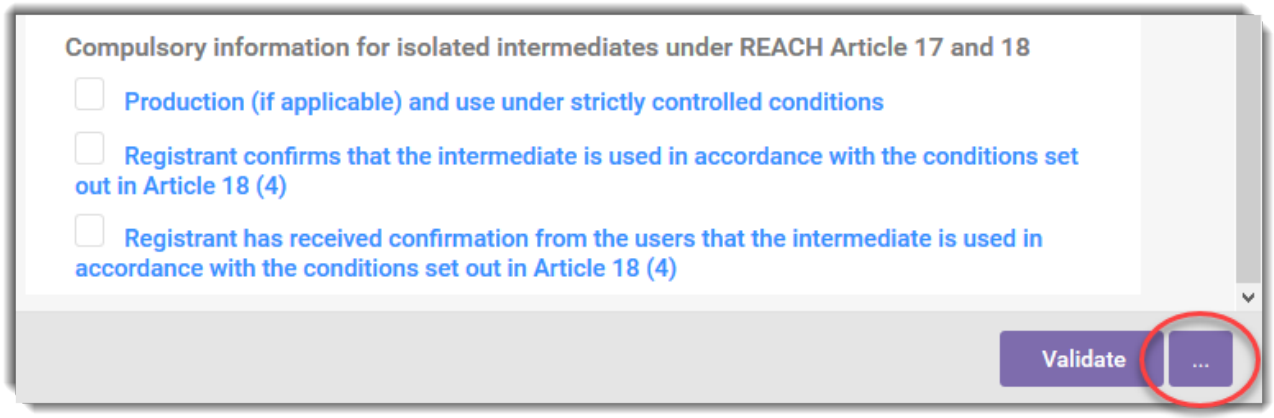
An example where to find the *Validate* button is shown for a *Substance* dataset.

Figure 176: Run the Validation assistant on a Substance dataset



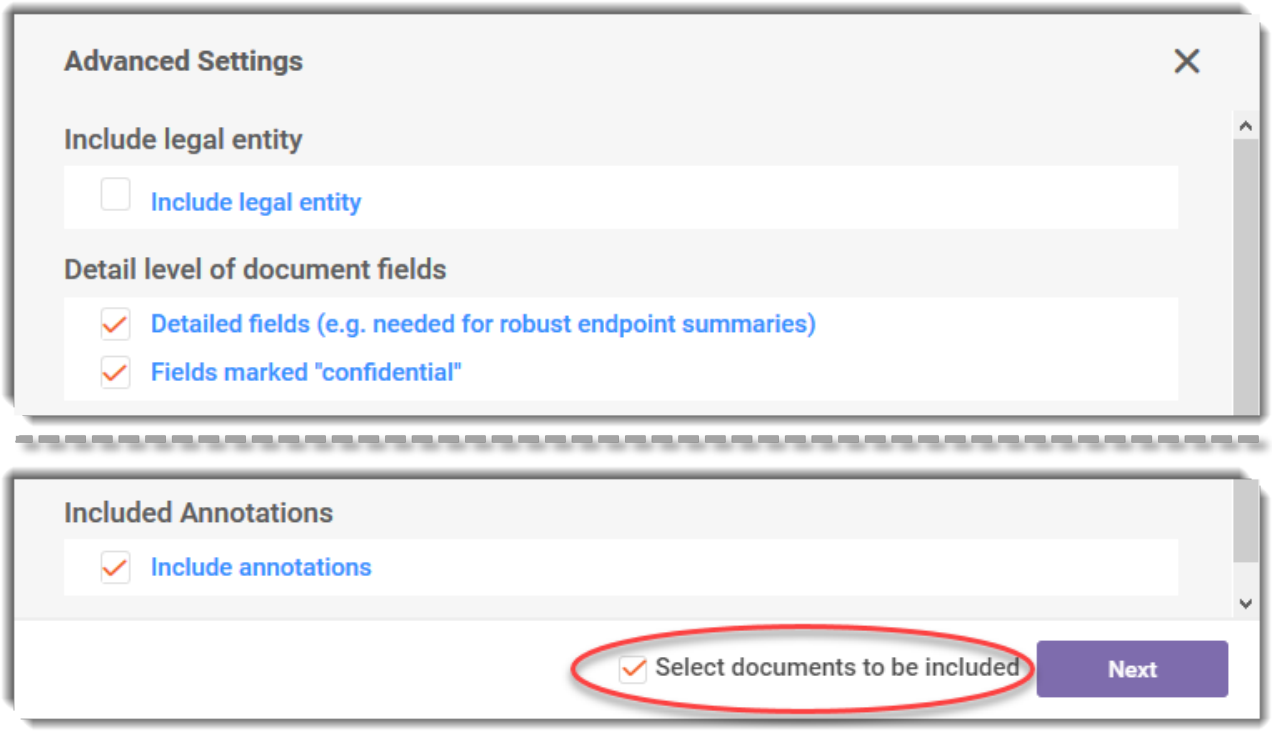
Fill out the *Dossier* header. To validate all of the dataset, click on the *Validate* button at the bottom right of the window. To exclude data from the validation, click on the button with three dots at the bottom right of the window, as indicated in the example below:

Figure 177: Validate a subset of a dataset



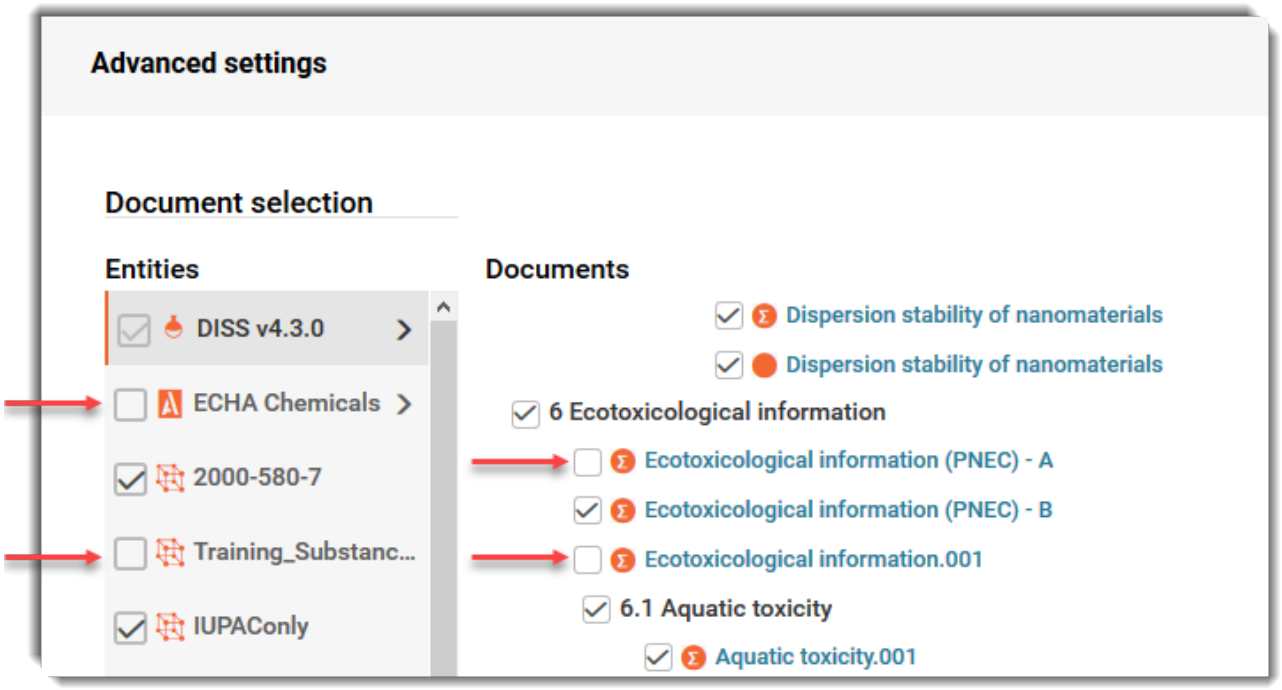
The three-dot icon opens the advanced settings. On the first page certain types of data can be excluded or included, for example according to flags. To select only specific entities, documents, and/or sections in the table of contents, tick the box labelled *Select documents to be included*, before clicking on *Next*. The option is highlighted below.

Figure 178: ***Select the entities, sections, and/or documents to be included*** **in the validation of a dataset**



In the example shown below, some entities and specific documents have been excluded from the validation. To exclude a whole section in the table of contents, untick title of the section.

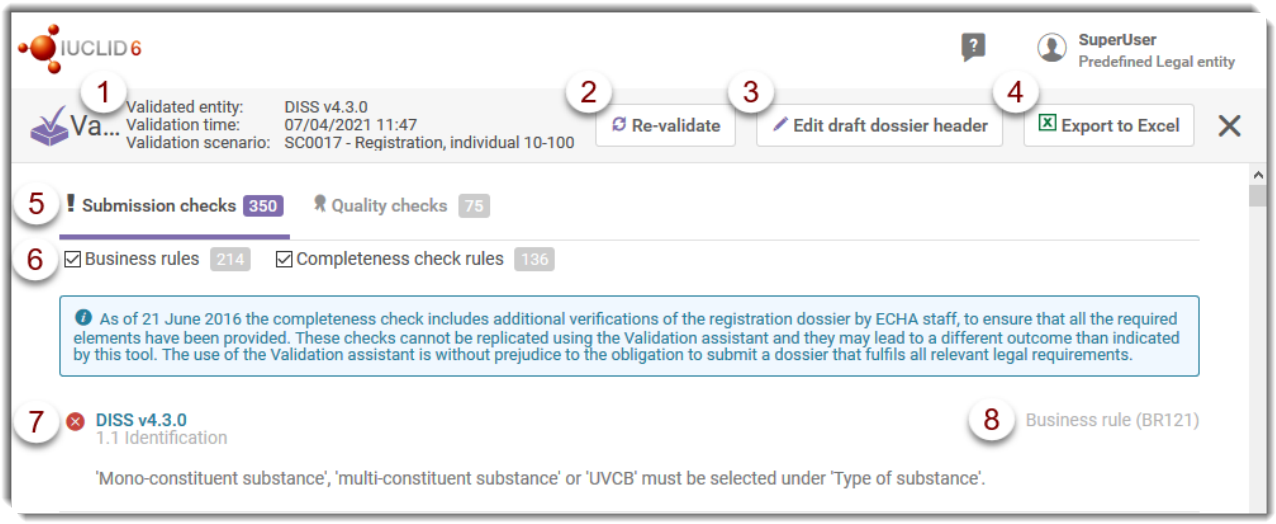
Figure 179: Exclude individual entities and documents from the Validation



If the validation assistant has been run at least once, to get back to the advanced settings after having run the validation assistant, click on *Edit draft dossier header*.

The *Validation assistant* produces a report. There are two tabs in the report: one named *Submission checks* which contains the *Business rules,* and the *Completeness check rules*, and another for the *Quality checks*. Annotated examples of the report are shown in the figures below.

Figure 180: The Validation assistant report: Submission checks

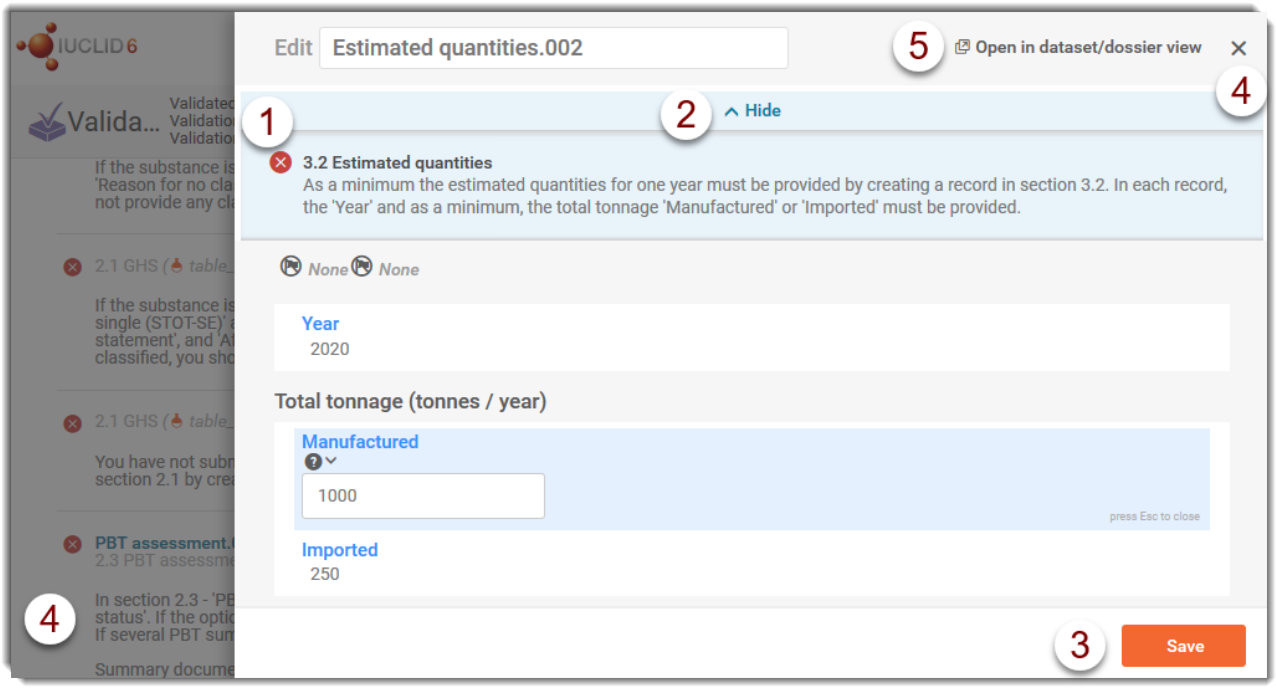


Legend for Figure 180

1. Information is provided about the validation;
2. Click here to run the *Validation assistant* again;
3. This link opens the draft dossier header for editing, and allows the advanced validation settings to be changed;
4. Export the report in Excel format;
5. Here are two tabs: *Submission checks*, and *Quality checks*. The selected tab is shown with a coloured bar under its title. By default, the tab *Submission checks* is selected, which contains *Business rules* and *Completeness check rules*. Under the other tab, failing *Quality checks* are shown. The number to the right is the total number of rules currently failing under that tab;
6. On the left there is the number of rules failing under the selected tab, by type. On the right there is the total number of rules failing under both tabs;
7. A list of the rules currently failing for the entity. For each rule there is a statement of why the entity fails the rule, and instructions on how to edit the data to pass the rule. A link in the name of the rule leads to the specific document that failed the rule. If the name does not have a link, it means that the required document does not exist, and must therefore be created;
8. The type of rule and its identifying code.

Following a link in the *Validation report* opens the document that fails the rule, so that it can be edited. The rule is presented at the top of the document page. An example is shown below.

Figure 181: Edit a document, and then go back to the validation assistant report



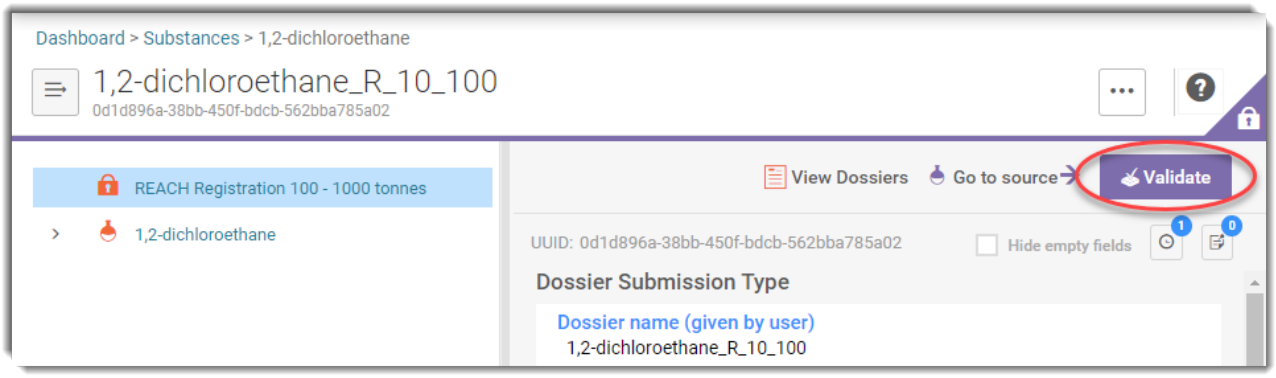
Legend for Figure 181

1. To help the user edit the document, instructions are given on how to pass the rule.
2. Clicking on *hide* closes the instructions to give the user more vertical space in the data entry window. Clicking on *Show* re-opens the instructions;
3. After editing the document, save changes by clicking on the *Save* button;
4. To go back to the *Validation assistant report* without saving unsaved changes, click on the cross icon at the top right, or the greyed-out area to the left of the data window. Note that the greyed-out area to the left, is visible only if the browser window is wide enough.
5. This opens the document in a new browser tab ( ). The document is displayed in the same view as the one used for viewing the data in datasets and dossiers. The user can switch back to the validation assistant by choosing its tab.

15.4. Run the Validation assistant on a Dossier

The *Validation assistant* is run on a *Dossier* from the top level of the record for the *Dossier*. An example is shown below.

Figure 182: Run the Validation assistant on a Dossier



Links in the *Validation report* lead to the read-only copies of documents within the dataset. To obtain a *Dossier* that passes all the *Validation checks*, edit the dataset upon which the *Dossier* is based until it passes all the checks, and then re-create the *Dossier*.

15.5. Update a registration - reduced information requirements

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 working context. 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.

15.6. Disclaimer

The checks performed by the *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.

16. Export to i6z

This exports data in the standard data exchange format of IUCLID, which has an extension i6z. The file format is a zip archive that contains data in XML format, and may also contain attachments in other formats. An i6z file can be imported into any instance of IUCLID that is the same or a newer major version. There is also an option to export in the previous major version.

Export to i6z exports acts at the highest level the currently viewed raw *Substance dataset*, raw *Mixture/Product dataset*, or *Dossier*. All types of entities contained within those high-level entities can be exported. The export options for *Dossiers* differ from those for raw datasets because a *Dossier* is treated as single read-only entity that should not be split up. The options for a *Dossier* apply to the whole *Dossier*, but for raw datasets there is an option to select which documents and entities are exported. The two different sets of options are described below, each in its own section.

A document within an entity cannot be exported individually to an i6z file, but it can be exported in PDF or RTF format, as described in *18.2 Create document PDF/RTF - Create PDF/RTF.* If *Export to i6z* is selected whilst a document is open in the data window, for example an endpoint study record, the export is applied in the same way as when the parent entity is selected at its top level.

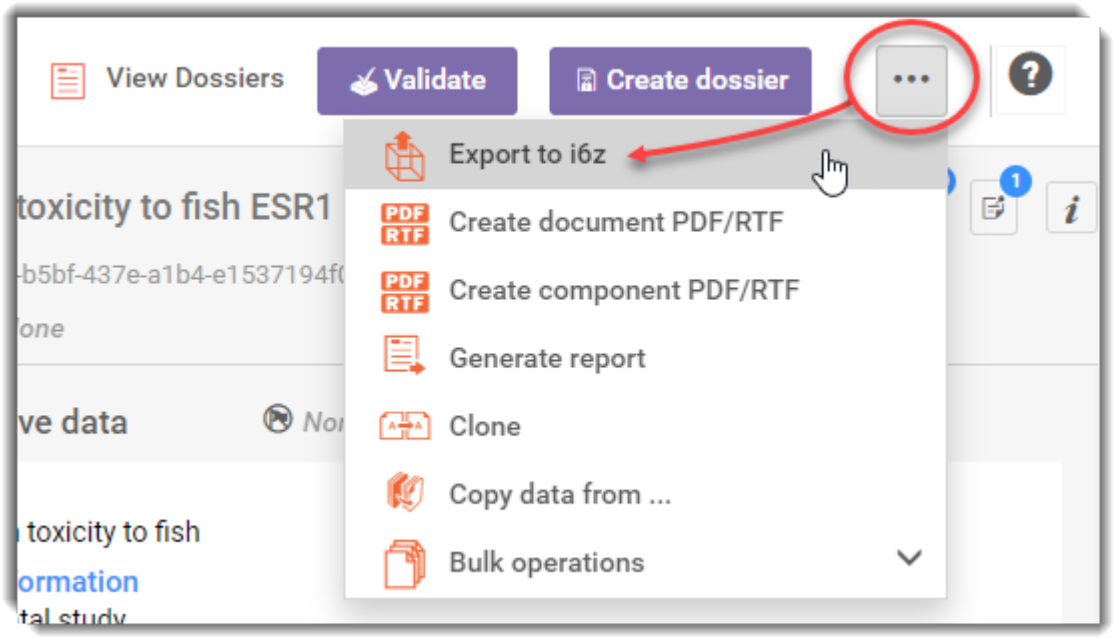
By default, entities and documents referred to directly by an entity are also exported. For example, by default, a *Reference substance* linked to a *Substance* is exported along with the *Substance*. For raw datasets, the default behaviour can be over-ridden using settings in the export process, as described below. *Export to i6z* is accessed from the menu under the three-dot button in the application window.

Export to i6z is run as a background task, as described in *23 Background tasks*.

16.1. Export to i6z – raw dataset

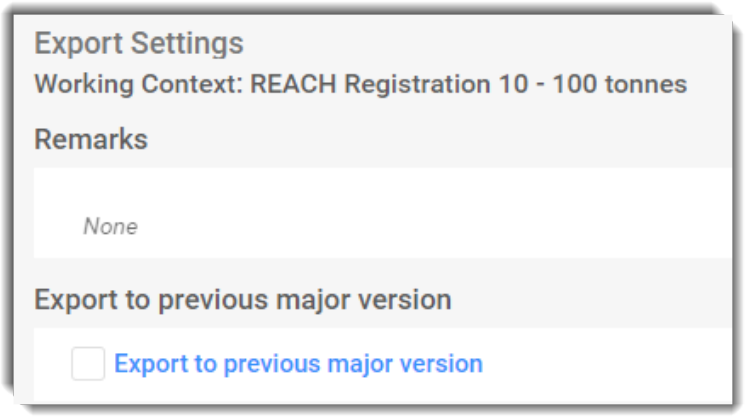
Export to i6z is run from the three dots button, as shown ringed in red in the example below.

Figure 183: Selecting Export to i6z for a Substance dataset



This opens the *Export* settings for a raw dataset, as shown below section by section.

Figure 184: The top of the page of settings for Export to i6z for a raw dataset



Note that the current working context is stated at the top of the settings, which can determine the sections of the table of contents that are exported. To see which sections are included, use the function *Set documents to be included*; as described later.

16.1.1. Remarks

This is a free text field in which you can record information about the export and its data.

16.1.2. Export to previous major version

In each major release of IUCLID 6, changes are made to the underlying way that data is stored in IUCLID. In other words, the IUCLID format changes. This may be seen, for example, in changes to the way that data is organised across fields. When this happens, the version number after the 6 goes up by one: for example, from IUCLID 6.4 to IUCLID 6.5. Data exported from IUCLID can be imported into the same version, and optionally into the previous major release. This latter option is switched on using *Export to previous major version*. Data cannot be exported to be compatible with a major release, that was two or more releases in the past. For example, data cannot be exported from IUCLID 6.5 into the format for IUCLID 6.2.

If you need to send data to a IUCLID user who is using IUCLID from the previous major version, and you know that the data is not critically affected by the most recent format changes, export the data with *Export to previous major version* enabled. This will allow the data to be imported. However, it is always recommended to use the latest version of IUCLID.

Be aware that *Export to previous major version* does not reverse all the actions that can occur on migration forwards between major versions, e.g. from IUCLID 6.4 to IUCLID 6.5.

The differences between major versions of IUCLID 6 are documented on the IUCLID website under the section IUCLID format.

Example

In some cases, migration of data between major versions involves the merging of the text from two text fields into 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 into 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, even when *Export to a previous major version* is enabled. However, any text that was placed in an attachment is available in the IUCLID from which data is being exported, so if required, it can be pasted back into the original field.

An attachment created during migration begins with the name and path of the field from which it 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 …
```

16.1.3. Detail level of document fields

See section *6.2.1.2 Detail level of document fields*.

16.1.4. Flags for confidentiality

See section *6.2.1.3 Flags for confidentiality*.

16.1.5. Flags for regulatory programmes

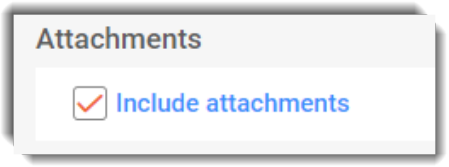
See section *6.2.1.4 Flags for regulatory programme*.

16.1.6. Included annotations

See section *6.2.1.5 Included Annotations*.

16.1.7. Included attachments

If the box is ticked, attachments will be exported.



16.1.8. Modification history

See section *1.7.16 Modification History*.

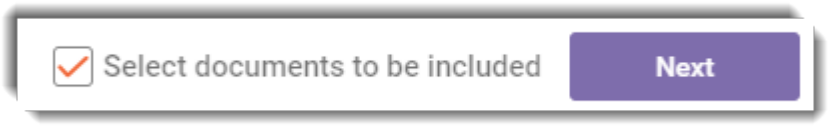
16.1.9. Reduced category content

See section *6.2.1.6 Reduced category content*.

16.1.10. Select documents to be included

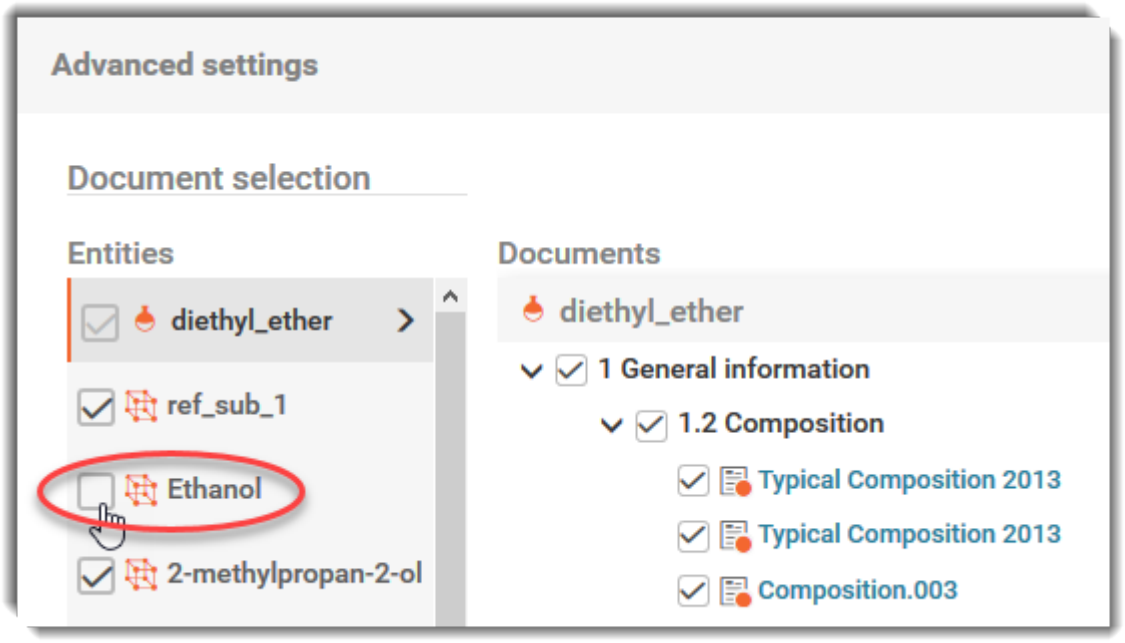
This allows entities and documents to be excluded individually. It over-rides exclusion for other reasons. If the box is ticked, the button to the right changes to *Next*, as shown below.

Figure 185: Select documents to be included in export to i6z from a raw dataset



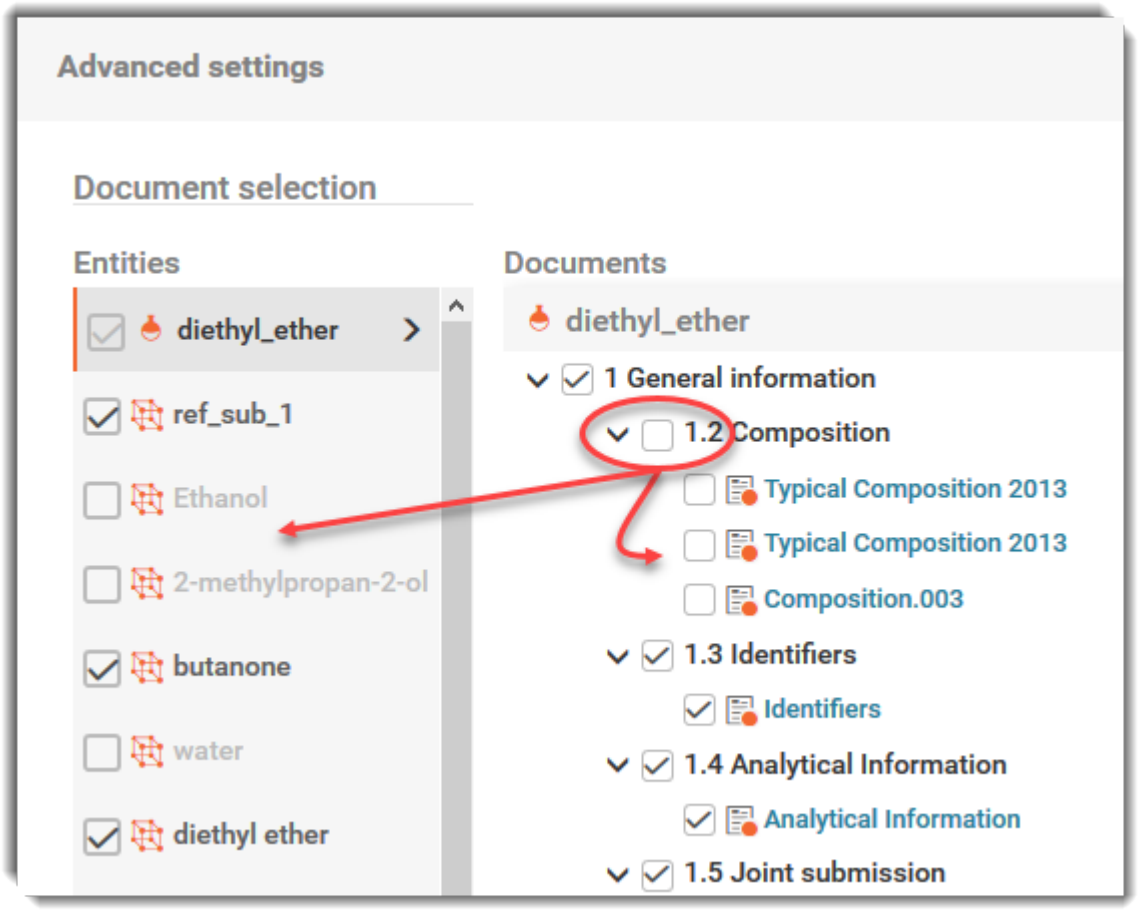
Clicking on *Next*, opens a selection panel that has *Entities* on the left and *Documents* on the right. On the left, entities can be excluded individually by unticking their boxes. In the example shown below, this has been done for the *Reference substance* ethanol. There are no documents in the *Reference substance*, so the right-hand side remains unchanged.

Figure 186: Exclude an entity from an Export to i6z file



The dependencies of excluded *Documents* are excluded. In the example shown below, all *Documents* in section *1.2 Composition* have been excluded by unticking the box adjacent to the section name. This has automatically unticked the *Documents* in the section 1.2 on the right. It has also excluded the *Reference substance*s on the left that are referred to only in section 1.2.

Figure 187: Exclude all the documents in a section from an Export to i6z file



16.2. Export to i6z – Dossier

The following options for *Export to i6z* apply to only *Dossiers*.

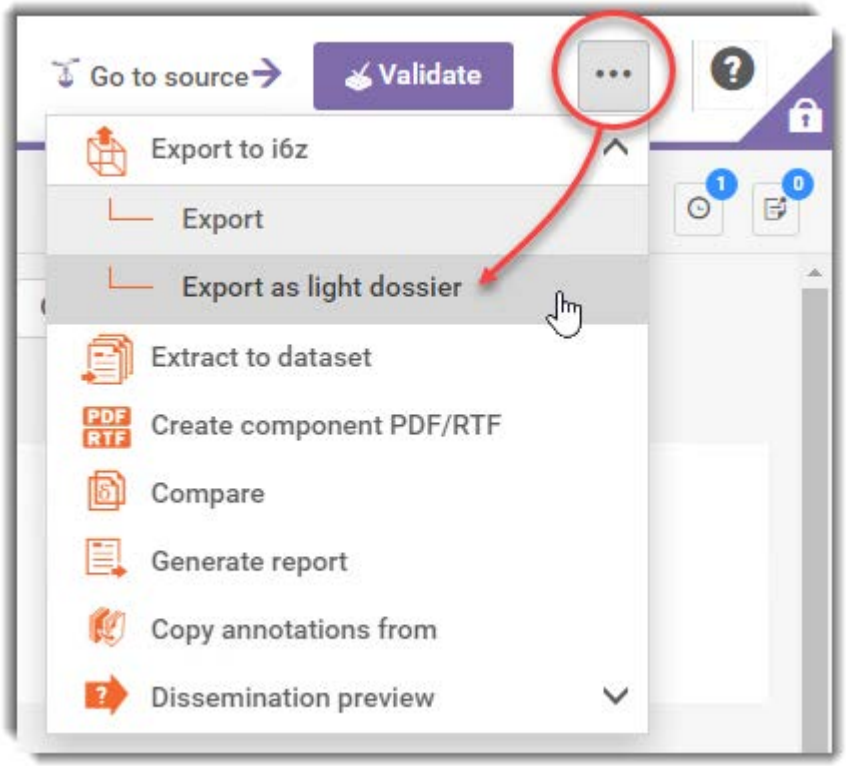
16.2.1. Export only annotations

This exports to a zip archive, only the *Annotations* for a *Dossier*. Each *Annotation* is in its own i6z file within the zip archive. The export is the same no matter from where it is launched in the *Dossier*. *Annotations* that were in the subject of the *Dossier* when the *Dossier* was created are not exported. These are shown in the *Annotations* window with a locked icon.

16.2.2. Export as light dossier

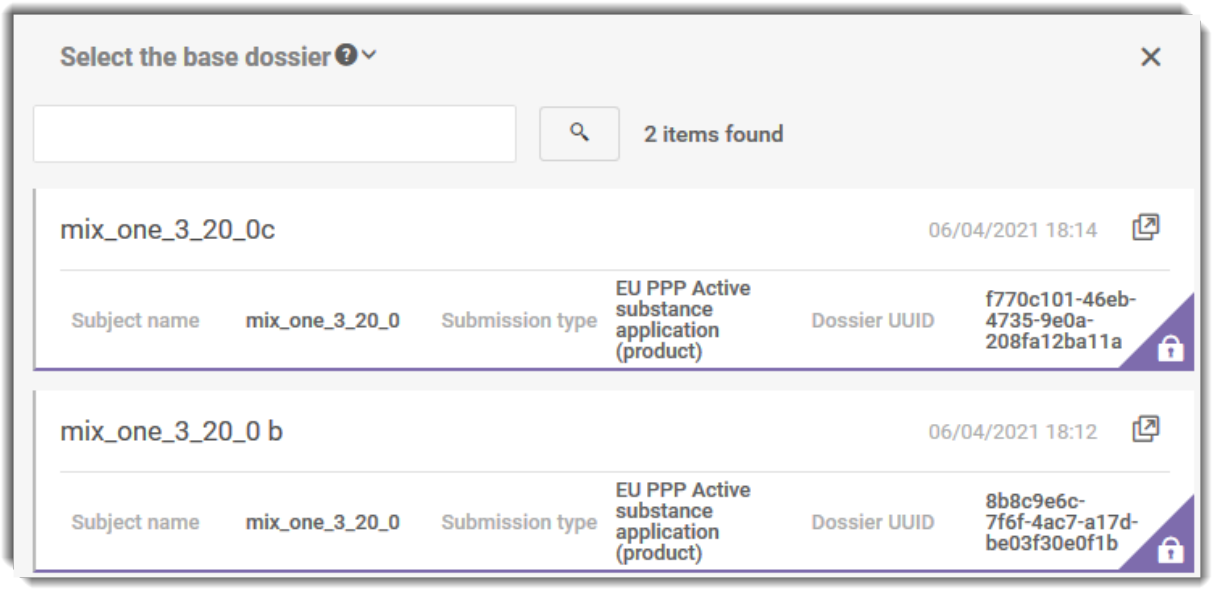
For working contexts relevant to *Plant Protection Products (PPP) in the EU*, under *Export to i6z*, there is an option to export to a *light dossier*. A *light dossier* contains only the attachments that have changed compared to a *base* dossier that is selected during the export.

Figure 188: Export as light dossier



The base dossier is selected from those that are available in the database, and are derived from the same dataset, with the same working context.

Figure 189: Selecting the base dossier for a light dossier



The working contexts supported are:

EU PPP Active substance application (product)

EU PPP Basic substance application

EU PPP Microorganisms - active substance application (product)

EU PPP Microorganisms - plant protection product authorization

EU PPP MRL Application

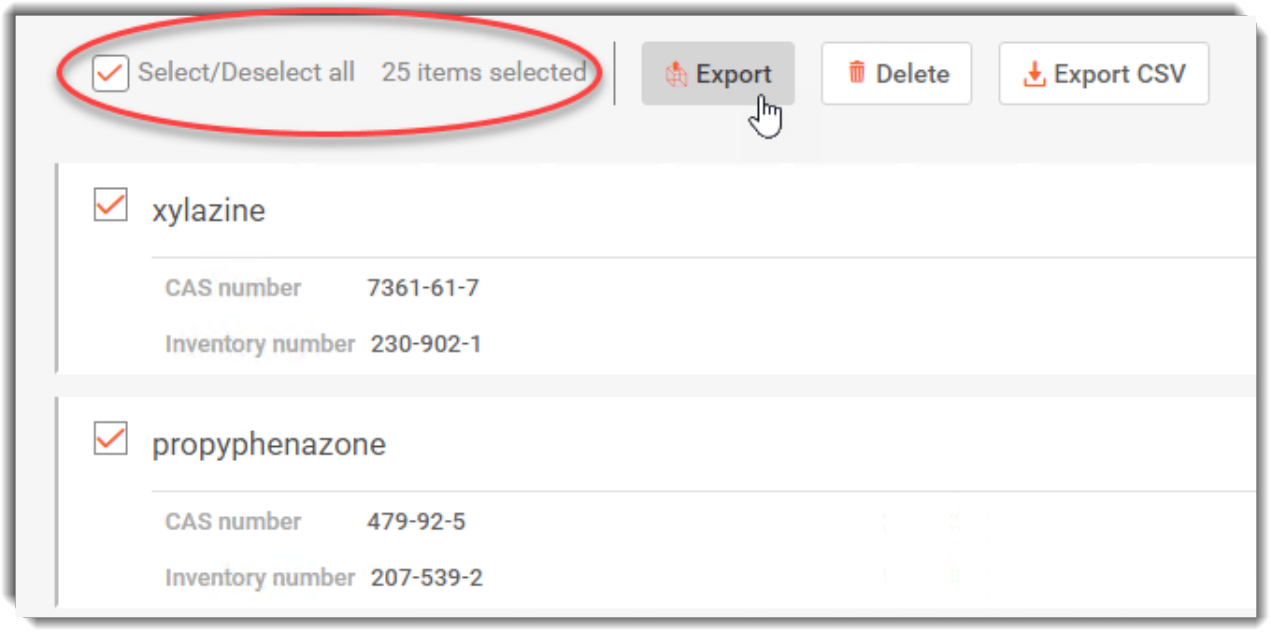
EU PPP Plant protection product authorisation

A light dossier cannot be imported into an instance of IUCLID in which the base dossier does not exist. This is because the attachments are not available. The error message on import contains the message, “You are importing a light dossier and the attachments that were omitted cannot be found in the target database. Please verify that the base dossier from which you created the light dossier was successfully submitted to this recipient in the past. Otherwise, a standard dossier can be exported and submitted.”.

17. Export from the list page in bulk

To export more than one entity of a particular type in a single action, select the entities from the list page, and then click on the *Export* button that is situated above the list. The selection can be made individually across multiple pages in a listing, or all entities can be selected at once. An example is shown below in which all the *Reference substances* are being exported.

Figure 190: Export in bulk



Certain data can be excluded in the same way as is defined on the first page of the individual export, as described in the previous section. Thus, exclusion is not possible per entity. The options apply in the same way to all the exported entities.

The output is a zip archive that contains i6z files. The default name of the archive is the type of entity, e.g. `MIXTURE.zip`, but you can set whatever name you like. Such an archive can be imported in to IUCLID in a single action.

Export is run as a background task, as described in *23 Background tasks*.

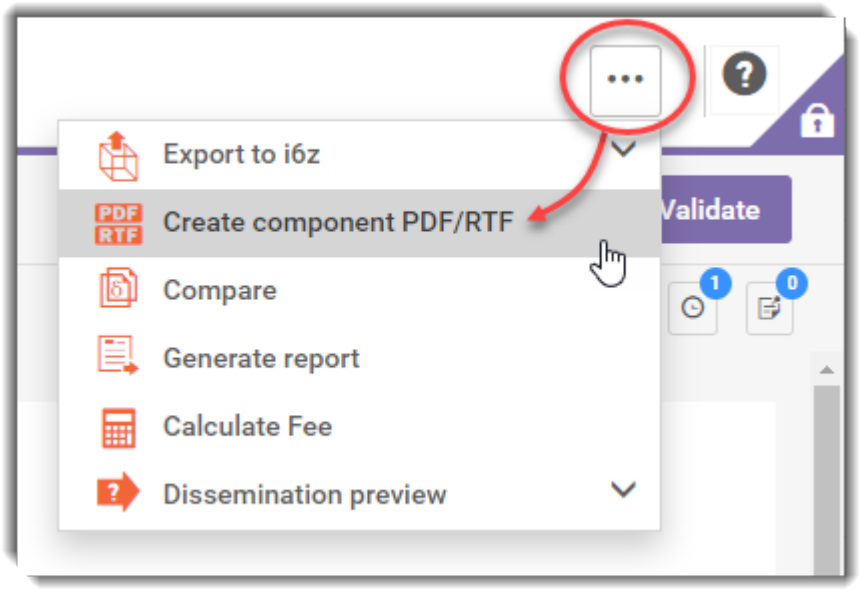
18. Output data to files of format PDF or RTF

Documents and entities in raw datasets or Dossiers can be exported to files of standard formats that differ from the internal standard format of IUCLID (i6z). The options are PDF, and Rich Text Format (RTF). The latter can be opened in Microsoft Word. The options shown differ depending on what type of component is selected, as described below.

18.1. Create component PDF/RTF

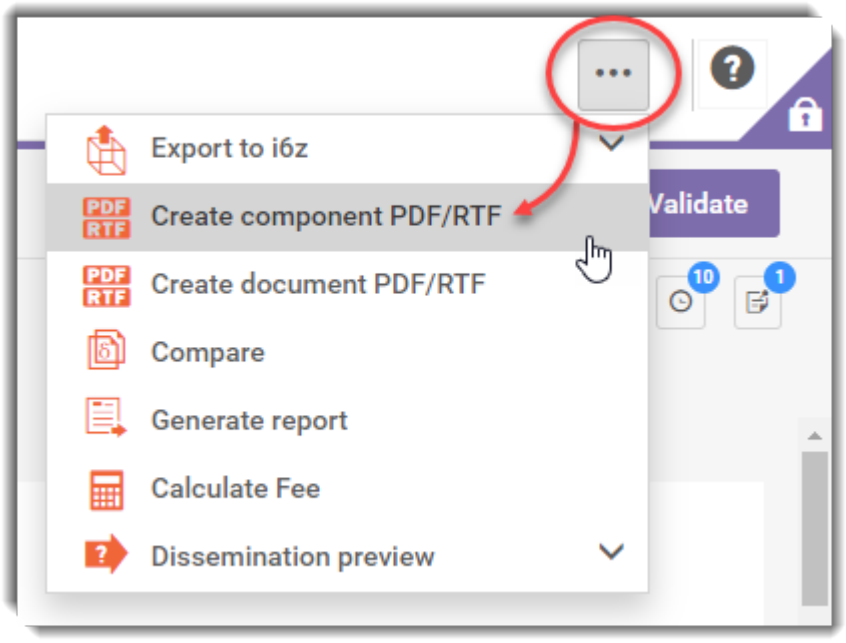
This option prints a whole raw dataset or Dossier. For example, where the Dossier header is selected it is the only option because the selection effectively means the whole Dossier.

Figure 191: Output all of a Dossier to a file whilst the Dossier header is selected



Where a document is selected, the component option is shown alongside an option to print only that document instead of the whole dossier.

Figure 192: Output all of a Dossier to a file whilst a document is selected



18.2. Create document PDF/RTF - Create PDF/RTF

This prints only the currently selected document or simple entity such as an endpoint study record, or a *Reference substance*.

Figure 193: Output a single entity from a raw dataset

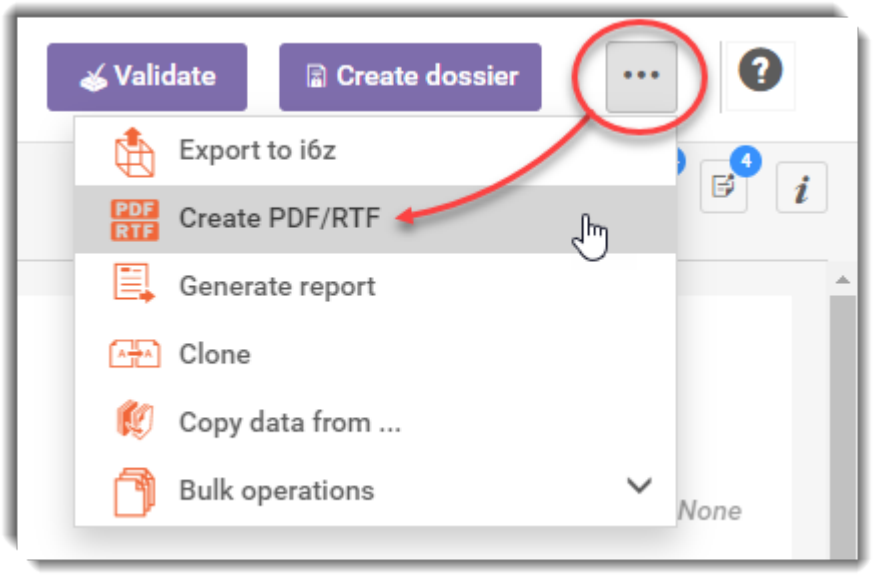
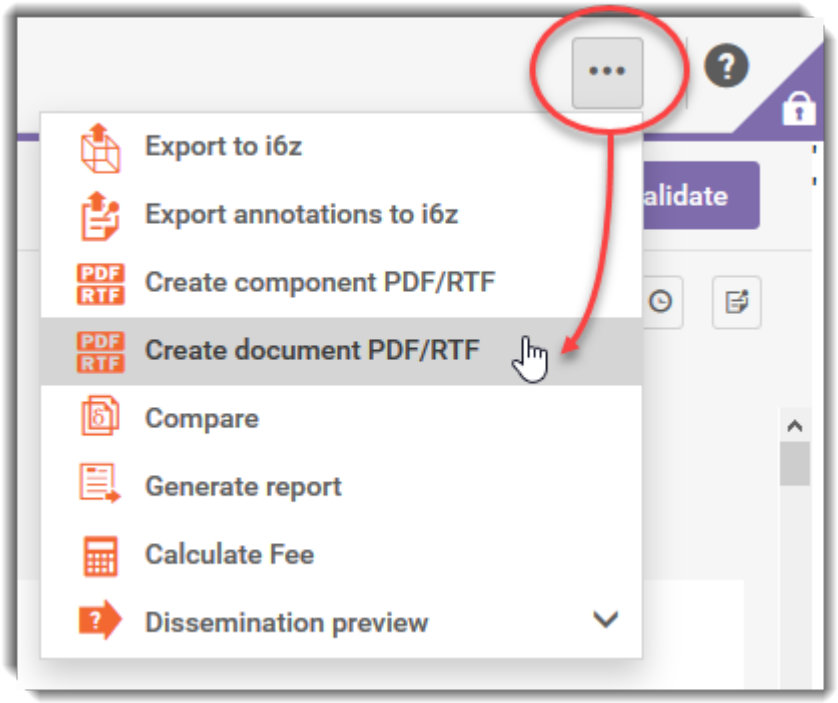


Figure 194: Export only the currently selected document from a Dossier to a file



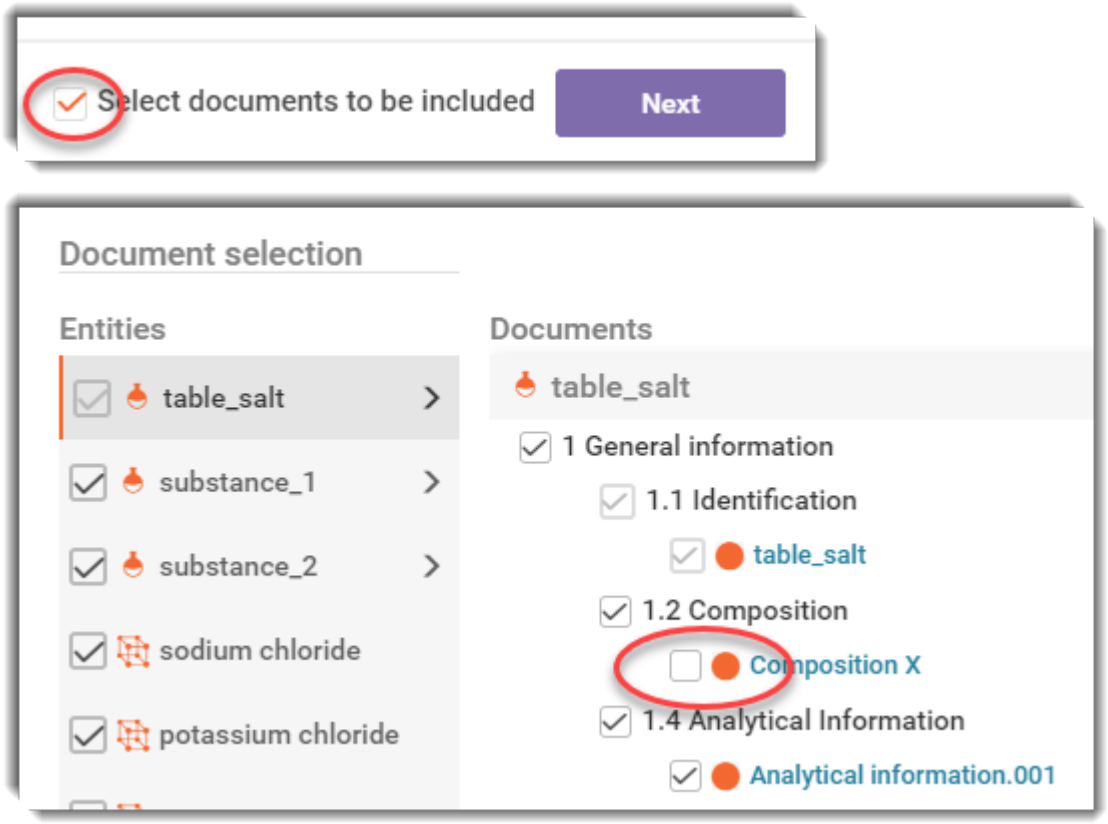
18.3. PDF/RTF Settings

On the first page, the features to exclude data work in the same way as for *Export to i6z file*, and for *Create Dossier*, but there are two options unique to creating PDF/RTF which are:

1. Include cover page;
2. Include fields with no value.

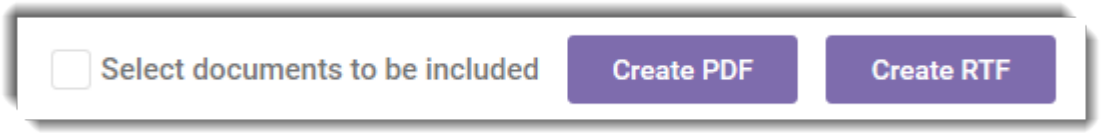
If the file is being created for a whole dossier, or a whole dataset, there is an option at the foot of the first page labelled *Select documents to be included*. This allows only certain individual documents to be excluded from the file. On the next page, documents can be excluded by un-ticking their boxes.

Figure 195: Exclusion of a document from the PDF file



After selecting what is to be output to the file, select the type of file.

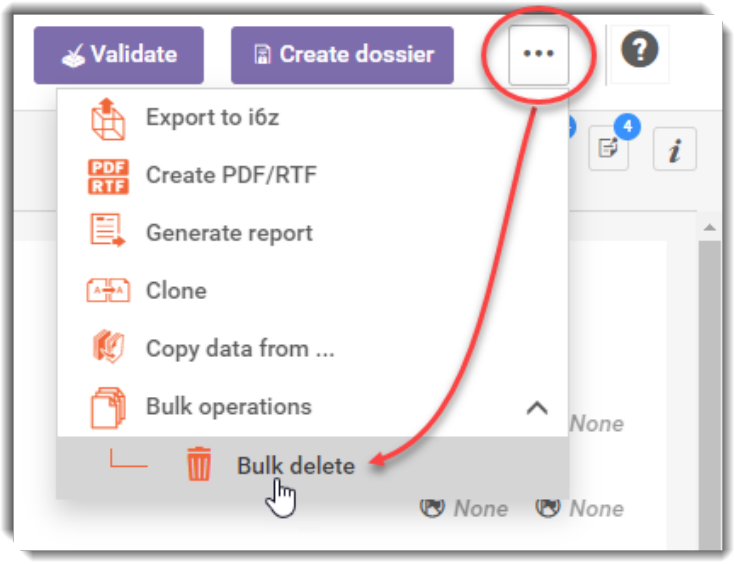
Figure 196: Select the type of file to be exported



19. Bulk operations - Bulk delete

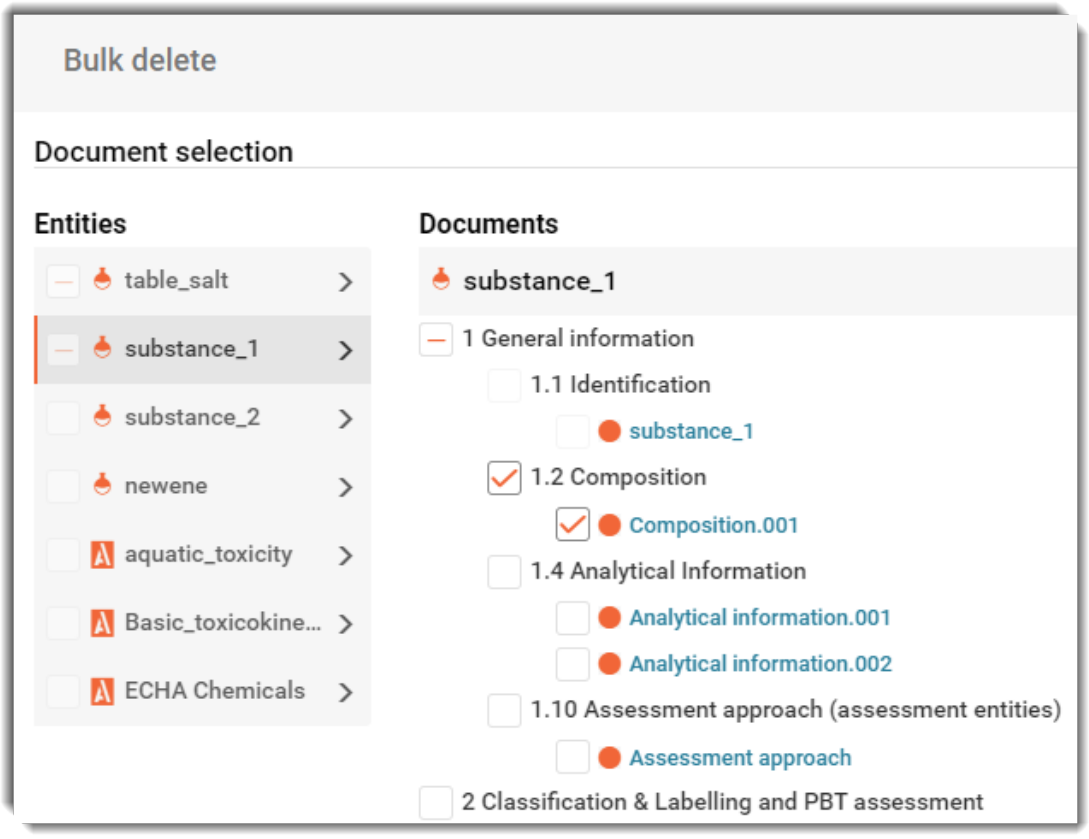
This feature allows data to be deleted across multiple entities at once. It is opened from the three-dot menu, as shown below.

Figure 197: Open bulk delete



Select an entity on the left and the documents to delete from it on the right. Multiple documents and sections can be selected independently across the entities.

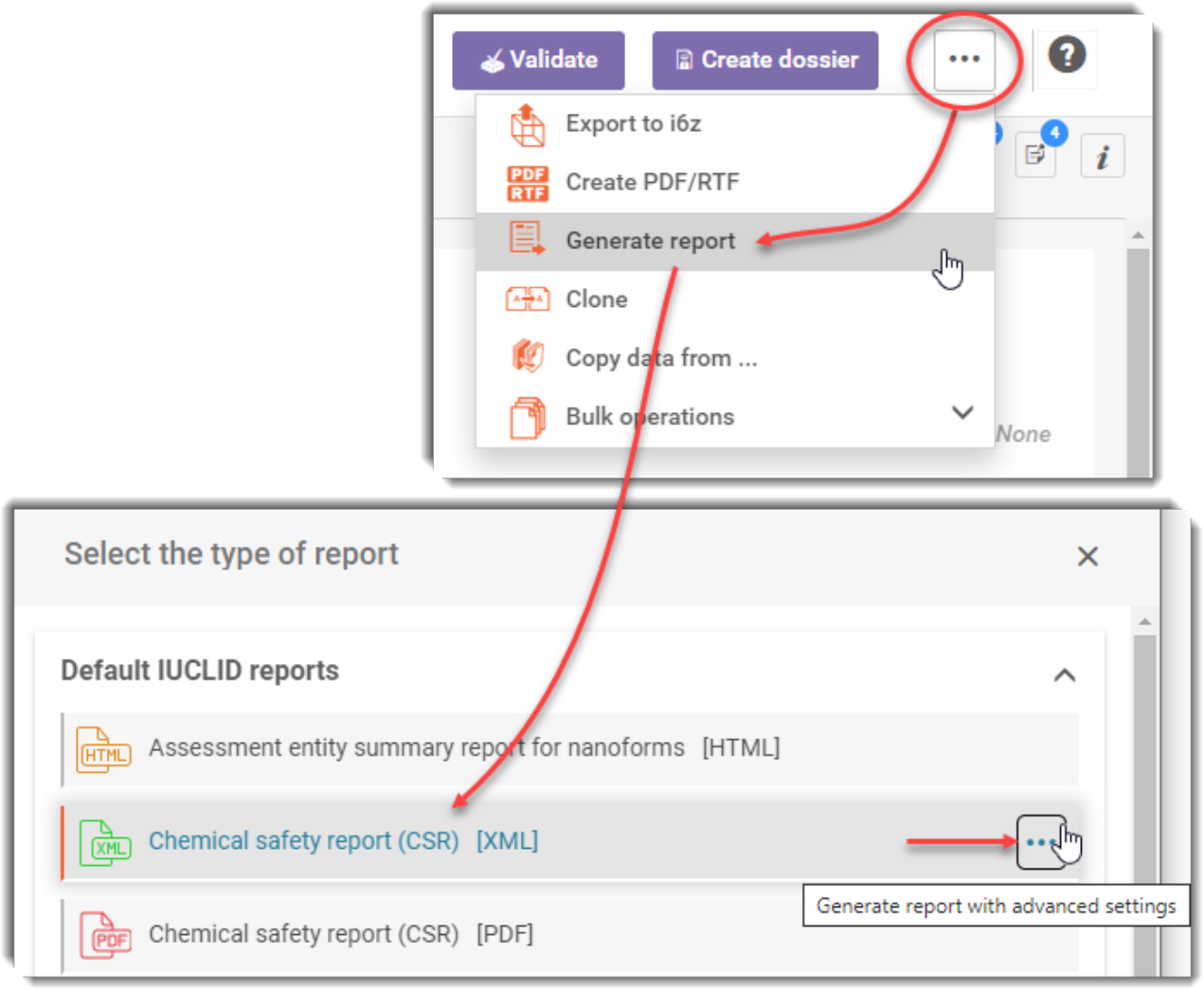
Figure 198: Bulk delete - Select documents to delete individually and by section



20. Generate Report

The function *Generate report* exports data from a dataset or a *Dossier* to an external file that can be downloaded from the browser used to view the user interface. It is accessed from the menu under the three-dot menu in the application bar. Select the required type of report and its output format from the menu. An example is shown below for a *Chemical safety report (CSR) [XML]*. Note that the report can be run with default settings by clicking anywhere in its row, or with advanced settings from the three-dot icon that appears on hovering over the row. The advanced settings allow data to be included and excluded in the same way as for *Export to i6z*, *Create PDF/RTF*, and *Create Dossier*.

Figure 199: Generate report – example of Chemical Safety Report (CSR)



Reports are defined per dossier *working context*. If *Generate report* is greyed out and cannot be selected, there are no reports available for the current dossier *working context*.

Reports can be defined outside IUCLID, and then uploaded to be used in the *Report generator*. Once a report has been uploaded, it is available beneath the default built-in reports. Uploading reports is described in the next section.

Generate report is run as a background task, as described in section *23 Background tasks*.

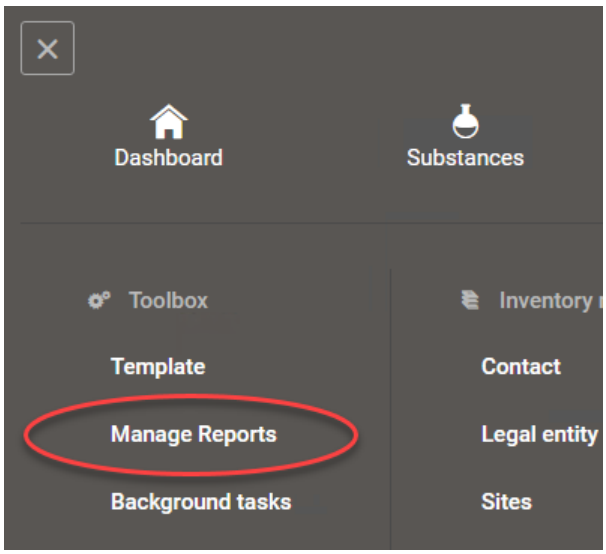
20.1. Manage reports

The format and structure of report is defined outside IUCLID, and then imported in to IUCLID for use in the *Report generator*. For more information about defining reports, see the IUCLID website at the address:

https://iuclid6.echa.europa.eu/reports.

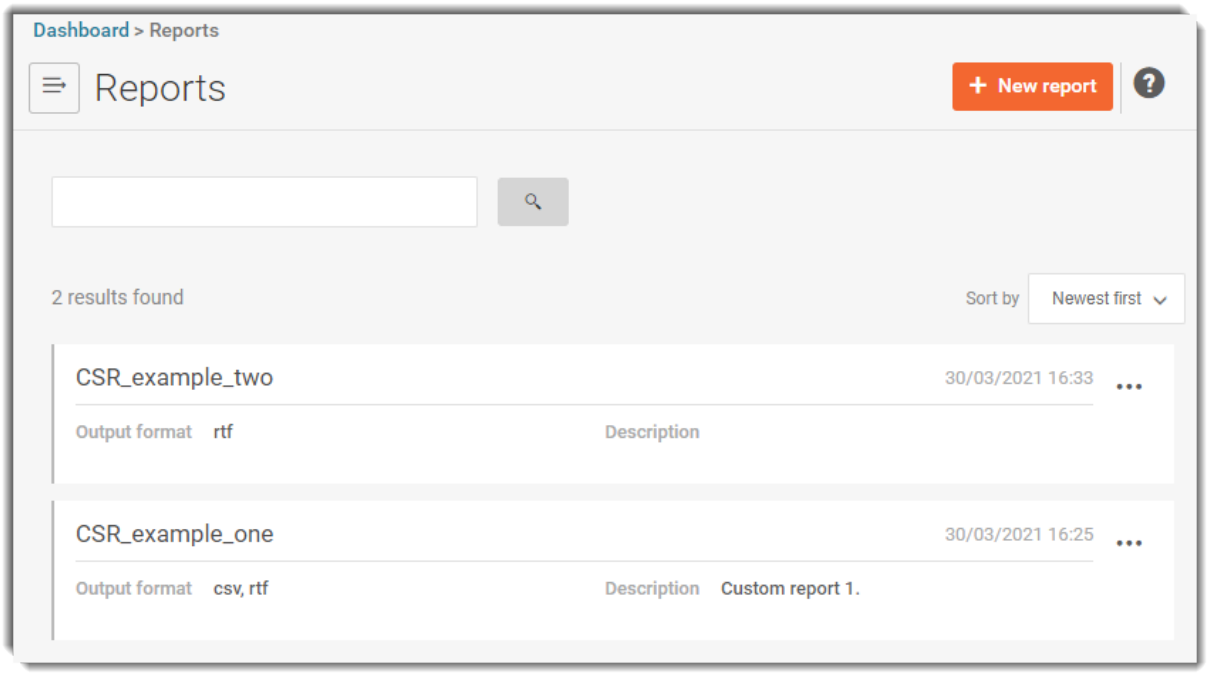
The definition of a report is imported as one or more templates in to a IUCLID entity of type *Report*. To open the list page of *Reports*, click on *Manage reports* on the main menu, as shown below.

Figure 200: Open the list page for Manage Reports



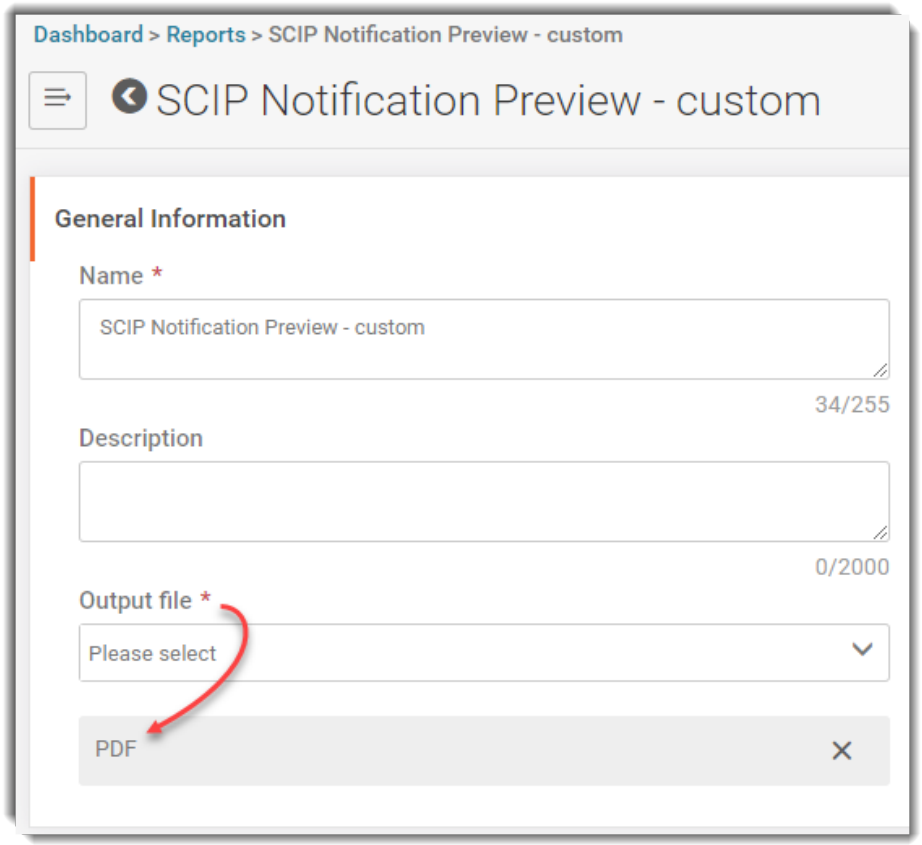
On the list page, *Report* entities can be created, modified, and deleted. In the example below, there are two *Reports* listed.

Figure 201: The list page for reports



A report must have a name, and at least one type of file must be selected in the field *Output file*. In the example below, there is only one type of file that is appropriate, which is PDF.

Figure 202: Selecting file types for a Report



Which file types that may be used for a *Report* are defined in its template. The compatible file types for reports that are available on the IUCLID website are indicated in the filename, and at the point of download, as shown in the example below.

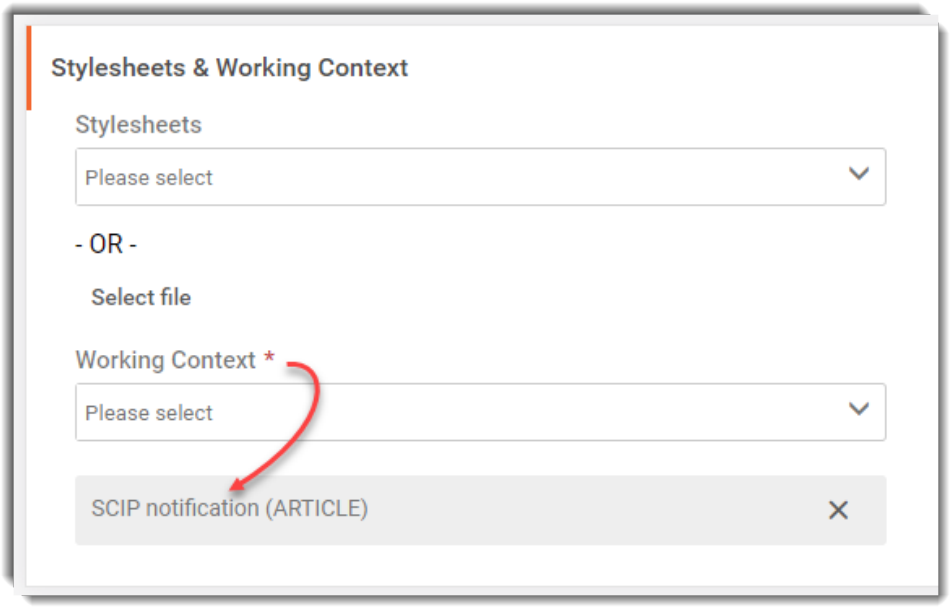
Figure 203: An example of a report template on the IUCLID website

Upload a *main* template file and any additional template files required. The file extension is *ftl*. An example is shown below for a report definition available on the IUCLID website. *Main* templates have the word *main* in the filename.

Figure 204: Upload report definition files

The next step is to define the format of the output of the report using either a style sheet, or by selecting a *working context*. If a *working context* is selected, the report will be available in the *Report generator* only where that *working context* is currently selected for the source of data.

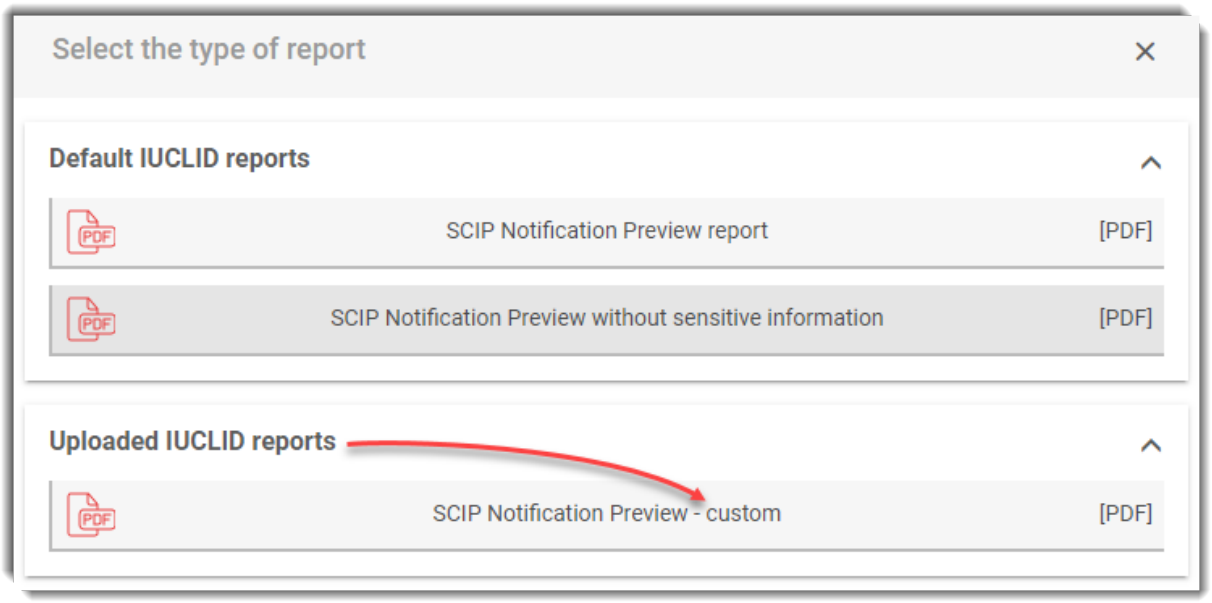
Figure 205: Select a working context for a Report



If a *working context* is selected, the report will be available in the *Report generator* only where that *working context* is currently selected for the source of data.

Uploaded reports are run from the *Report generator*, where they are shown under the default built-in reports, as shown in an example below.

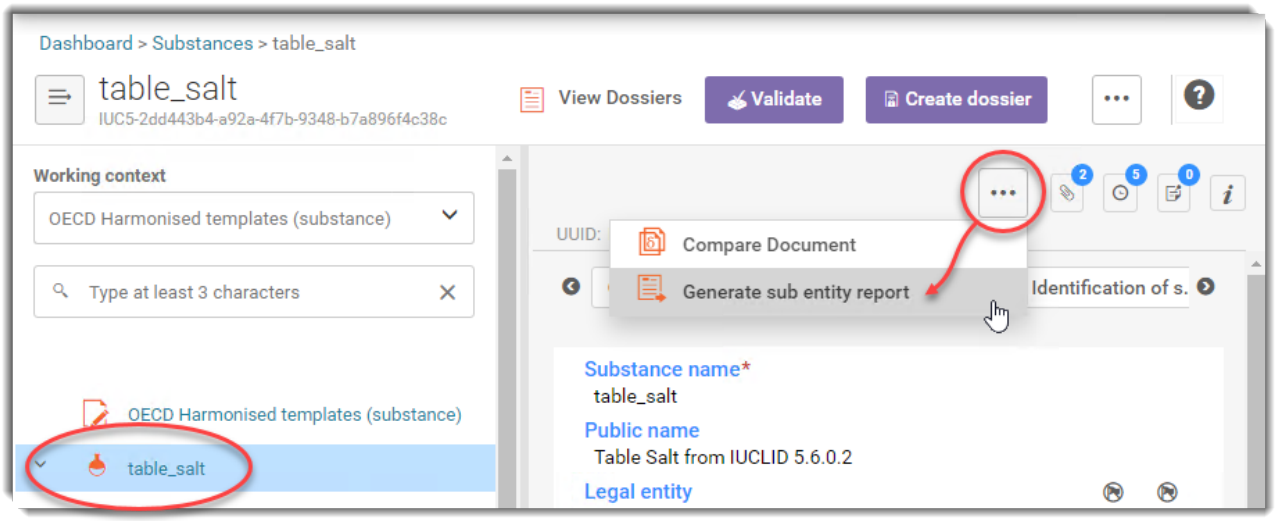
Figure 206: Selecting an uploaded definition of a report in the Report generator



20.2. Generate sub entity report

Generate sub-entity report is accessed from the three-dot icon at the top of the data window when the record of a dataset is open and selected, as shown in the example below for a *Substance*.

Figure 207: Generate sub-entity report



In this context, a sub-entity is a dataset that is referred to by a *Mixture/Product*. This can be either a *Substance* or a *Mixture/Product*. The function *Generate sub-entity report* is intended for use only with custom reports that are run from inside a *Mixture/Product*. A custom report can be created that includes data only from the sub-entity, and not the whole *Mixture/Product*. The types of report that are delivered with IUCLID produce the same output for both *Generate sub-entity report* and *Generate report*.

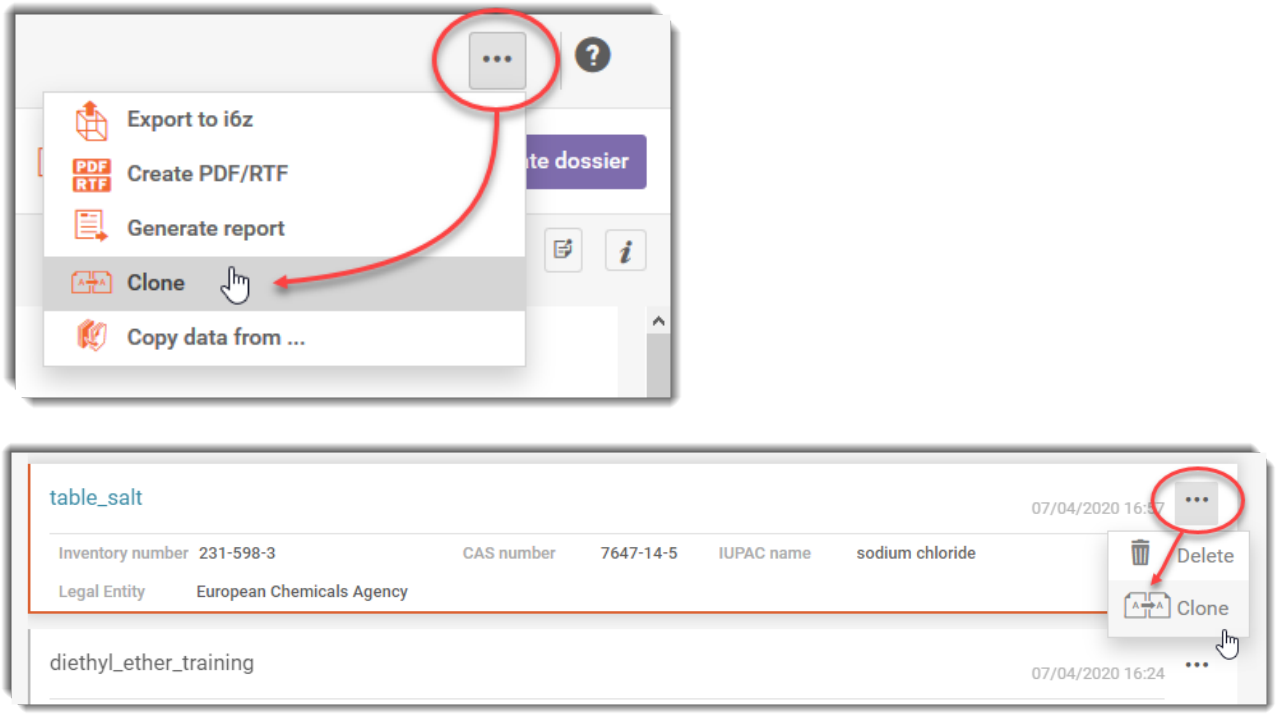
For information about custom reports, see the information on the IUCLID website at:

https://iuclid6.echa.europa.eu/reports

21. Clone

Clone creates an exact copy of a dataset. The name must be unique within the instance of IUCLID. A new UUID is generated. Referenced documents are not touched. The option can be selected from the menu either whilst viewing the dataset, or from the record of the dataset in a listing.

Figure 208: Clone a dataset

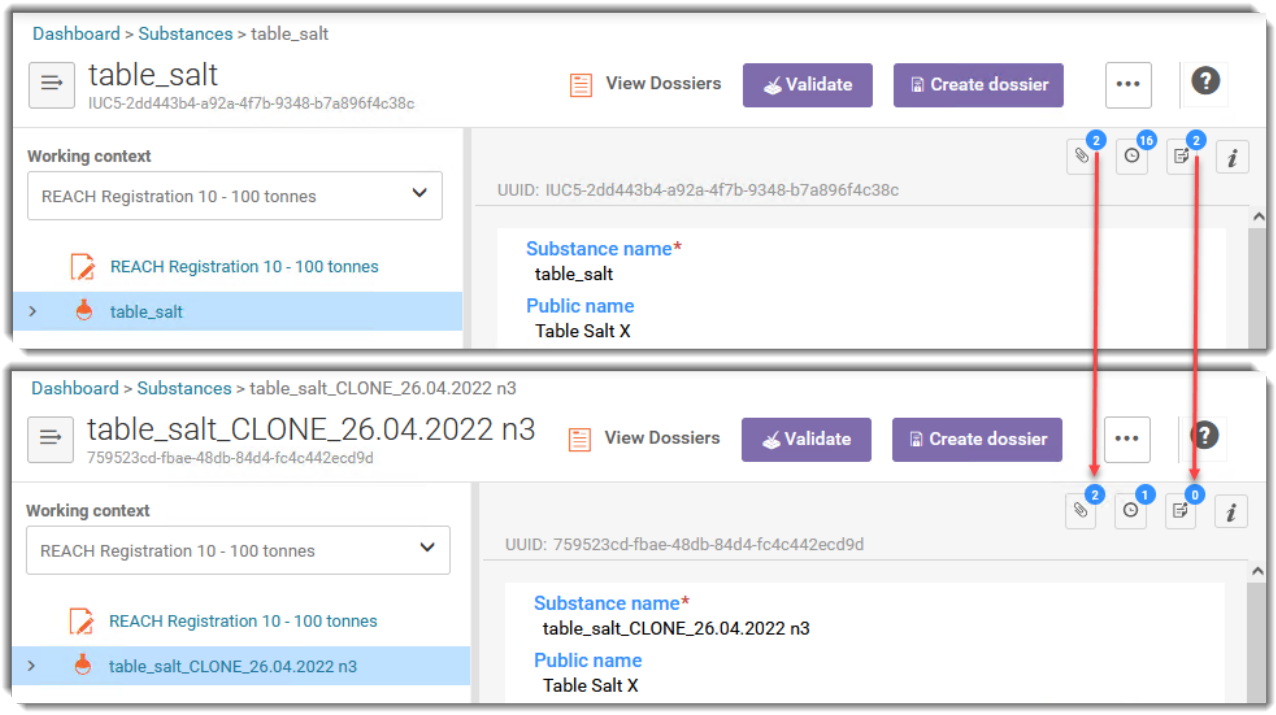


Cloning takes into consideration the direction of references. Outbound references are cloned; inbound references are not. The reason for having entities is that they can be referred to from multiple entities, thus avoiding duplication and improving consistency. For example, a *Substance* refers to a *Reference substance*. When a *Substance* is cloned, the reference is copied into the new cloned entity. Referenced documents are not touched, which also applies to entities. A newly cloned *Substance* refers to the same *Reference substance* as the document that was cloned. The UUID of the *Reference substance* does not change. On cloning, a document in a data section is copied into the clone, and given a new UUID. Documents cannot be cloned individually.

Another example of an outbound references is from an entity to an attachment. These are handled like a reference to an entity. On cloning, a new reference to an attachment is made. The attachment file in the database is not touched. There can be multiple references to an attachment, but there is only one file in the database. The uniqueness of an attachment file is confirmed and managed using a file checksum in the database.

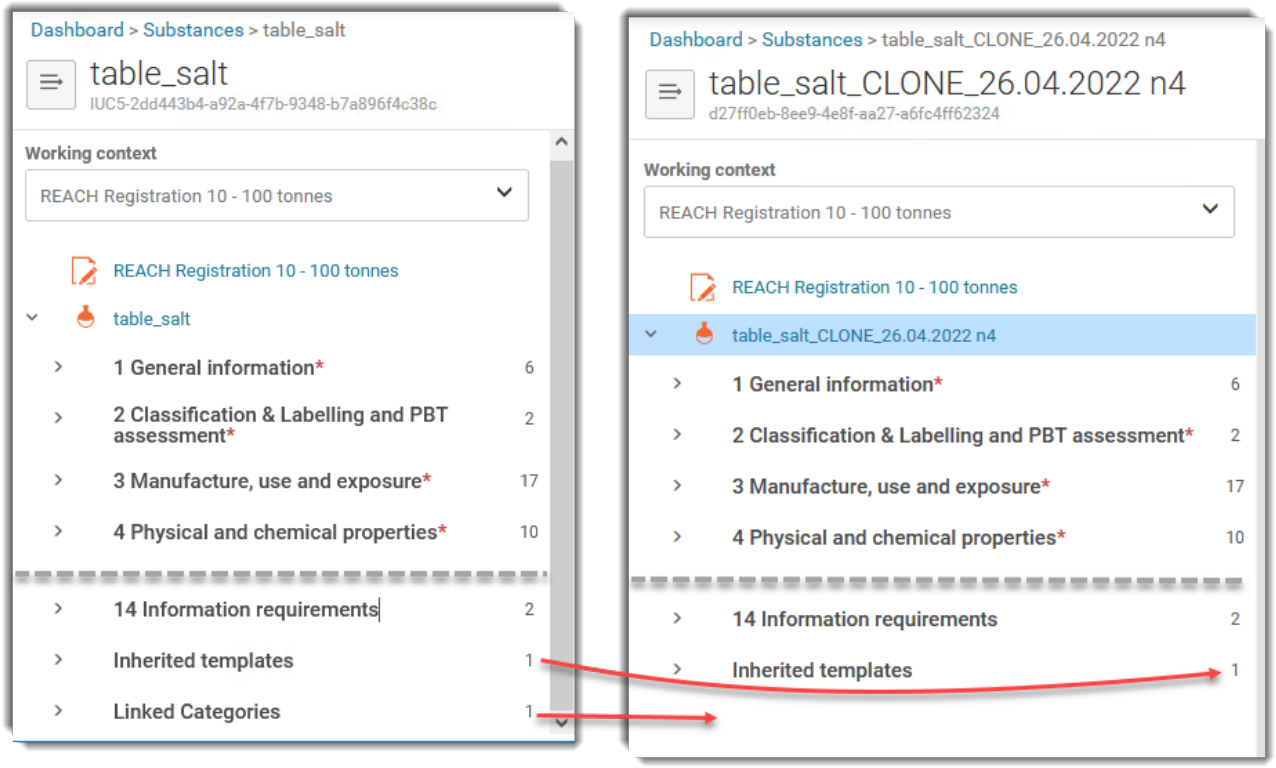
An example of an inbound reference is an *Assessment entity*. To illustrate the difference between attachment and *Assessment entity*, see the figure below that shows what happens on cloning a *Substance*. The number of attachments is the same, but the *Assessment entities* have **not** been cloned.

Figure 209: Cloning a substance dataset that has Assessment entities attached



On cloning a *Substance*, the behaviour of *Template* and *Category* differ for the same reasons. A *Substance* refers to a *Template*. A *Category* refers to a *Substance*. See below for cloning from left to right.

Figure 210: Cloning a substance dataset that is in a Category



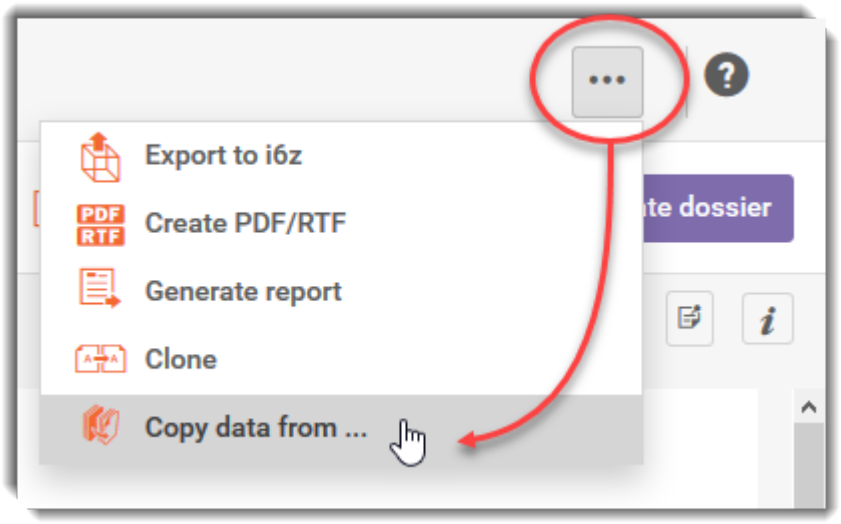
To add a link of the type shown on the left to the cloned *Substance* on the right, go to the *Category*, and create a reference to the cloned *Substance*. It is also possible to clone the *Category*, then create a reference to the cloned *Substance*.

Copy data from…, see below, is only for copying documents from a dataset. It handles referencing in the same way as cloning. Outbound references are copied, but the targets of the references are not touched. *Copy data from…* also works inside *Templates*.

22. Copy data from …

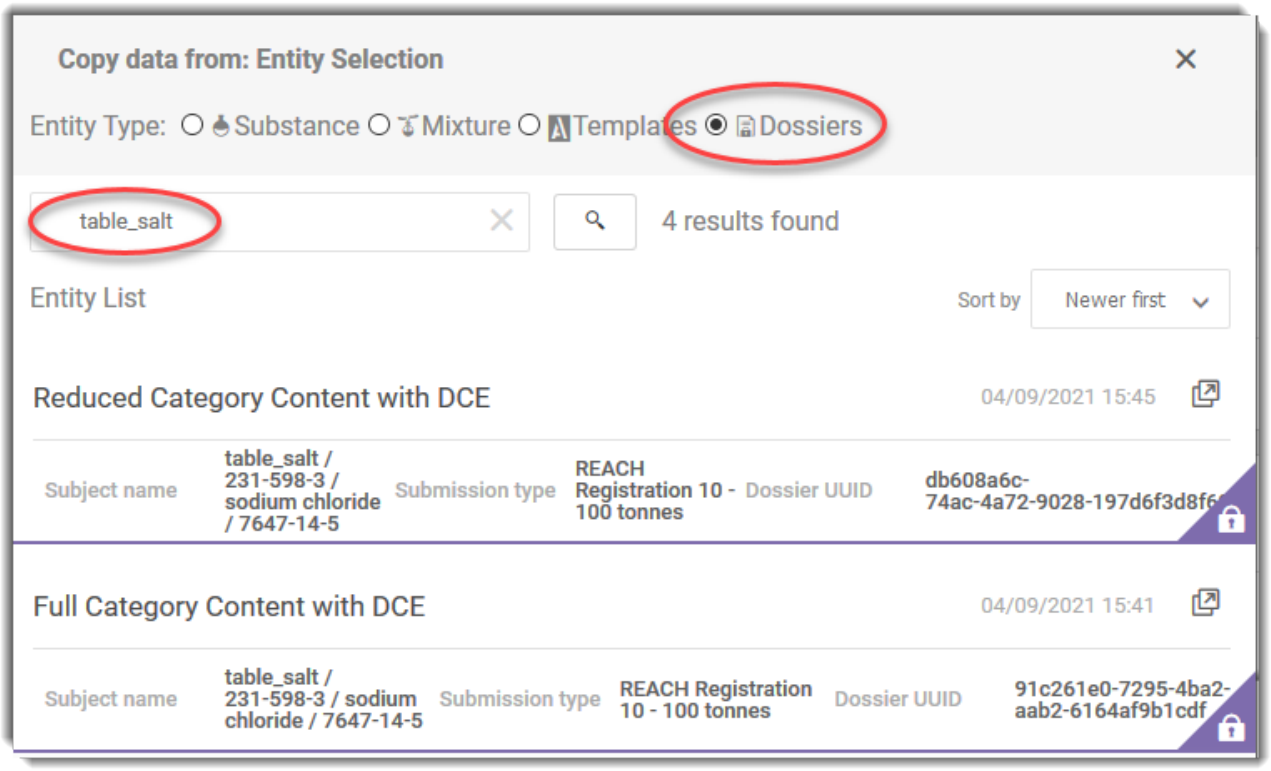
Copy data from is used to copy data between datasets. Start by viewing the record of the destination dataset. Open *Copy data from* from the menu, as shown below.

Figure 211: Copy data from …



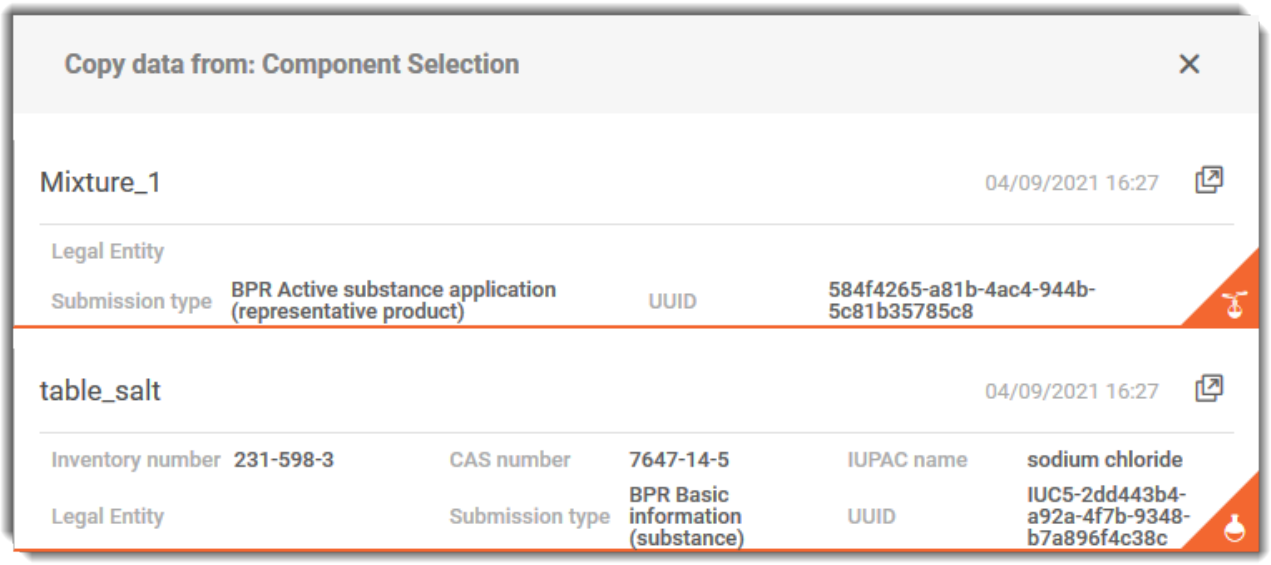
Next, select the type of entity from which data is to be copied. In the example below, data is to be copied from a *Dossier* that has the text *table_salt* in the subject.

Figure 212: Select the top-level source of the data to be copied



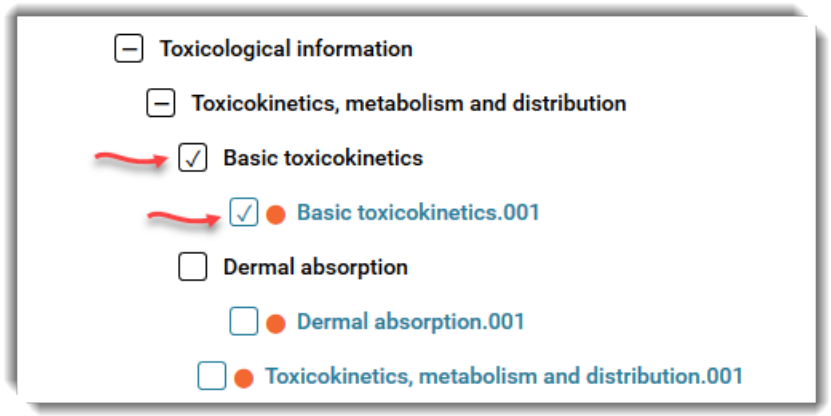
If the entity selected is a *Dossier*, and more than one dataset or component is in the *Dossier*, the next window offers a selection. In the example below, a *Substance* and a *Mixture/Product* are available in the *Dossier*.

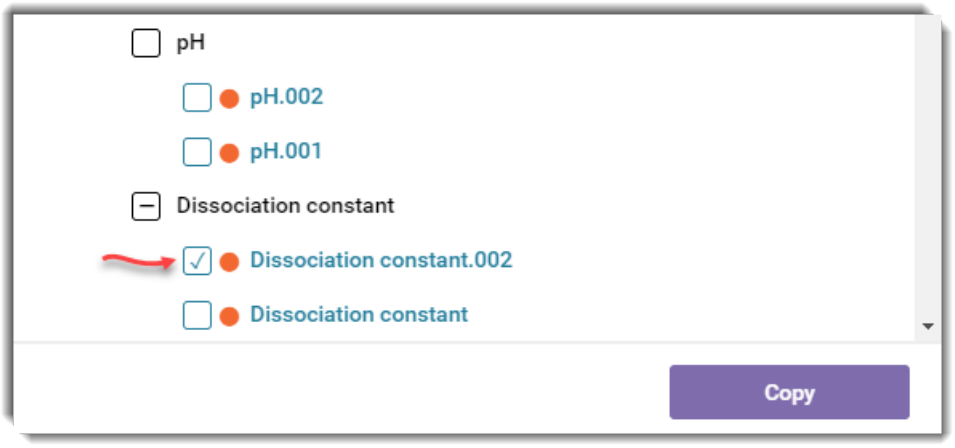
Figure 213: Select source of the data to be copied at the component level



Selecting an entity opens a window that shows the data from the source in a tree structure. Select the required documents by ticking the boxes, and then click on *Copy*.

Figure 214: Select the document(s) to be copied

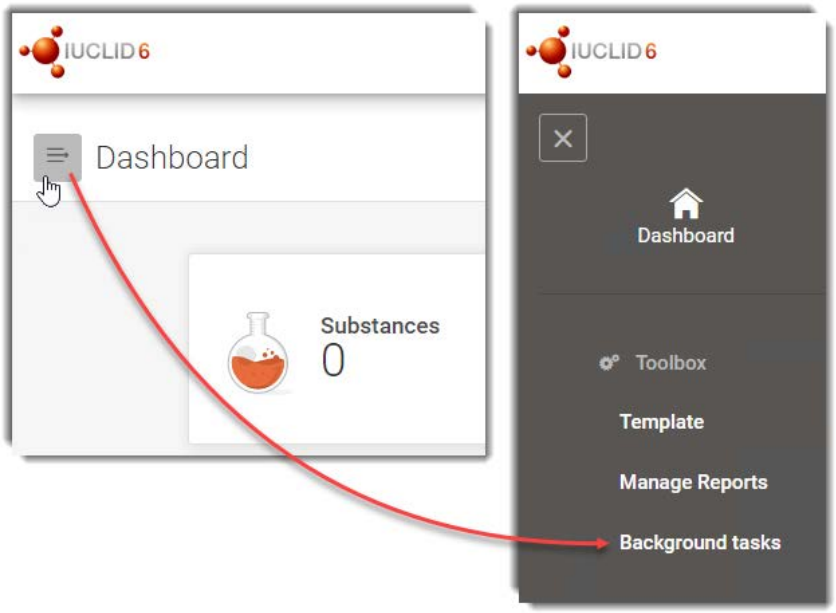



pH
pH.002
pH.001
Dissociation constant
Dissociation constant.002
Dissociation constant
Copy

23. Background tasks

Some tasks that are started from the user interface may take longer than a few seconds to complete. To allow a user to carry on working whilst the task is under way, some types of tasks are run in the background. On starting the task, the user interface remains accessible, and the task appears as an item on a page dedicated to background tasks. This applies to *Import*, *Export* and *Generate report*. How to access the *Background tasks* is shown below.

Figure 215: Opening the list page of the Background tasks



A background task can be in one of two states: running or completed. On successful completion of a task, a green tick is shown. If the task is no longer running either because it was cancelled by the user, or an error occurred, a red cross is shown. The tasks are shown in order of their start times. The record of a task has a three-dot icon on the right, that gives access to actions that are specific to that type of task.

Import contains a link that opens the imported entity in the data window. If files are imported in bulk in a zip archive, a background task is created for each file.

Data are exported by starting the export process from either *Export* on a list page, or from the option *Export to i6z* in the three-bar menu at the top right of the data window. Once the background task has finished, dependent on browser settings the file is either automatically saved to the default location, or a dialogue opens asking where to download the file. In addition, the file is made available to download via the background task. It remains downloadable until the background task is deleted. The data can be either a single IUCLID entity, as for *Export to i6z* or, when exporting entities in bulk from a list page, it is a zip archive of the exported files.

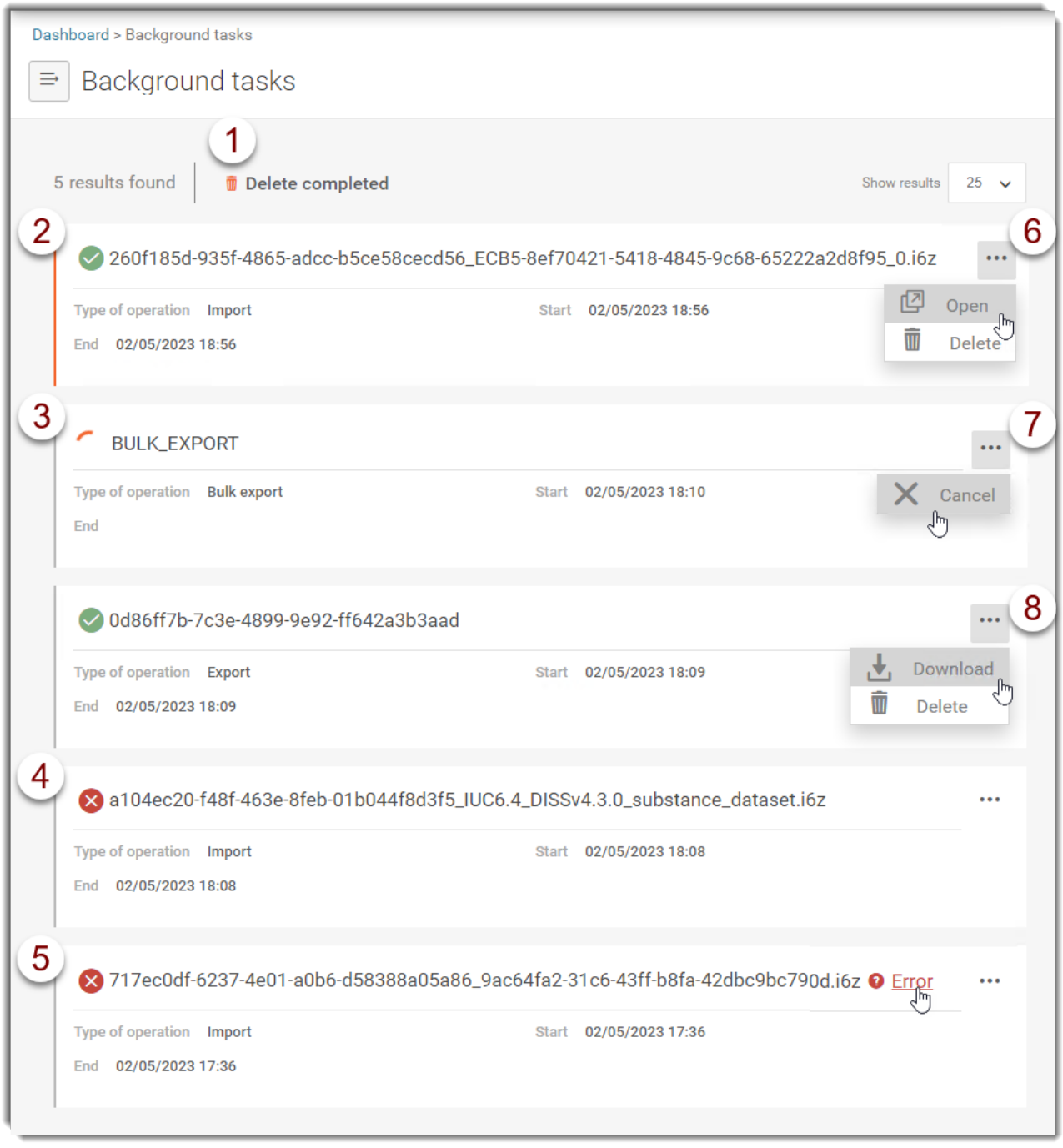
The downloading of generated reports behaves in the same way as exported data.

Background tasks in the completed state can be deleted, either all at once, or individually. Deletion removes the possibility to download the exported data via *Background tasks*, but it does not affect the source data. The same applies for *Import*.

If the user logs out of IUCLID whilst a background task is running, the task continues to run. Note that on importing multiple files it may take some time for all the background tasks to start. In that case, before logging out, check from the list page that all the background tasks have started.

An annotated example of the list of background tasks is shown below.

Figure 216: The list page for background tasks



Key for Figure 216

1. *Delete completed*, deletes all the background tasks that are not indicated as running with an orange spinning icon (3). This applies to all the tasks, not just those viewed on the current

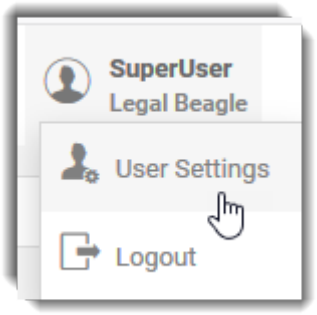
page. The deletion is done automatically at midnight every day for tasks that were completed more than 10 days ago;

2. The task has finished successfully, as indicated by the green tick icon ;
3. The task is still running, as indicated by the orange spinning icon ;
4. The task was cancelled by the user, as indicated by the icon and the absence of any error;
5. The task ended in error, as indicated by the icon and a link to the error message;
6. The data window for an imported entity can be opened from here;
7. A running task can be cancelled. All actions associated with it are undone, as though the process had not been started;
8. Once an export task has finished, the file to export is downloaded from here. There is no automatic download.

24. User management

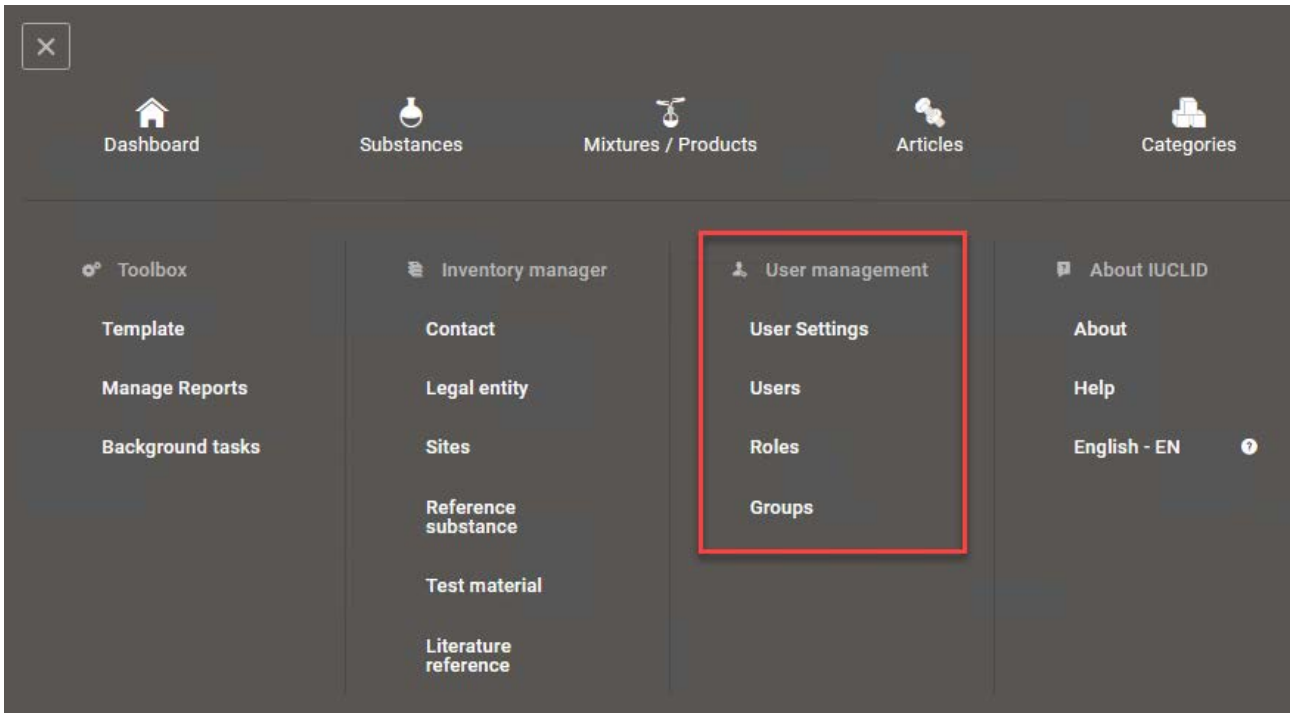
IUCLID 6 Desktop has only one User, which is *SuperUser*. All actions are carried out under the *SuperUser*. There is no log-in or lot-out process. However, access is provided to the record page of *SuperUser*, to allow the *working Legal entity* to be changed. For more information see section *7.1 Working Legal entity*. The access is via a menu at the top right of the interface, as shown below.

Figure 217: User settings of SuperUser in IUCLID 6 Desktop



IUCLID 6 Server is a multi-user environment, in which each user has its own username, password, and access rights to data. The IUCLID data objects associated with *User management* are: *User*, *Role* and *Group*. *Group* is accessible only if *Instance Based Security (IBS)* is active, which is described in section *24.4 Ownership and Sharing - Instance based security (IBS)*. The list pages for *User*, *Role* and *Group* are accessed from the main menu, as indicated in the figure below.

Figure 218: User management with Instance Based Security (IBS) active



User, *Role* and *Group* are described in their own sections that follow.

24.1. Overview of user management concepts

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.

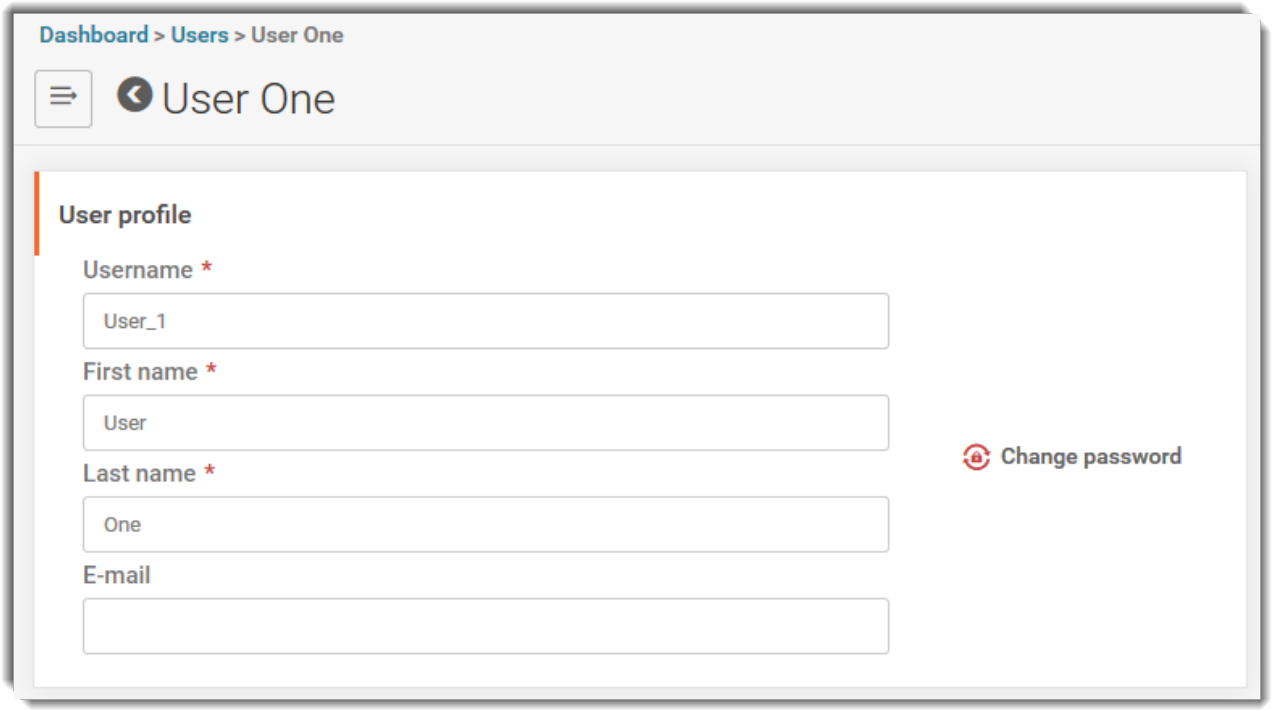
The username uniquely identifies the *User* throughout the interface. It is common to have a one-to-one relationship between a person using IUCLID 6 and a *User*, in which case only one person knows the authentication details of each *User*. More than one *User* can be logged in to IUCLID 6 Server at the same time, from any machine that has appropriate network access.

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. A document can be owned by only one *User* at a time, and ownership can be transferred between *Users*. 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, but, can act on behalf of only one *Legal entity* at a time. The access a *User* has to functions and to different types of data within IUCLID 6 is controlled via *Roles*. In addition, limits can be applied to specific documents, using *Instance Based Security (IBS)*, as described in section *24.4.*

24.2. User

User management can be performed by a *User* that has the rights provided by the pre-defined *Role* of *User Manager*. An example of the user management window is shown in the figure below, where a record for a *User* with username User_1 is defined.

Figure 219: User management via the record page of a User



The *Role* of *User Manager* permits a *User* to 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*. To manage a *User* that has administrator rights, the *User manager* must also have administrator rights.

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

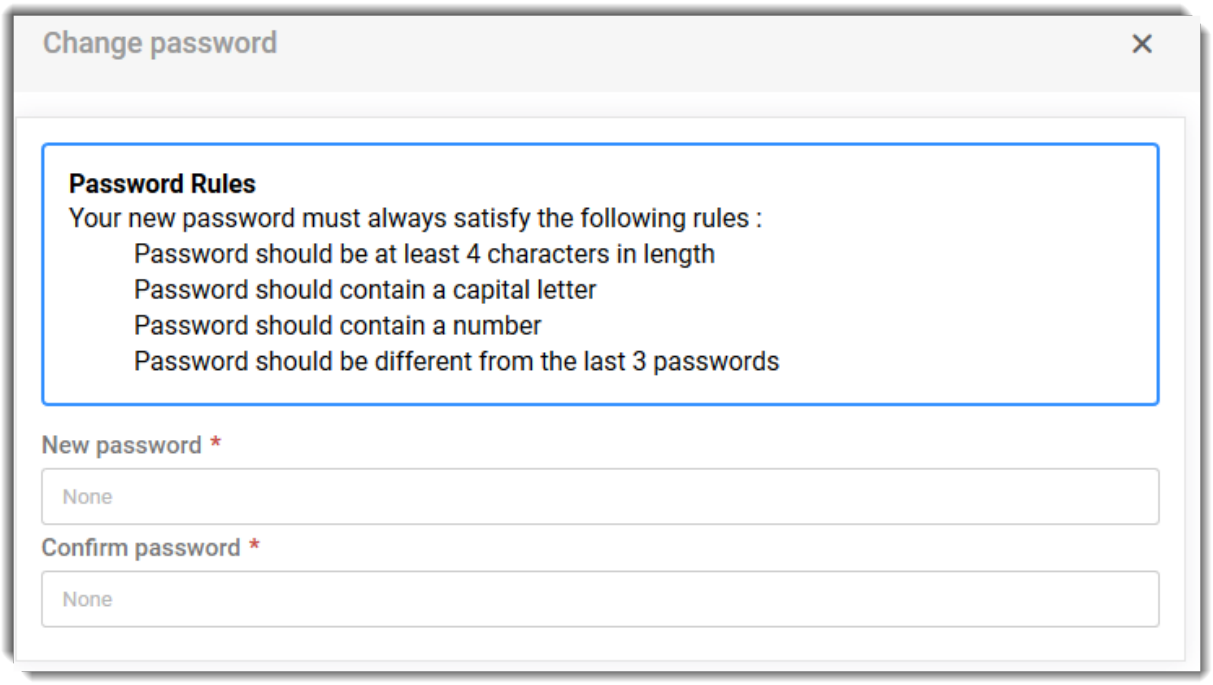
24.2.1. User profile

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.

24.2.1.1. Change password

The *password* is used in combination with the *username* to authenticate a person when logging in to a *User*. The password must conform to a minimal set of security criteria. The criteria are displayed when changing a password, as shown below.

Figure 220: Password management



The criteria are set by the system administrator of IUCLID. If a *User* changes its own password from the *User settings* menu at the top right, the current password must be entered. If the *User* has the right to manage other users, the old password does not need to be entered when changing a

password from the record of the *User*. For example, this allows the user manager to reset a forgotten password.

24.2.2. Contact person

For information purposes, a single *Contact* can be attached to a *User*. The *Contact* can be an existing one, or a *Contact* can be created from the selection window.

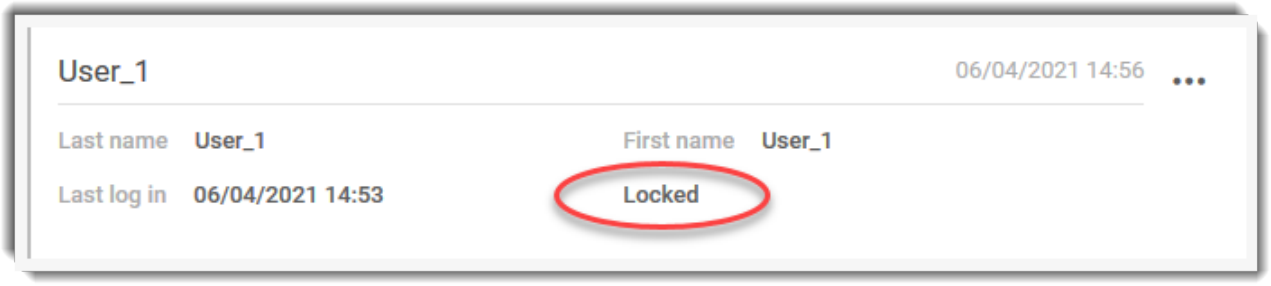
24.2.3. General

The option *Access All* is shown only when Instance Based Security (IBS) is active. For a description of IBS, see section *24.4 Ownership and Sharing - 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*. If a *User* is set to *Access All*, all the *Roles*, *Groups* and *Legal entities* in the instance of IUCLID are assigned to the *User*. If *Access All*, is subsequently removed from a *User*, its rights remain the same, but the *Roles*, *Groups* and *Legal entities* can be removed manually.

Locked means that the maximum number of attempts to log in to the *User* has been exceeded. 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*.

The states of *locked*, *suspended*, and *expired* are indicated per user on the list page of *Users*. In the example shown below, a user has entered an incorrect password too many times for the username *User_1*.

Figure 221: A locked User



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*.

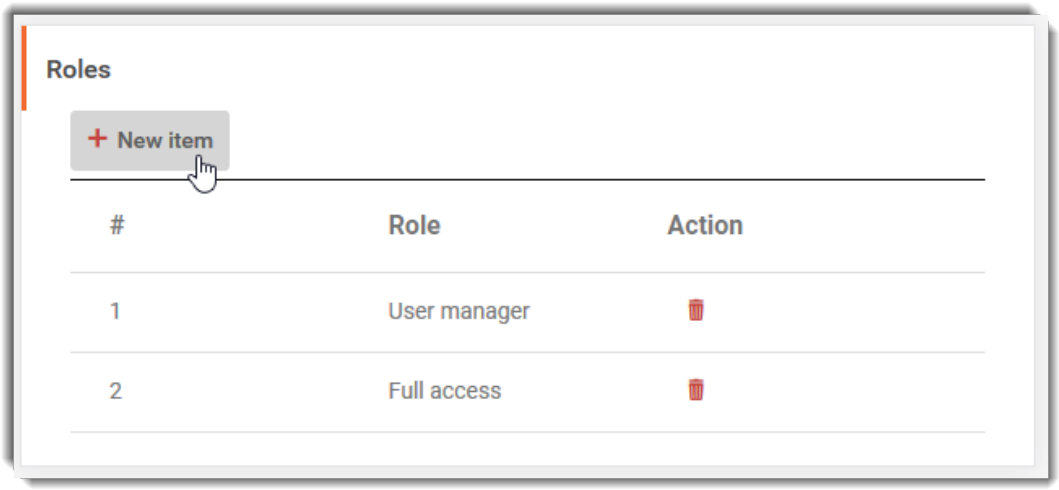
Expired means that no one has logged in to the *User* for the number of days set in the field *Admin / System administration / Security policy / Automatic expiry of unused accounts after x days*. The default value is sixty. To cancel the expiration, untick the box. The change takes effect as soon as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

Remarks is a free text field provided to allow the user manager to make notes about the *User*. It can contain up to 255 characters.

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

24.2.4. Roles

Figure 222: Adding a Role to a User under User management



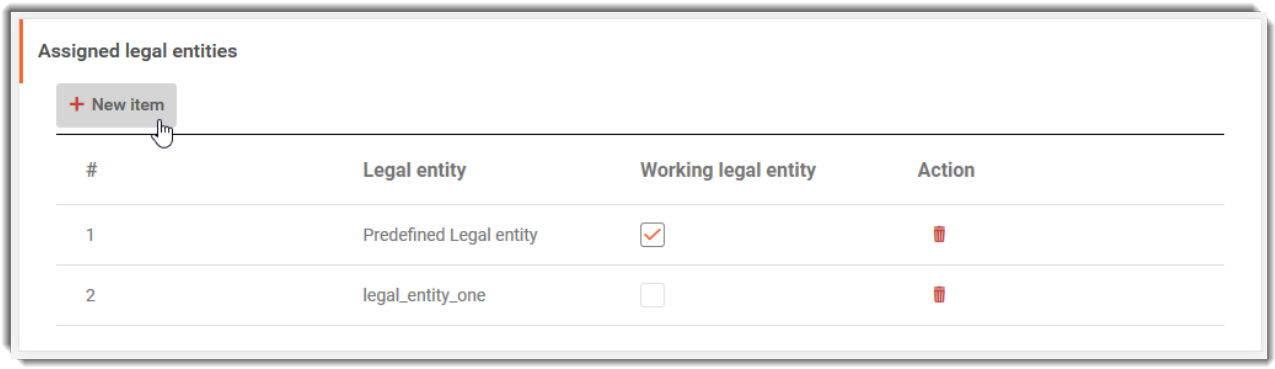
This field is used to set the *Roles* of the *User*. A *User* must have at least one *Role*. By default, a new user is given the predefined *Role* of *Read-only*. If a *User* has more than one *Role*, the rights given are additive. For example, if a *User* has a *Role* that allows only reading for a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

24.2.5. Assigned legal entities

A *User* must have at least one *Legal entity* assigned to it, and at least one *Working legal entity*. 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, tick the box *Working legal entity*.

Figure 223: Adding a Legal entity to a User under User management



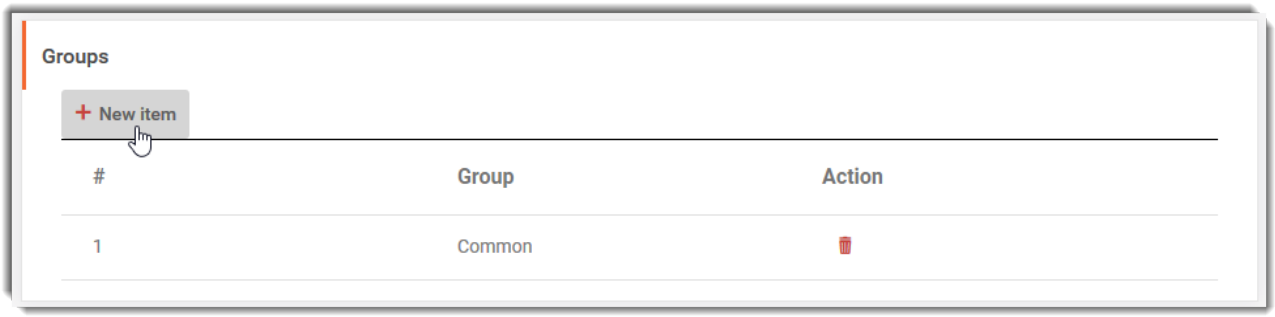
A *User manager* can assign only *Legal entities* to which it has access.

24.2.6. Groups

This field is shown only when Instance Based Security (IBS) is on. For a description of IBS, see section *24.4 Ownership and Sharing - 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 *Groups*.

Figure 224: Adding a User to a Group under User management



24.2.7. Default group access for a User

This is shown only when Instance Based Security (IBS) is active in the instance of IUCLID 6 Server.

The options shown 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. The *User* can modify these default values via *User Settings*, which is accessible via the user icon at the top right of the interface.

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*, select one of the following options from the drop-down menu: no access, R (read), R/W (read and write), R/W/D (read and write and delete).

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

Figure 225: Default group access for a User

24.2.8. 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.

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

24.2.8.1. 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. The locking of SuperUser can be prevented by setting a system parameter, as described in the document *Installation and Update Instructions for IUCLID 6 Server*, which is available on the IUCLID 6 website.

24.2.8.2. 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 and un-check *Expired*. *SuperUser* can do that.

24.3. 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.

24.3.1. Role information

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 2000 characters.

24.3.2. Permissions - access to operations

24.3.2.1. Basic Operations

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

24.3.2.2. Plugin operations

These fields control access to sets of functionalities which may not be required by all *Users*, for example the PNEC and DNEL calculators.

24.3.3. Permissions - access to data

24.3.3.1. 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, R (read), R/W (read and write), R/W/D (read and write and delete).

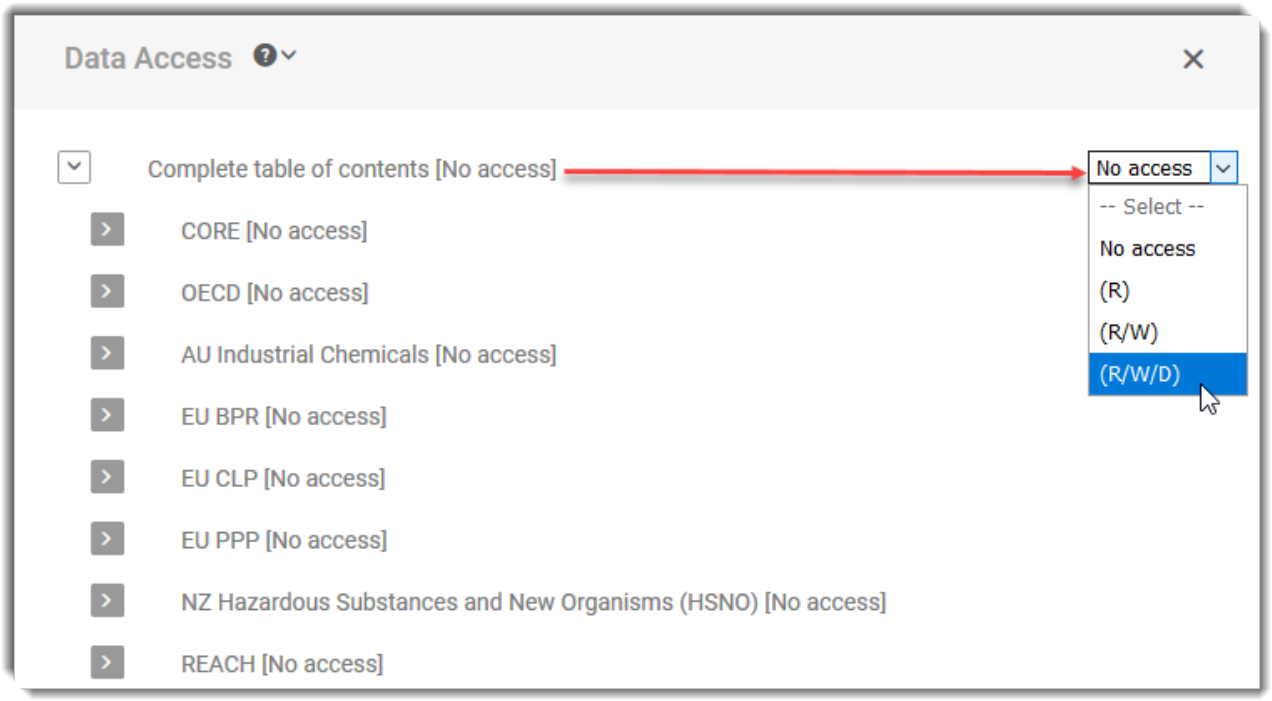
If Instance Based Security (IBS) is in use, the access must also be allowed through either ownership, or sharing within a *Group*.

24.3.3.2. Data access to section documents

Here, access to data in datasets can be controlled at the level of section. The sections are shown in the default tree structure. To open the view, hover the cursor over the text “please view and select…”, then click on the grey box.

To change a level of access, hover the cursor to the right of the node in the tree structure and then select the access from the box the menu that appears. The access is applied down the hierarchy from the node. In the example shown below, the access is being changed from the default of *No access* to R/W/D across the whole tree hierarchy by acting on the highest node.

Figure 226: Setting access rights to all documents in one action



The access rights are indicated at the right of the title of a node using a code: no access, R (read), R/W (read and write), R/W/D (read and write and delete).

To set access for a whole section in one action, edit the access value at the top of the section. In the example, below, all of section 7 under CORE is being changed from *no access* to *read and write*.

Figure 227: Set access to documents per section

To save changes to the Role, exit the view and then click on the orange *Save* button at the foot of the page.

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*.

24.3.4. Application management

24.3.4.1. System configuration

System configuration is not managed via the user interface, but in settings files. For more information contact your system administrator.

24.3.4.2. Security management

Security management is not managed via the user interface, but in settings files. For more information contact your system administrator.

24.3.4.3. *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, R (read), R/W (read and write), R/W/D (read and write and delete).

24.3.4.4. *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, R (read), R/W (read and write), R/W/D (read and write and delete).

24.3.4.5. *Assign Legal entities to users*

This right permits a *User* to assign a *Legal entity* to a *User*.

24.3.4.6. *Assign Roles to users*

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

24.3.4.7. *Remove Roles from users*

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

24.3.5. Assigned Users

The field *assigned users*, lists the *Users* that have the selected *Role*, and provides a means of adding the *Role* to *Users*. The assignment of *Roles* to *Users* can also be done per *User* from the record of the *User*. A *User* can assign only *Roles* that are assigned to it.

24.3.5.1. *IBS management*

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

24.3.5.1.1. Manage Groups

Here, access can be defined to the entity *Group*, which can be: no access, R (read), R/W (read and write), R/W/D (read and write and delete).

24.3.5.1.2. Assign users to groups

This right permits the changing of *Group* membership.

24.3.5.1.3. Manage private groups

This right permits the changing of ownership of a document. For more information see section *24.4.3 Ownership*.

24.3.6. Predefined Roles

IUCLID 6 is supplied with various *Roles* predefined for the convenience of users. Predefined *Roles* can neither be edited nor deleted. The predefined *Roles* are described below.

24.3.6.1. System administrator

Grants all possible permissions that can be granted from within the functionality of *Role*.

24.3.6.2. Full access

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

24.3.6.3. Read-only

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

24.3.6.4. 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*.

24.3.6.5. Group manager

This *Role* is available only when instance based security (IBS) is active.

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*.

24.4. Ownership and Sharing - Instance based security (IBS)

Instance based security (IBS) is intended for use with only IUCLID 6 Server, and not with IUCLID 6 Desktop.

When IBS is in use, each entity has an owner, and can be shared among groups of *Users* to different levels of access per group.

Instance based security allows access within IUCLID 6 to be controlled per entity per *User*. *Users* can be organised into *Groups*. Access to an entity can be defined per *Group* using the *Share* functionality. When a *User* creates an entity, the *User* becomes the owner of the entity. Ownership allows the *User* to *Share* an entity to the members of any *Group* to which it belongs. The system can be set up to *Share* entities automatically on creation, and to allow *Users* to decide to which *Group(s)* they share the entities they create. Contact your system administrator for details on how your system is set up. If you are unsure of the behaviour, it is always possible to view how an entity is currently being shared, as described later in this section.

The levels of access that can be applied to a document under IBS are shown in the table below:

Table 8: The levels of access under Instance based security

Access
No Access
Read
Read/Write
Read/Write/Delete

Access to a document can be determined in four ways:

1. on creation of the document according to the settings in *Default group access*;
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.

Example of using IBS

Members of a team in an organisation need to work on a subset of *Substances* in a centralised database. *Users* not in the team cannot access the *Substances*. Team members have complete

control over the *Substances* they create, and by default, read-only access to *Substances* created by other members of the team.

The team members are given personal *Users* which are placed in a *Group* for the team. The administrator sets the system so that *Substances* created by any member of the *Group* are automatically shared to the *Group* with read-only access. When a member of the team imports a *Substance*, the team member can decide on the level of access to provide to the team. This can be changed later if required.

24.4.1. 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*.

24.4.1.1. Common Group

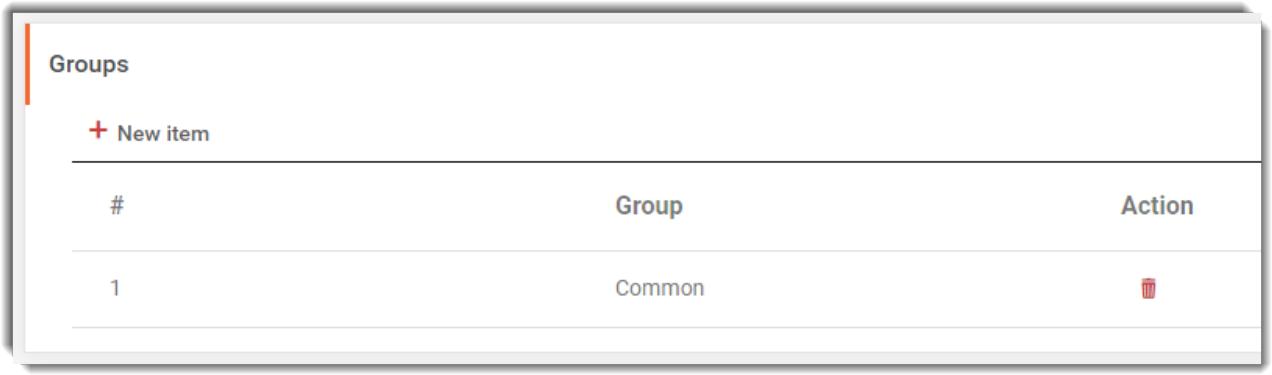
Common is a *Group* to which all *Users* belong, by default. In that sense, common has the same meaning as public. In contrast, a *Group* created within IUCLID 6 is inherently private, because only members of the *Group* have access to the data shared within the *Group*.

24.4.1.2. Group Management

Membership of a *Group* can be set either by editing a *User* or a *Group*.

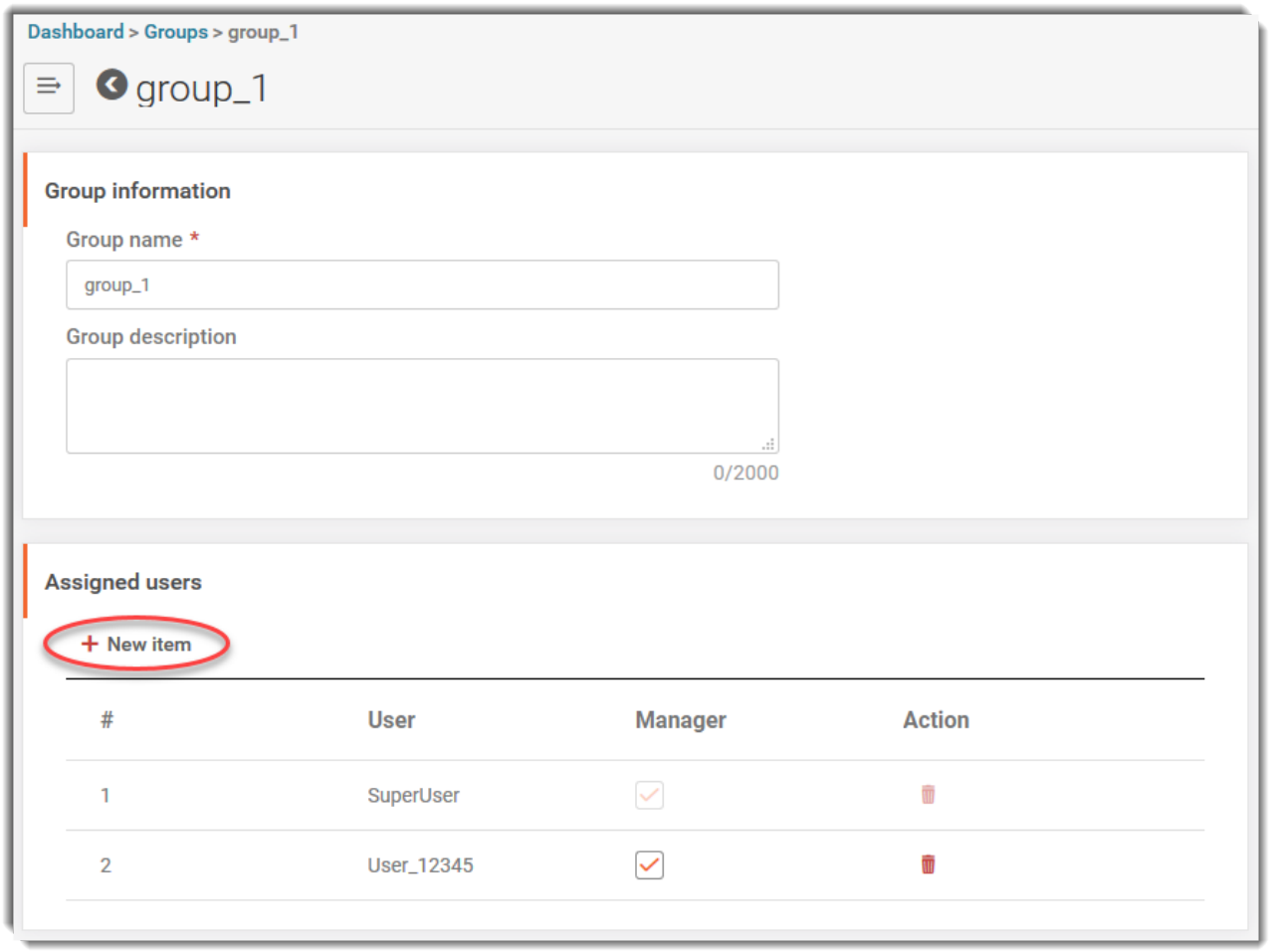
The *Groups* to which a *User* belongs can be controlled from the record of the *User*, under the heading *Groups*, as shown below. To add a *Group*, click on *New item* and then select a *Group* from the window on the right. To remove the *User* from a *Group*, click on the dustbin icon for the *Group*.

Figure 228: Add a User to a Group from the record of the User



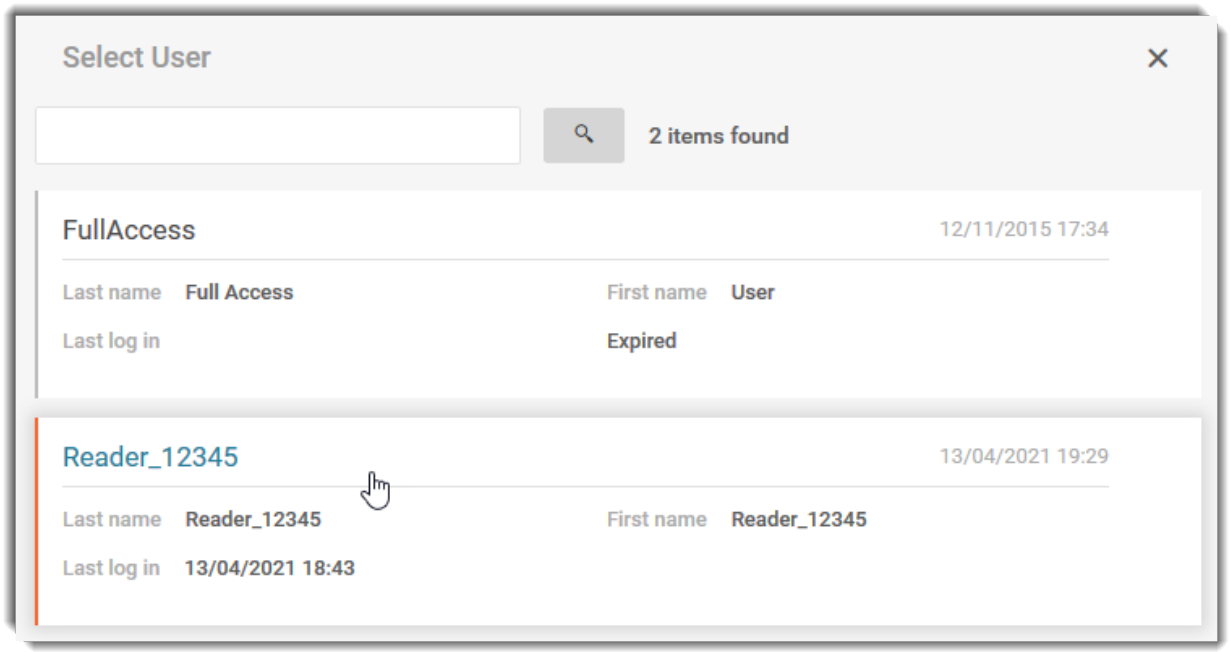
An equivalent action can be done from the record of a *Group*. To add a *User* to a *Group*, open the record of the *Group* from the list page, and then click on *New item*, as indicated below.

Figure 229: Add a User to a Group from the record of the Group



Select the *User* from those available. In the example below *User* Reader_12345 is selected.

Figure 230: Select a User for membership of a Group



To set a *User* as a manager of the *Group* tick the box in the column headed *Manager*. This is possible only where the *User* has sufficient access rights. These are granted by the pre-defined *Role* of *Group Manager*.

24.4.2. Share

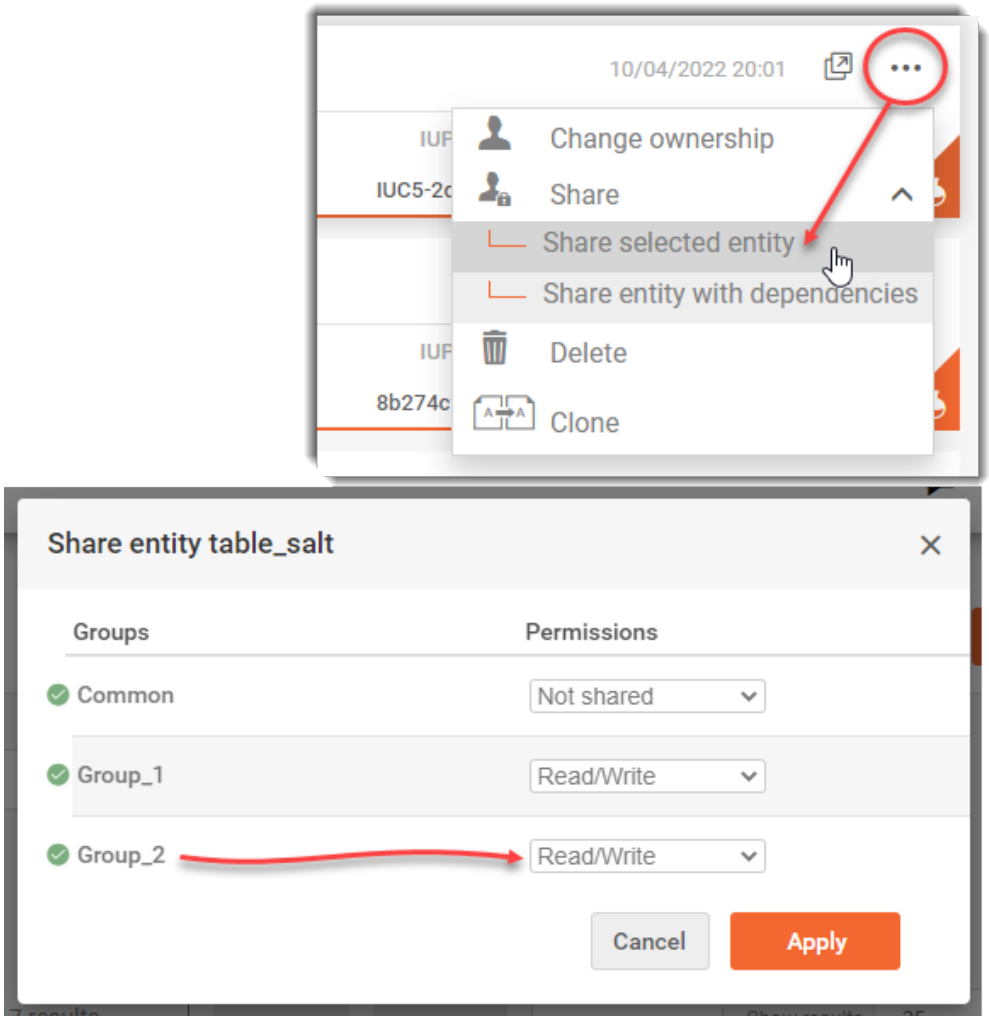
Share is an action in which the *Users* in a *Group* are granted access to an entity with one of the four permissions shown in the table below:

Table 9: The permissions grantable to a Group using the functionality Share

Permissions
Not Shared
Read
Read/Write
Read/Write/Delete

To view the permissions for an entity, click on the three-dot icon to the right of its entry in the list of entities, and then select the option *Share*. This opens a list of the *Groups*. For each *Group*, the current permissions are stated, as shown in the example below.

Figure 231: View the permissions of an entity, e.g. a Substance dataset



To change a permission for a *Group*, click on the arrowhead icon for a *Group*, and then select the required option.

If a *User* is in more than one *Group*, the combined effect for that *User* of a *Share* is additive. Thus, the combination of *Not Shared* and *Read/Write* is *Read/Write*.

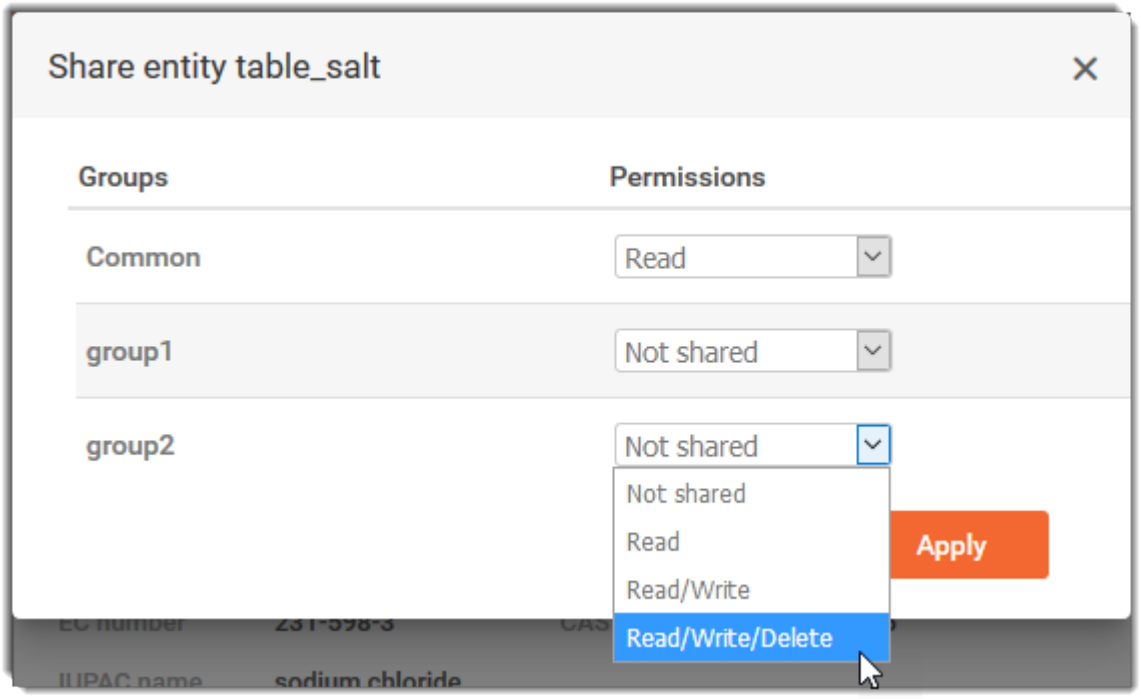
A *User* that has access to an entity only because of sharing, cannot edit the sharing of the entity.

The owner of an entity can set any level of sharing for it, to any of the *Groups*. It does not need to be a member of the *Group*, and it does not have to have the *Role* of *Group Manager*.

A *User* that has the built-in *Role* of *Group Manager* can apply any sharing to an entity to which it has at least read access. This applies across all *Groups*, irrespective of whether the *User* is a member.

Example of Share

Figure 232: Example of sharing a Substance dataset

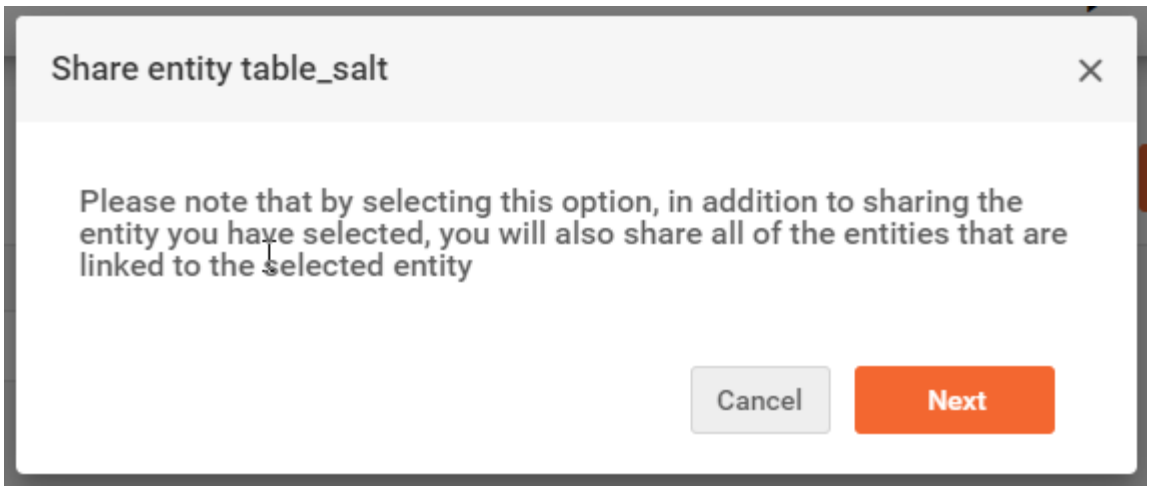


For *group2*, the permissions are being changed from *Not shared*, to *Read/Write/Delete*.

24.4.2.1. Share entity with dependencies

This option is shown only for entities that have dependent entities, for example, a *Substance dataset* that refers to *Reference substances*. In that example it would apply the same sharing to the *Reference substances* referred to in the *Substance dataset*. The following notice is displayed:

Figure 233: Share entity with dependencies



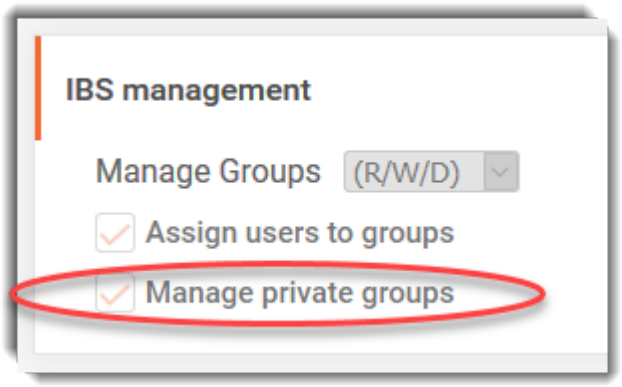
24.4.3. Ownership

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 active.

24.4.3.1. Change ownership

When an entity is created or imported, its ownership is set to that of the current *User*. An entity can have only one owner at a time. Ownership can be transferred only within the *Group* of the owner. Ownership can be transferred only by a *User* that is a manager of a *Group*, and has a *Role* in which *Manage private groups* is enabled, as shown below.

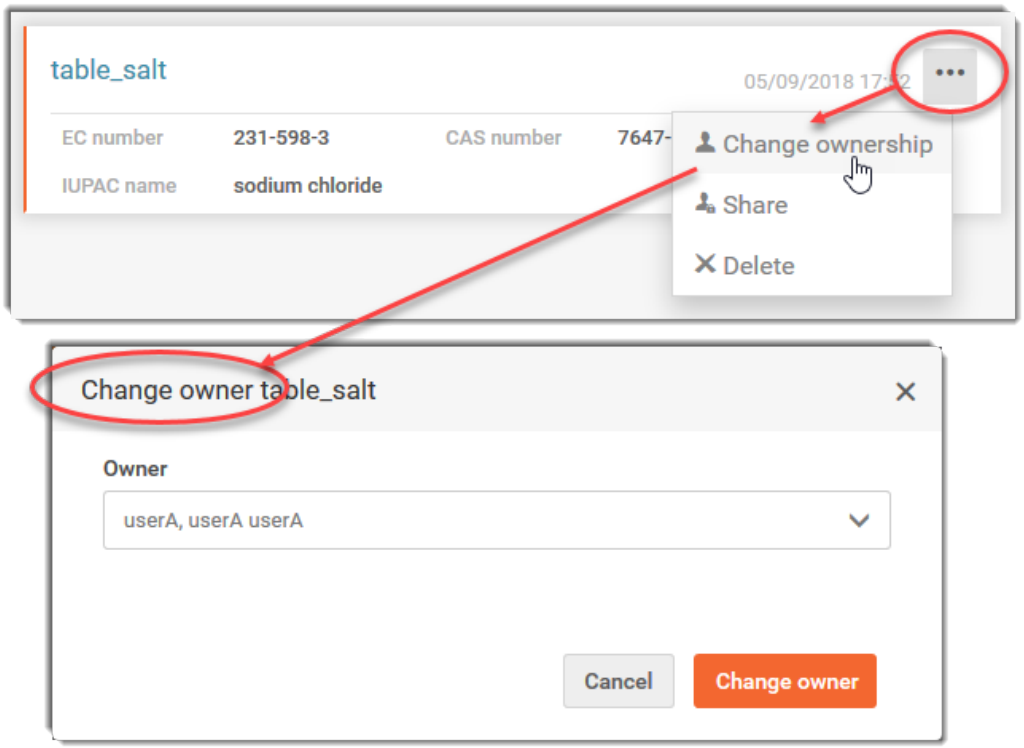
Figure 234: The right to change ownership



The predefined *Roles* that provide this right are *Administrator* and *Group manager*.

Ownership of an entity is viewed and changed from a window opened via the three-dot icon accessible from the list of entities, as shown in the example below.

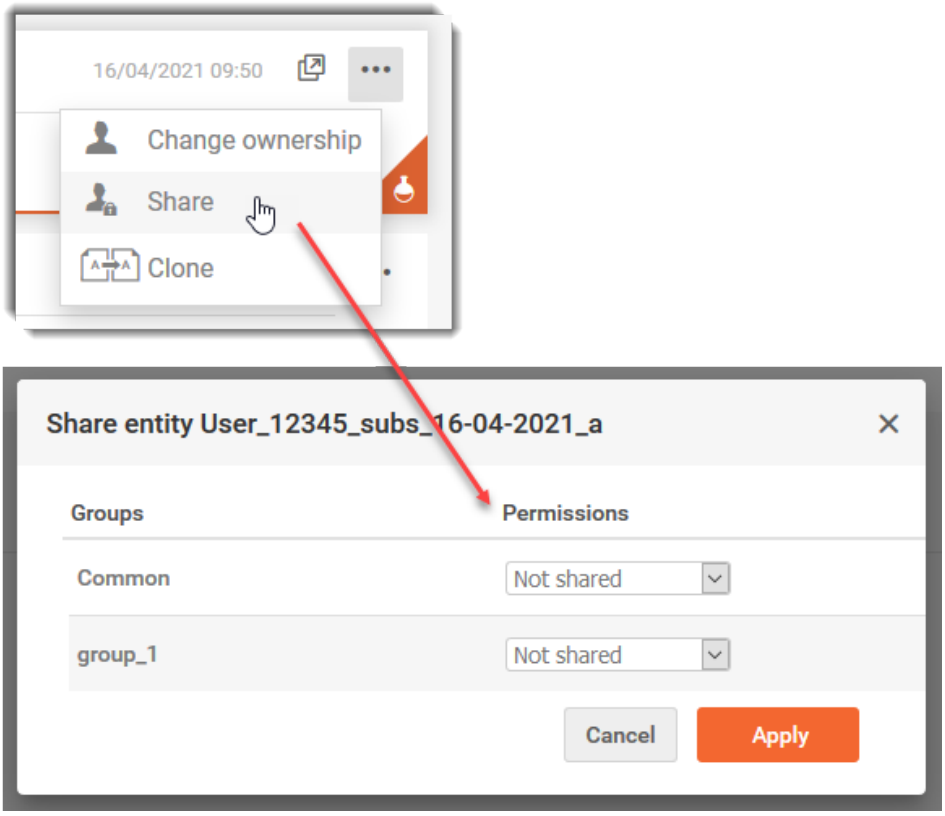
Figure 235: Viewing and changing the ownership of an entity, e.g. a Substance dataset



24.4.3.2. User manager access to an entity it does not own

A *User* that has the right *Manage private groups* and is a manager of a *Group* has the same level of access to the sharing and ownership of entities as the owners in the *Group*, except it cannot delete entities it does not own. A consequence of this, a scenario is possible in which the *Group manager* opens the sharing menu of an entity, and sees that it has not been explicitly shared to the *Group*. This is not a contradiction. The *Group manager* has the access because the entity is owned by a member of the *Group*. An example is shown below for a *Group manager* of group_1 who does not own the entity.

Figure 236: User manager access to an entity it does not own



24.4.4. 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 *Resources* \ *Substance* for userA mean that when userA creates a *Substance*, all members of group1 are automatically given rwd rights to it. No rights are given for *Dossiers*.
userC			There are no settings under *Resources* for userA that automatically confer access rights to userC for *Substances* or *Dossiers*.
userD			There are no settings under *Resources* for userA that automatically confer access rights to userD for *Substances* or *Dossiers*.

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

result 2: The following access has been granted.

Table 12: IBS exercise - result 2

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

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

result 3: The sharing allowed is shown below.

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

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

result 4: The sharing allowed is shown below.

Table 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 *share* the document. The permissions are rwd because the settings under

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

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

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

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

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

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

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

Table 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 *Users* have been granted that right as part of this

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

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

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

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

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

25. 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 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). The assessor should always make sure to add to the DNEL calculator all the needed information, so that the calculator can then perform the algorithm to select the starting dose descriptor(s) for the specific route, as described.
2. The DNEL calculator performs the following for deriving DNELs for workers and the general population for a route of exposure.
    a. Analyses the dose descriptors available in the endpoint summaries in 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 25.1.5 Step 1: selection of relevant dose descriptors*.
    b. Analyses 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 *25.1.6 Step 2: modification of relevant dose descriptors* and section *25.1.8 Step 3: application of assessment factors*, 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, as described in section *25.3 Modifying defaults from the DNEL calculator*.

5. The DNEL calculator reports the outcome of the calculation and related explanations when relevant in the IUCLID endpoint summary section 7.

25.1. 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*.

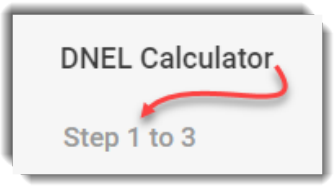
The IUCLID endpoint summary is the document that summarises the information available in all the endpoint study records of a given Endpoint section. Therefore, it is expected that before running the DNEL calculator, the assessor should have already carried out the assessment of the available studies, 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 in the endpoint summaries of sections 7.1, 7.5 and 7.8.

The data for reporting on the hazard assessment conclusions for human health (workers and general population) are in an endpoint summary at the top level of section 7 *Toxicological information* in a *Substance*. To launch the DNEL calculator, navigate to the endpoint summary, and then click on the button at the right of the interface, as shown in the example below.

Figure 237: Open the DNEL calculator

The DNEL calculator has three steps. The current step is indicated as shown below:

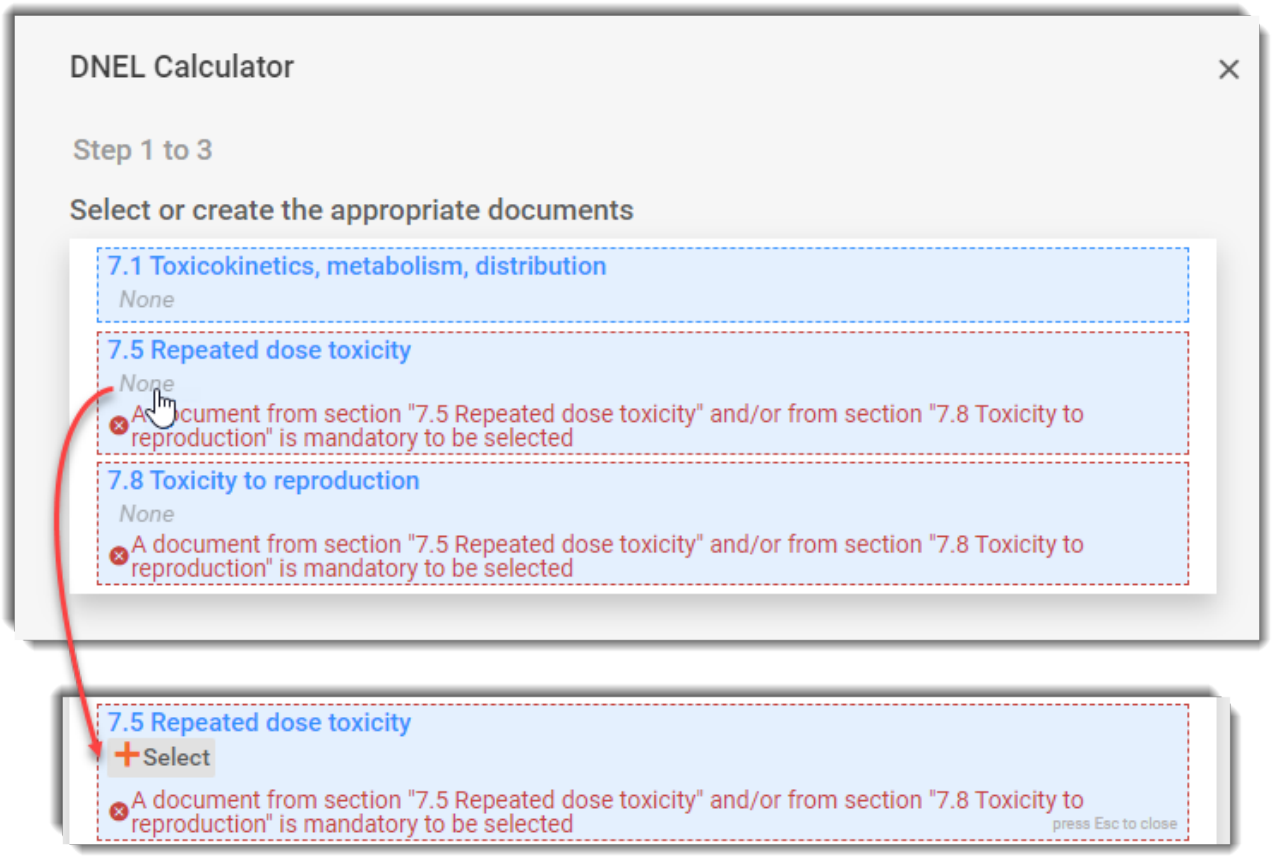
Figure 238: Steps in the DNEL calculator wizard



Guidance on entering data into the different steps of the calculator is provided in later sections.

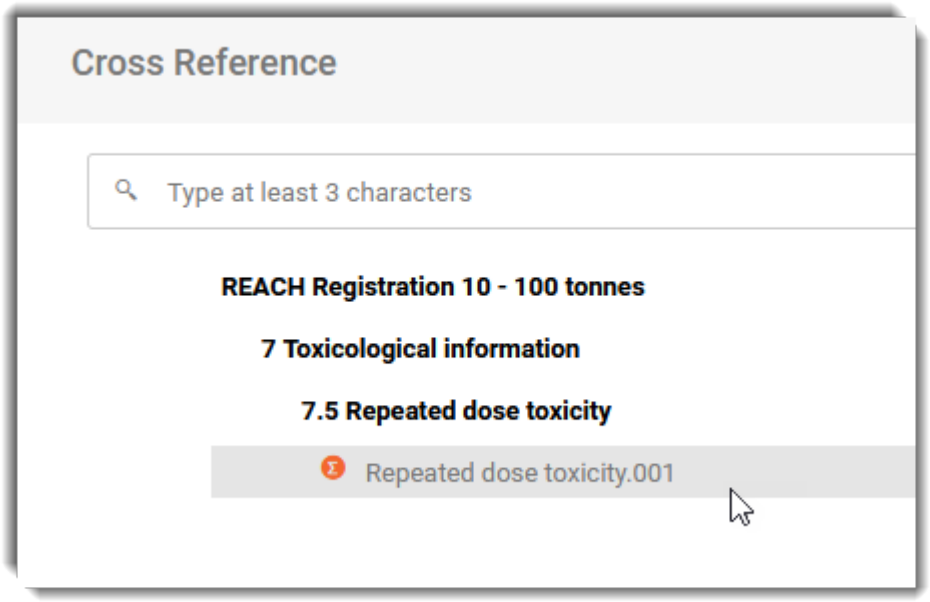
In the first step, the endpoint study summaries needed for the DNEL calculation are selected. Where nothing has been selected, there is a greyed-out comment *None*. To select a summary, click on the endpoint. Where a summary is mandatory and nothing is selected, a warning message is shown. An example is shown below.

Figure 239: Selecting summaries in step 1 of the DNEL calculator



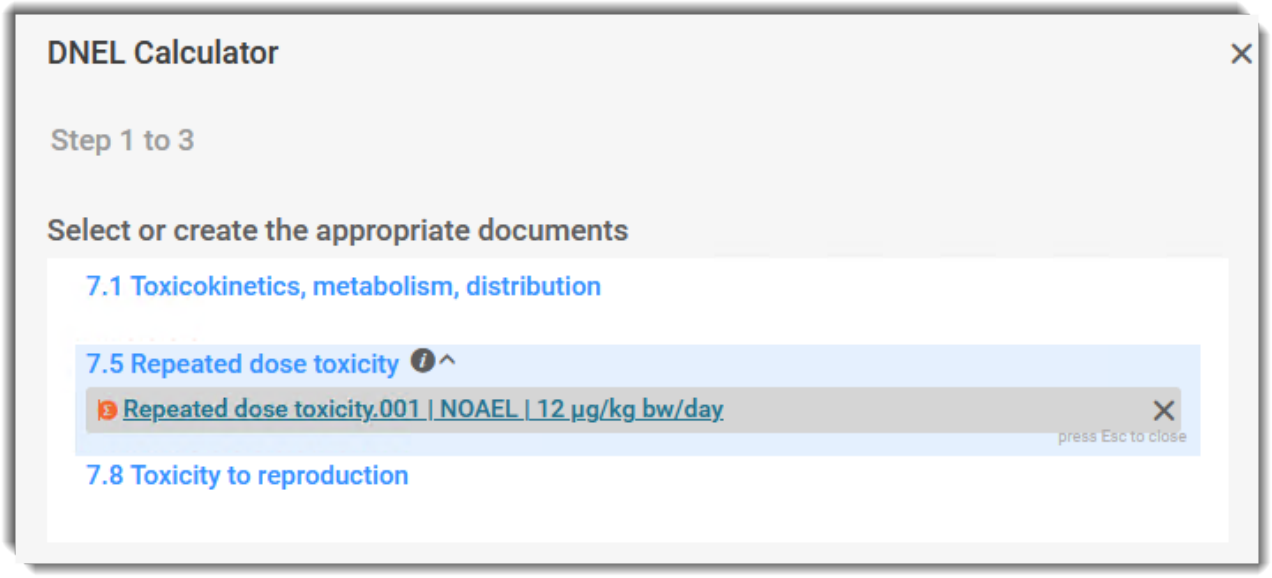
After clicking on the button labelled *+Select*, a window is shown in which you can select the needed endpoint study summary, as shown in the example.

Figure 240: Select an Endpoint study summary in section 1 of the DNEL calculator



Click on the endpoint summary in the Cross Reference window. This goes back to step 1 of the DNEL calculator, where the summary is shown in a grey box.

Figure 241: An endpoint study summary selected in step 1 of the DNEL calculator



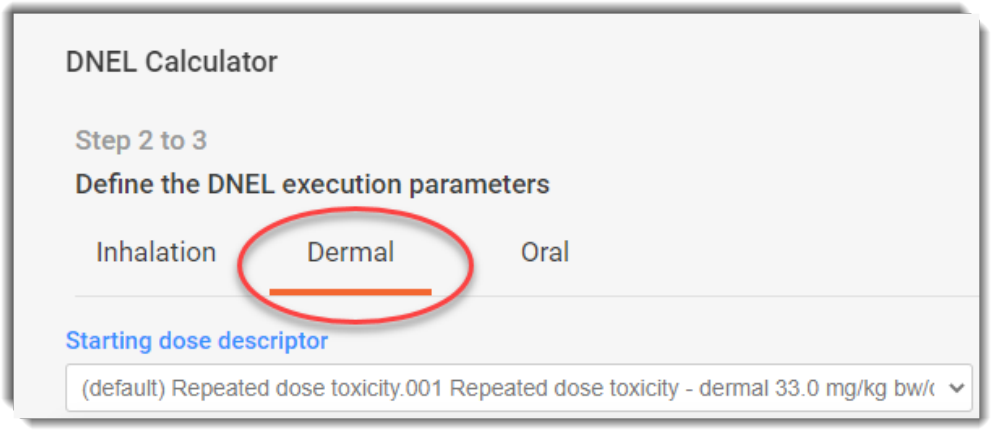
A selected endpoint summary can be deselected by clicking on the cross icon to its right.

The *Next* button is available only if enough information has been provided to proceed with the calculation of DNELs.

Note that to allow a proper calculation of the DNELs, the assessor has the responsibility to select all relevant information available in the dataset.

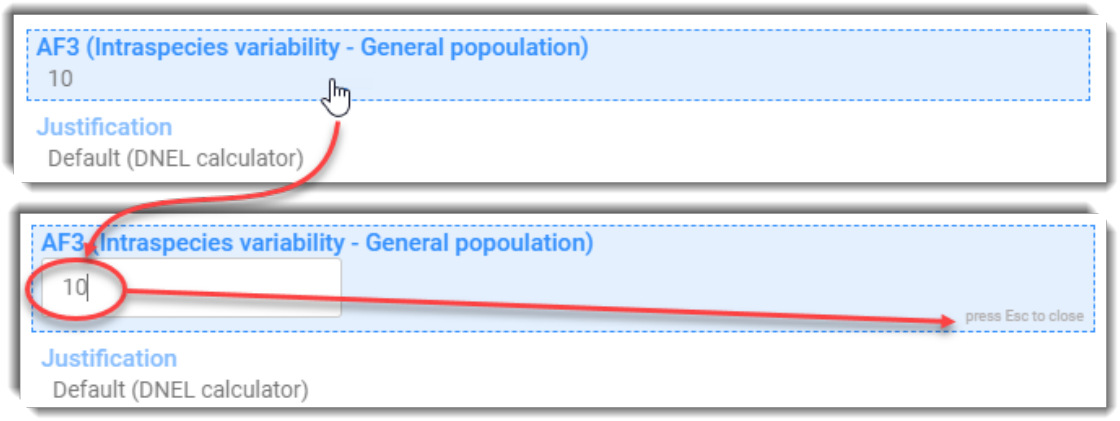
In steps 2 and 3, the data for different routes of exposure are grouped under tabs which are accessed by clicking on the tab. A selected tab is indicated by an orange bar under its title, as shown below in the example for *Dermal*. On moving between tabs, changes to data are remembered.

Figure 242: Tab for the exposure route Dermal in the DNEL calculator



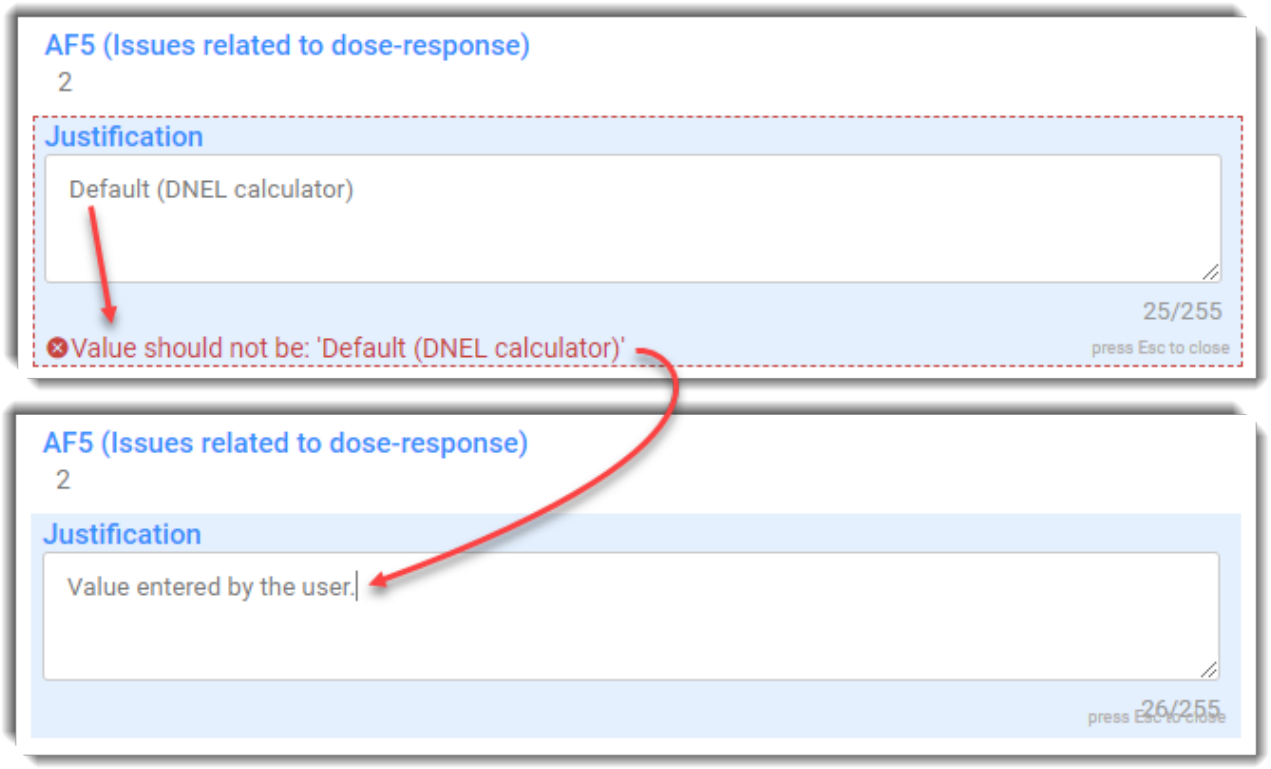
In these tabs, it is possible to verify the values for the starting dose descriptors and assessment factors that will be used in the calculations of DNELs. Where a numerical value can be entered into a field, hovering the cursor over the field causes a blue box to appear. To open the field for editing, click in the box. To close the box and keep the value, press the *Escape* key on the keyboard. This process is shown below.

Figure 243: Entering a data value in to the DNEL calculator



If it is necessary to change one or more of the default values, the change must be justified by the user. Such changes are described in section *25.3 Modifying defaults from the DNEL calculator*. Where this is the case, a warning is shown telling the user to enter a justification. The justification field is a free text field of up to 255 characters. To close the box and keep the text value, press the *Escape* key on the keyboard. An example is shown below.

Figure 244: Entering a justification in to the DNEL calculator.



Clicking on the button labelled *Back*, goes back to the previous step of the calculator, without saving any changes.

25.1.1. 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.

25.1.2. 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.

25.1.3. 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.

25.1.4. 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 linked to the DNEL calculator 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.

25.1.5. Step 1: selection of relevant dose descriptors

The DNEL calculator requires the assessor to link 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 and 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 NOAE(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 *25.1.6* and *25.1.8*, and selects the lowest DNEL.

25.1.6. 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.

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

25.1.7. 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. If a route1-to-route2 extrapolation is made, the following correction factor is

applied: Absorption(route1-animal)/Absorption(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

25.1.7.1. 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(human 70 kg, 8h) = 6.7 m3/person/8h

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(human 70 kg, 8h) = 6.7 / 70 kg = 0.0957 m3/kg bw/8h

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

sRV(rat, 8h) = sRV(human, 8h) x allometric scaling factor = 0.0957 x 4 = 0.38 m3/kg bw/8h

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

sRV(rat, 24h) = sRV(rat, 8h) x 24/8 = 1.35 m3/kg bw/24h 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

		DNEL inhalation		DNEL dermal		DNEL oral
Route for dose descriptor	Species	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

25.1.7.2. 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.

25.1.7.3. 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).

	DNEL inhalation		DNEL dermal		DNEL oral	
Route for dose descriptor	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.

25.1.8. Step 3: application of assessment factors

To derive a DNEL for human health variability, allowance is made for the uncertainties in experimental data. 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.

25.1.8.1. 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

25.1.8.2. 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.

25.1.8.3. 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..

25.1.8.4. 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.

25.1.8.5. 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.

25.1.8.6. 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.

25.1.9. 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 *25.1.6 Step 2: modification of relevant dose descriptors* and the assessment factors explained in section *25.1.8 Step 3: application of assessment factors*.

It is important to note that if more than one dose descriptor remains after applying the prioritisation criteria described in section *25.1.5 Step 1: selection of relevant dose descriptors* above, the DNEL calculator derives the corresponding DNELs will all the dose descriptors as starting point but will select only the lowest DNEL.

25.1.9.1. Worker-DNEL for inhalation route

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

DNEL = (dose descriptor* ABS * WORKER * EXPCOND)/(AF1 * AF2 * AF3 * AF4 * AF5 * AF6)

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

DNEL = (dose descriptor * (1/SRV) * ABS * WORKER * EXPCOND)/(AF1 * AF2 * AF3 * AF4 * AF5 * AF6)

25.1.9.2. General population-DNEL for inhalation route

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

DNEL = (dose descriptor * ABS * EXPCOND)/(AF1 * AF2 * AF3 * AF4 * AF5 * AF6)

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

DNEL = (dose descriptor * (1/SRV) * ABS * EXPCOND)/(AF1 * AF2 * AF3 * AF4 * AF5 * AF6)

25.1.9.3. Worker-DNEL for dermal route

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

DNEL = (dose descriptor * SRV * ABS * EXPCOND)/(AF1 * AF2 * AF3 * AF4 * AF5 * AF6)

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

DNEL = (dose descriptor * ABS * EXPCOND)/(AF1 * AF2 * AF3 * AF4 * AF5 * AF6)

25.1.9.4. General population-DNEL for dermal route

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

DNEL = (dose descriptor * SRV * ABS * EXPCOND)/(AF1 * AF2 * AF3 * AF4 * AF5 * AF6)

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

DNEL = (dose descriptor * ABS * EXPCOND)/(AF1 * AF2 * AF3 * AF4 * AF5 * AF6)

25.1.9.5. General population-DNEL for oral route

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

DNEL = (dose descriptor * SRV * ABS * EXPCOND)/(AF1 * AF2 * AF3 * AF4 * AF5 * AF6)

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

DNEL = (dose descriptor * ABS * EXPCOND)/(AF1 * AF2 * AF3 * AF4 * AF5 * AF6)

25.2. Output information

The output of the DNEL calculator is shown in step 3 of the DNEL calculator wizard.

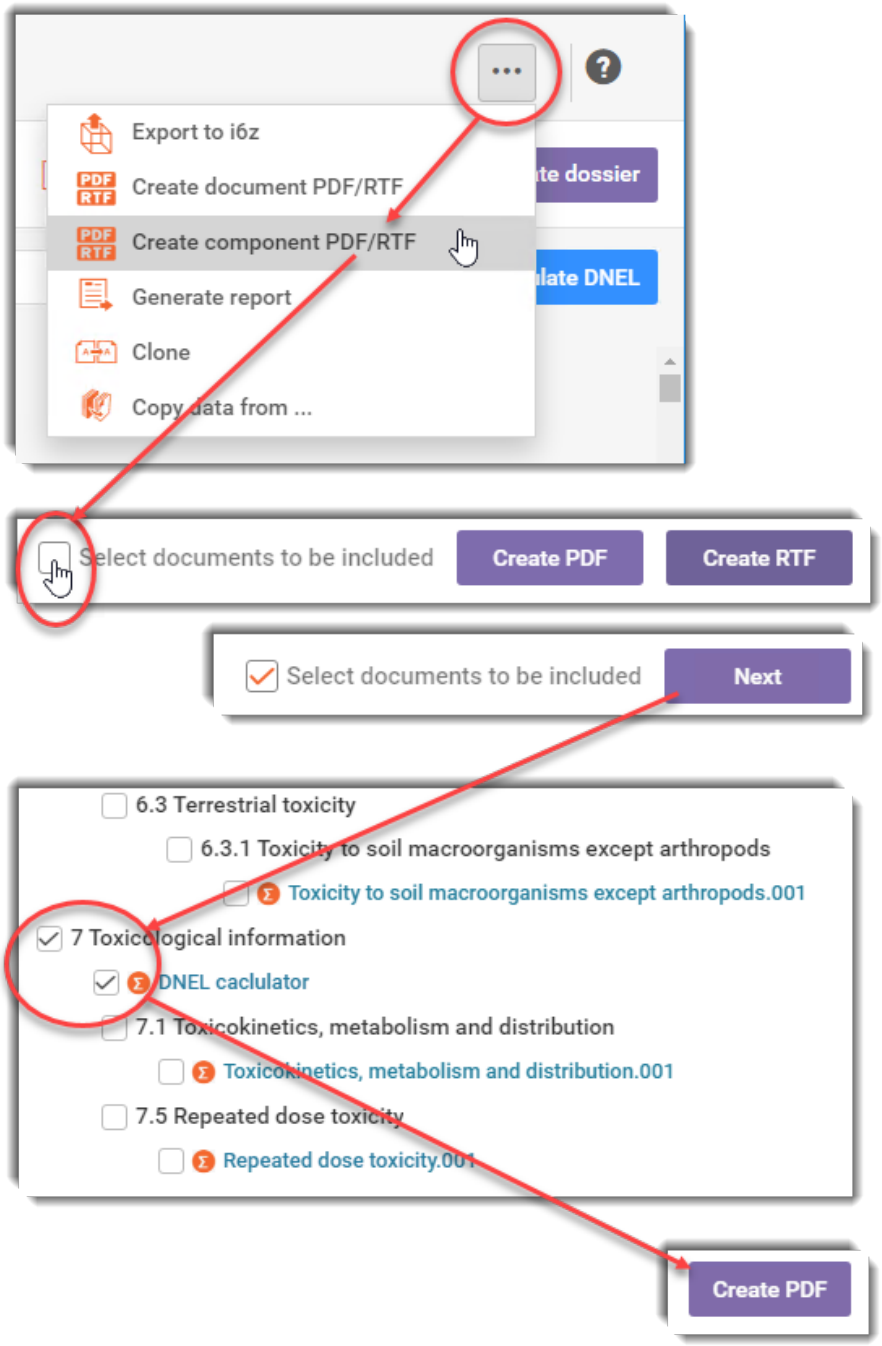
The button in step 3, *Apply DNEL calculations* closes the DNEL calculator, and the relevant data is then transferred automatically to the relevant fields in the summary of section 7 *toxicological information* from which the DNEL calculator was launched.

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.

Before navigating away from the summary in section 7 *toxicological information*, click *Save* to record the output of the DNEL calculator.

The data in the summary in section 7 *toxicological information*, can be printed using the standard method for documents. To print only the summary, from the document menu select, *Create component PDF/RTF*, *Select documents to be included*, and then select only the summary. The steps are shown below.

Figure 245: Print the endpoint summary that contains the output of the DNEL calculator



25.3. 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 by editing values in steps 2, and then re-doing the calculation by proceeding to step 3.

Fields are edited as described in section *25.1 Input data*:

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 the above section *25.1.5 Step 1: selection of relevant dose descriptors*. 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 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 the above section *25.1.7.3 Correction for differences between human and experimental exposure conditions (EXPCOND)*. If the experimental exposure conditions have been different from the default values, the assessor can modify this correction factor. 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. However, the assessor needs to provide a detailed justification explaining how the factors in Annex I, Section 1.4.1. of the REACH Regulation are taken into account.

To see the result of a modification, go to step 3 of the calculator.

25.4. Disclaimer

ECHA recommends the use of the optional DNEL calculator in IUCLID. Note that the registrants should link to the calculator all relevant endpoint summary(-ies) and that they remain responsible for the calculated DNELs.

26. 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 PNECoral used for the assessment of secondary poisoning.

The workflow followed by the PNEC calculator is the following:

1. The assessor selects the relevant endpoint summaries 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 summaries of section 6 enable the reporting of the hazard assessment conclusions for the environmental protection targets.
2. The PNEC calculator performs the following for deriving PNECs
    d. Handles 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.
    e. 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.
    f. 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 Koc is retrieved from the endpoint summary in IUCLID section 5.4.1.
    g. 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, as described in section *26.4 Modifying defaults from the PNEC calculator*.
5. The PNEC calculator reports the outcome of the calculations, and related explanations when relevant, in the IUCLID endpoint summary section 6.

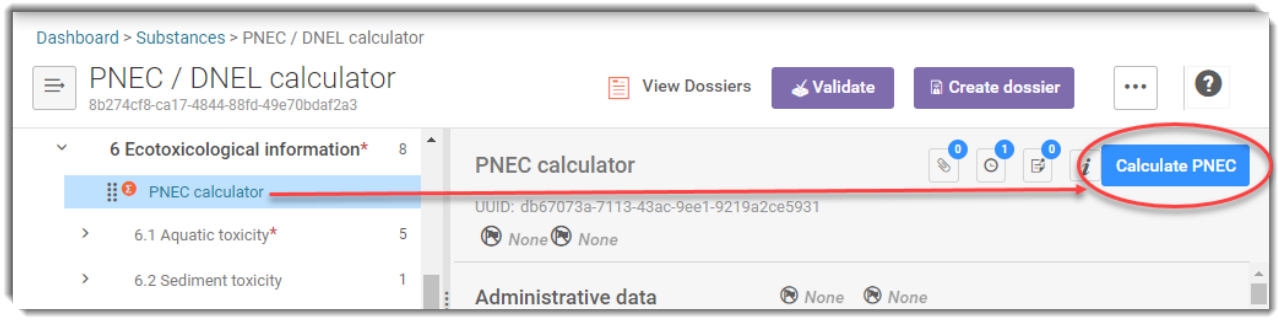
26.1. Input data

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.

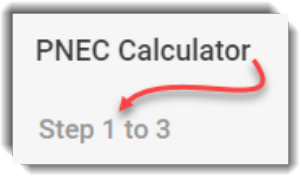
To launch the PNEC calculator, navigate to the endpoint summary *6 Ecotoxicological information*, and then click on the button at the right of the interface, as shown in the example below.

Figure 246: Open the PNEC calculator



The PNEC calculator has three steps. The current step is indicated as shown below:

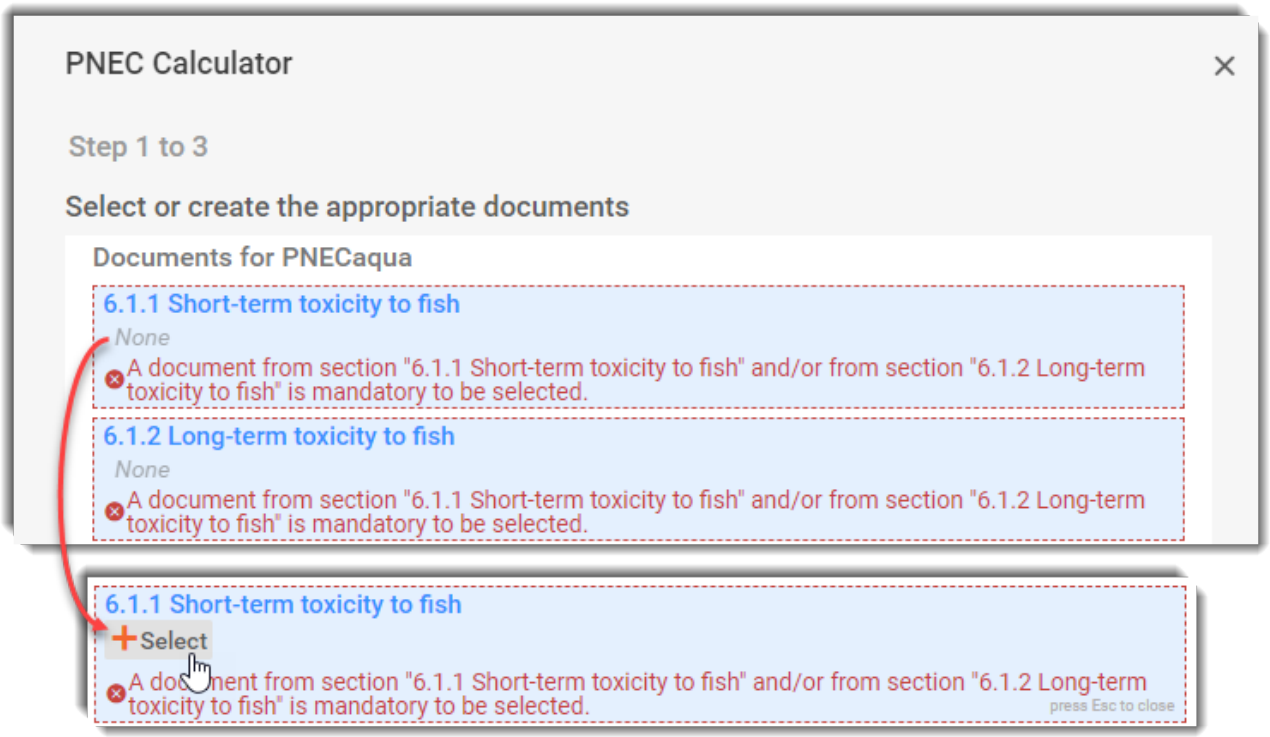
Figure 247: Steps in the PNEC calculator wizard



Guidance on entering data into the different steps of the calculator is provided in later sections.

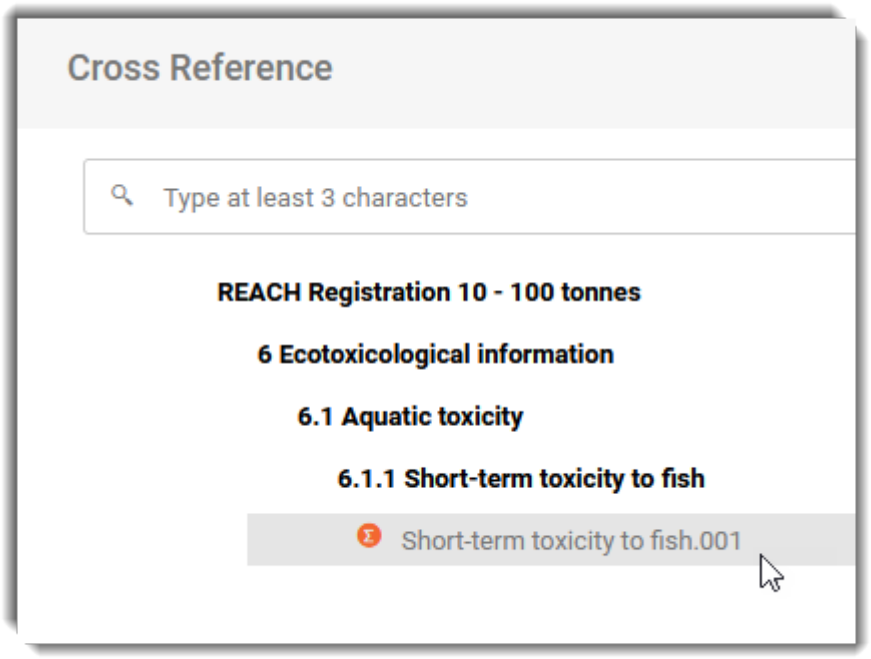
In the first step, the assessor needs to link the relevant endpoint study summaries to be used by the PNEC calculator. To select a summary, click on the endpoint. Where a summary is mandatory and nothing is selected, a warning message is shown. An example is shown below.

Figure 248: Selecting summaries in step 1 of the PNEC calculator



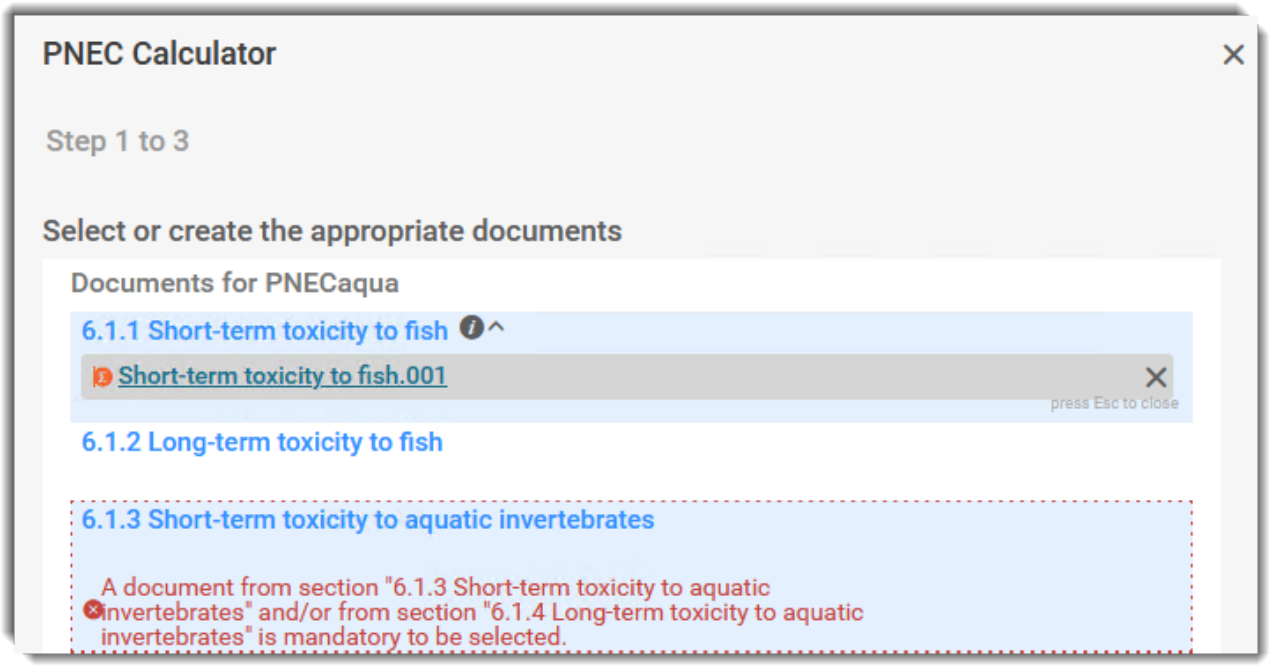
After clicking on the button labelled *+Select*, a window is shown in which you can select the relevant endpoint summary.

Figure 249: Select an Endpoint study summary in section 1 of the PNEC calculator



When clicking on the endpoint summary, the selection window closes and the PNEC calculator goes back to step 1 of the PNEC calculator, where the summary is indicated in a grey box, as shown in the example below.

Figure 250: An endpoint study summary selected in step 1 of the PNEC calculator



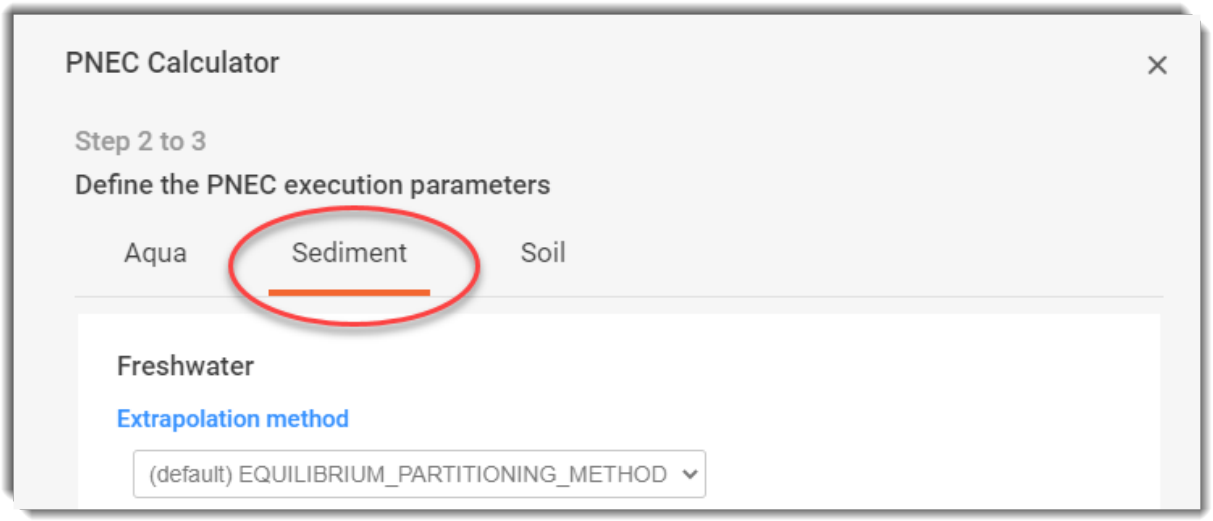
A selected endpoint summary can be deselected by clicking on the cross icon to its right.

The *Next* button is available only if enough information has been provided to proceed with the calculation of the PNECs.

Note that to allow a proper calculation of the PNECs, the assessor has the responsibility to select all relevant information available in the dataset.

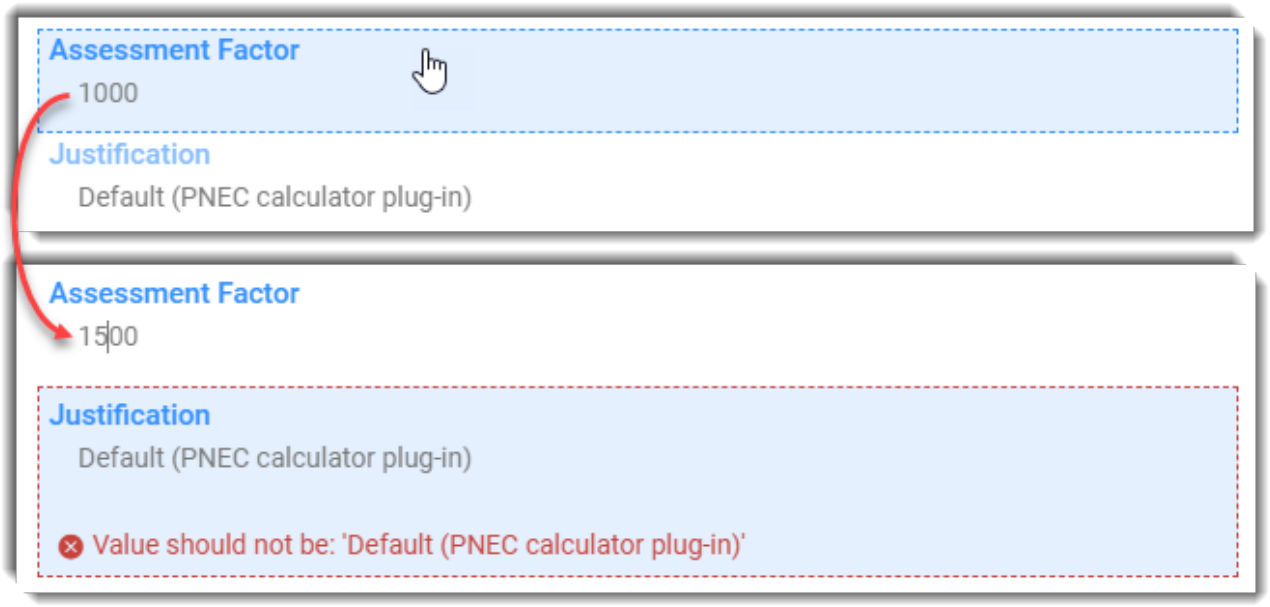
In steps 2 and 3, the data for different compartments are grouped under tabs which are accessed by clicking on the tab. A selected tab is indicated by an orange bar under its title, as shown below in the example for *Sediment*. On moving between tabs, changes to data are remembered.

Figure 251: Tab for the exposure route Dermal in the PNEC calculator



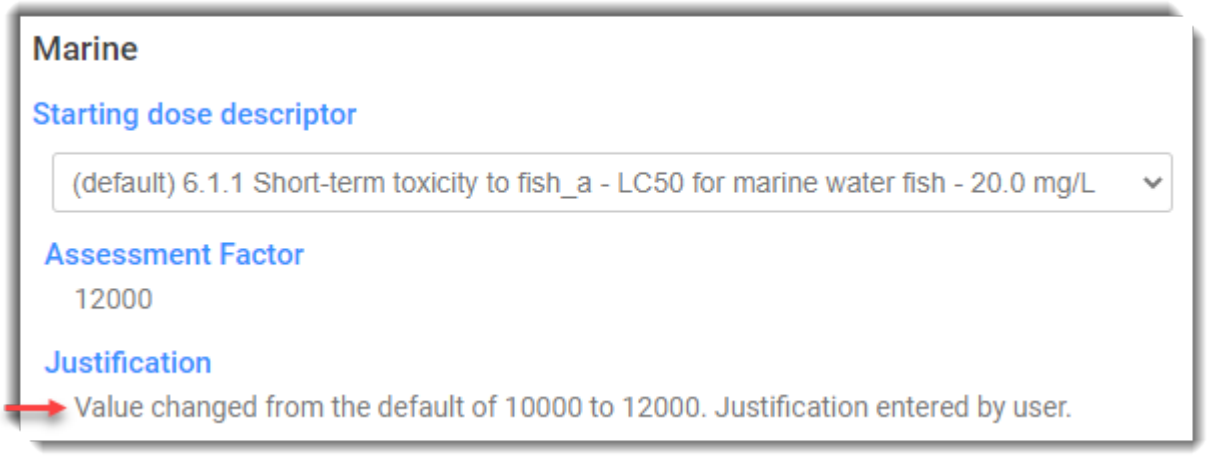
In these tabs, it is possible to verify the values for the starting dose descriptors and assessment factors that will be used in the calculations of PNECs. Where a numerical value can be entered into a field, hovering the cursor over the field causes a blue box to appear. To open the field for editing, click in the box.

Figure 252: Entering a data value in to the PNEC calculator



If a value of a field is changed from the default, the change must be justified by the user. Such changes are described in section *26.4 Modifying defaults from the PNEC calculator*. A warning is shown telling the user to enter a justification. The justification field is a free text field of up to 255 characters. To close the box and keep the value, click outside the field. An example is shown below.

Figure 253: Entering a justification in to the PNEC calculator.



Clicking on the button labelled *Back*, goes back to the previous step of the calculator, without saving any changes.

26.1.1. 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^logKoc

26.1.2. 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.

26.1.3. 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.

26.1.4. 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.

26.2. How the calculations are made

26.2.1. 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, as described in section *26.4 Modifying defaults from the PNEC calculator*.

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:

   PNECaqua,freshwater = Lowest “EC50/LC50” / 1000

PNECaqua,marine = 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

      PNECaqua,freshwater = Effect concentration / AF for freshwater
      PNECaqua,marine = Effect concentration / 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	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

      PNECaqua,freshwater = Effect concentration / AF for freshwater
      PNECaqua,marine = Effect concentration / 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	Lowest of "EC50/LC50" and "EC10, LC10 or NOEC"	100	1000

and no "EC10, LC10 or NOEC" available for the species having the lowest "EC50/LC50"			
“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 having the lowest "EC50/LC50"	Lowest "EC10, LC10 or NOEC"	50	500
“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.

26.2.2. 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.

26.2.3. 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 from IUCLID section 5.4.1 (and linked to the calculator) 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, as described in section *26.4 Modifying defaults from the PNEC calculator*.

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, as described in section *26.4 Modifying defaults from the PNEC calculator*.

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:

PNECsediment,freshwater = PNECaqua,freshwater * (3.6 + 0.1*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:

PNECsediment,marine = PNECaqua,marine * (3.6 + 0.1*Koc)

26.2.4. 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 from IUCLID section 5.4.1 is available and the PNECaqua,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, as described in section *26.4 Modifying defaults from the PNEC calculator*.

If there is no experimental data, the PNECsoil is calculated with EPM:

PNECsoil = PNECaqua,freshwater * (0.133 + 0.02*Koc)

If there is only one effect concentration available the PNECsoil 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, PNECsoil 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", PNECsoil 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", PNECsoil 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.

26.3. Output information

The output of the PNEC calculator is shown in step 3.

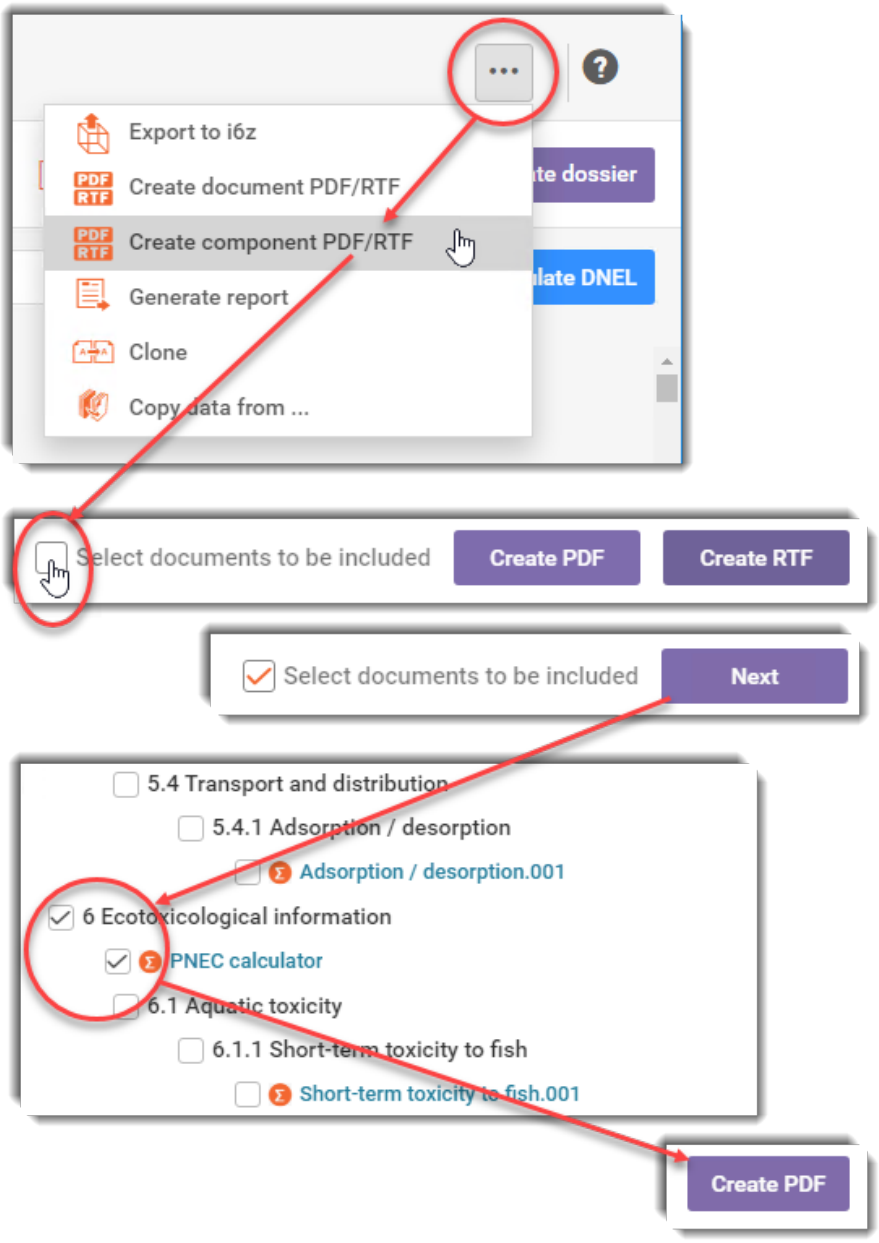
The button in step 3, *Apply PNEC calculations* closes the PNEC calculator, and the relevant data is transferred automatically to the relevant fields in the summary of section 6 *Ecotoxicological information* from which the PNEC calculator was launched.

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.

Before navigating away from the summary in section *6 Ecotoxicological information*, click *Save* to record the output of the PNEC calculator.

The data in the summary in section *6 Ecotoxicological information*, can be printed using the standard method for documents. To print only the summary, from the document menu select, *Create component PDF/RTF*, *Select documents to be included*, and then select only the summary. The steps are shown below.

Figure 254: Print the endpoint summary that contains the output of the PNEC calculator



26.4. Modifying defaults from the PNEC calculator

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. This is done by editing values in steps 2, and then re-doing the calculation by proceeding to step 3.

Fields are edited as described in section *26.4 Modifying defaults from the PNEC calculator*:

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 also needs to provide the relevant assessment factor for the calculation, and a detailed justification explaining why the new starting effect concentration is 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. However, in that case, the assessor needs to provide a detailed justification explaining why the new assessment factor is 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 an 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, for example 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 more relevant. In addition, if the new extrapolation method is "assessment factor" the assessor will be required as well to select an effect concentration from the picklist containing all relevant effect concentrations and an assessment factor.

To see the result of a modification, go to step 3 of the calculator.

26.5. Disclaimer

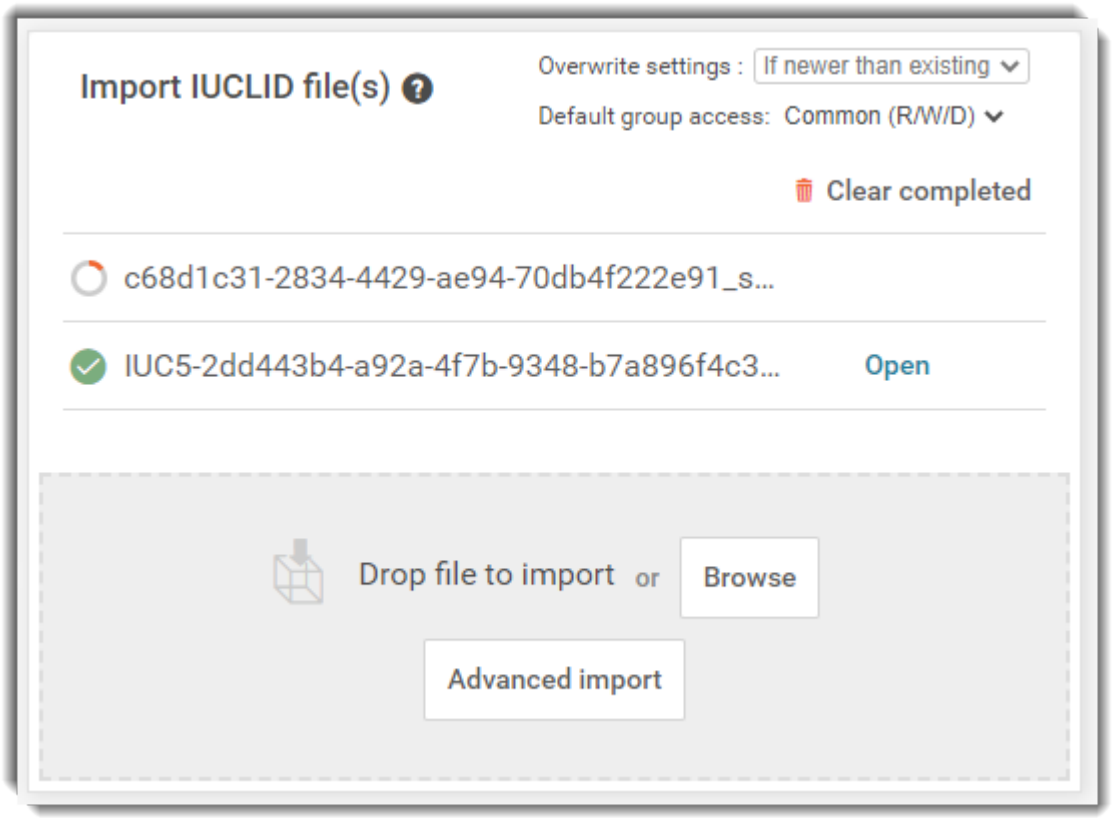
ECHA recommends the use of the optional PNEC calculator in IUCLID. Note that the registrants should link to the calculator all relevant endpoint summary(-ies) and that they remain responsible for the calculated PNECs.

27. Shutting down IUCLID

Before shutting down the IUCLID application, ensure that all processes have been completed.

For example, if data is being imported, the circular icon for the job still has some grey showing ( ). The import will be cancelled if IUCLID is shut down before the green tick icon appears.

Figure 255: Data is being imported

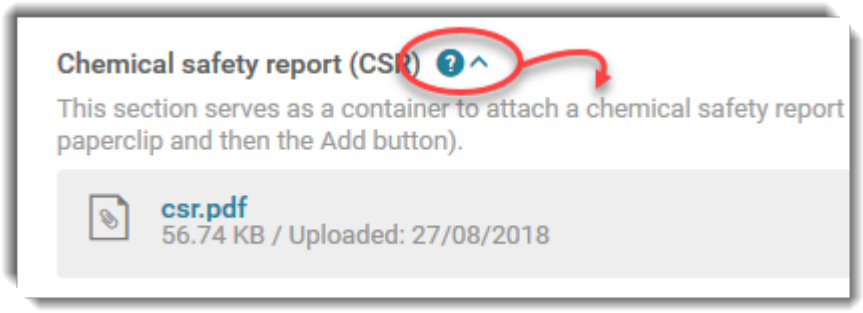


To shut down the IUCLID 6 Desktop application, close the window that opened when the application started.

28. Getting help

Field specific help inside the records of an entity is accessed from the question mark and arrowhead icons to the right of the field header, as shown in the example below:

Figure 256: Field specific help



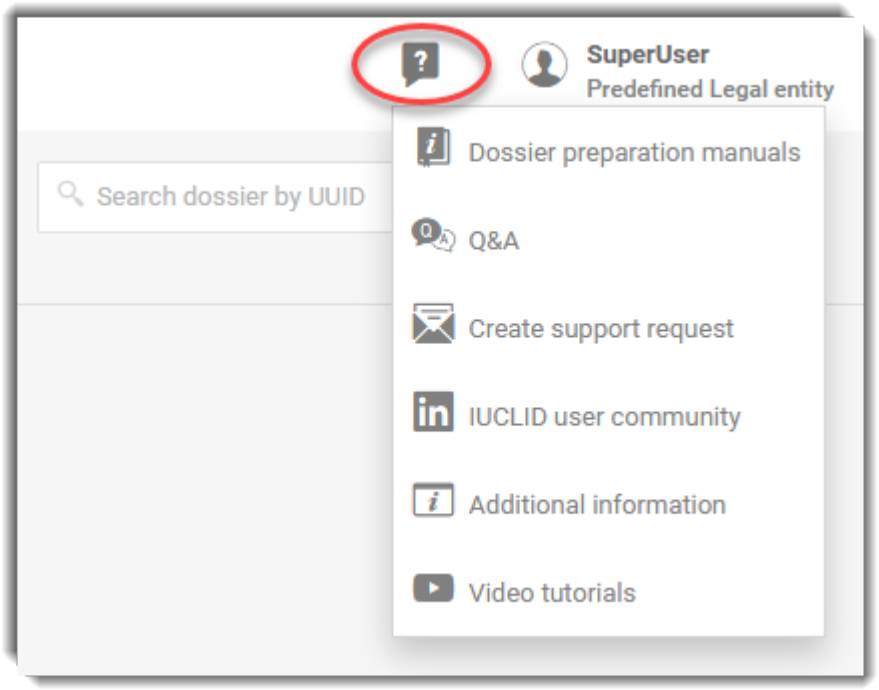
This manual is accessed from a large question mark icon at the upper right of the interface, as shown in (1) below. Also, there are various pop-up texts under smaller question marks, shown below in (2).

Figure 257: Function specific help

The dialogue icon with the question mark in the top bar of the interface contains links to external sources of help. An example of the links is shown below.

Create support request is a link to the European Chemicals Agency.

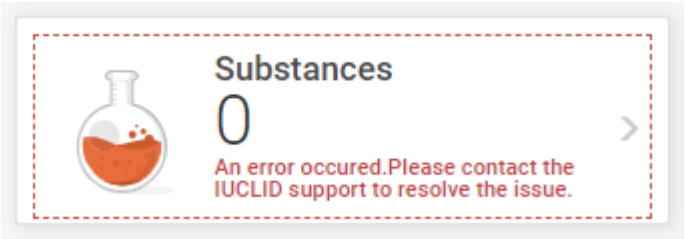
Figure 258: External sources of help



28.1. Error message on the dashboard

If the user interface of IUCLID cannot connect to IUCLID, the following message may be displayed, "An error occurred. Please contact the IUCLID support to resolve the issue". An example is given below:

Figure 259: An error occurred



The lack of connection may be temporary, for example when IUCLID has recently been started but is not yet available. If you see this message, first wait a few minutes, then try refreshing the browser. For IUCLID 6 Server, you may have to log back in again. For some browsers, the page can be forcibly reloaded using CTRL F5. If the problem persists, contact your local system administrator.

29. Glossary

2D structure	2-dimensional structure formula of a chemical molecule
ATP	Adaptation to Technical Progress
BMC	Benchmark Concentration
BMD	Benchmark Dose
BPD	Biocidal Products Directive (98/8/EC)
BPR	EU Biocidal Products Regulation (528/2012/EC)
C&L	Classification & Labelling
CA	Competent Authority
CAS	Chemical Abstracts Service
CBI	Confidential Business Information
CCOHS	Canadian Centre for Occupational Health and Safety
CEFIC	Conseil Européen de l'Industrie Chimique / European Chemical Industry Council
CMR	Substances which present at least one of the following properties: Carcinogen, Mutagen, Reprotoxic (Toxic to reproduction)
CSA	Chemical Safety Assessment
CSF	R-Phrases Chemicals Stakeholder Forum - risk phrases
CSR	Chemical Safety Report
DMEL	Derived Minimal Effect Level
DNEL	Derived No-Effect Level
DU	Downstream User
EC	European Commission
EC number	European Chemical number: EINECS, ELINCS or NLP
ECB	European Chemicals Bureau
ECHA	European Chemicals Agency
EFSA	European Food Safety Authority
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
EPA	Environment Protection Agency (United States)
EU	European Union
GHS	Globally Harmonised System for classification and labelling of chemicals
GLP	Good Laboratory Practice

HPV	High Production Volume
HPVC	High Production Volume Chemicals
HTML	HyperText Markup Language
i5z	The file format of IUCLID 5
i6z	The file format of IUCLID 6
ICCA	International Council of Chemical Associations
IFCS	Intergovernmental Forum on Chemical Safety
IP	Intellectual Property
IRPTC	International Register of Potentially Toxic Chemicals
ISO	International Standards Organisation
IUCLID	International Uniform ChemicaL Information Database
IUPAC	International Union of Pure and Applied Chemistry
JRC	Joint Research Centre
LOAEL	Lowest Observed Adverse Effect Level
LOEL	Lowest Observed Effect Level
MS	Member State
MSCA	Member State Competent Authority
NCD	New Chemicals Database
NLP	No-Longer Polymer
NOAEL	No Observed Adverse Effect Level
NOEL	No Observed Effect Level
OECD	Organisation for Economic Cooperation and Development
OECD TG	OECD Test Guidelines
OSOR	One Substance One Registration
PBT	Substances which are Persistent, Bioaccumulative and Toxic
PIC	Prior Informed Consent (The Rotterdam Convention on Prior Informed Consent sets up a system to control international trade in certain hazardous substances)
PNEC	Predicted No-Effect Concentration
POP	Persistent Organic Pollutant
PPORD	Product and Process Orientated Research and Development
PPP	Plant Protection Product
QSAR	Quantitative Structure Activity Relationship
RA	Risk Assessment

RAR	Risk Assessment Report
REACH	Registration, Evaluation and Authorisation of CHemicals
RIP	REACH Implementation Project
SAR	Structure Activity Relationship
SDS	Safety Data Sheet
SIDS	Screening Information Data Set (OECD Existing Chemicals Programme)
SIEF	Substance Information Exchange Forum
SME	Small and Medium Sized Enterprises
SVHC	Substance of Very High Concern
TGD	Technical Guidance Document
TNsG	Technical Notes for Guidance
TSCA	Toxic Substance Control Act Inventory in the USA
UI	User interface
US-EPA	United States Environment Protection Agency
UUID	Universal Unique IDentifier
vPvB	Very Persistent Very Bio-accumulative substance
WTO	World Trade Organisation
XML	eXtensible Markup Language
XSD	XML Schema Definition