

# Functionalities of IUCLID in the web interface

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## European Chemicals Agency

Mailing address: P.O. Box 400, FI-00121 Helsinki, Finland

Visiting address: Telakkakatu 6, FI-00150 Helsinki, Finland

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## 1. The IUCLID web interface and the IUCLID client

The IUCLID 6.6 application comes with an interface that is displayed in a web browser. The old interface is not delivered with the current version of IUCLID.

In the next section, there are some notes to help users who are familiar with the older client interface, to move over to using the web interface.

## 2. Help for users familiar with the IUCLID client

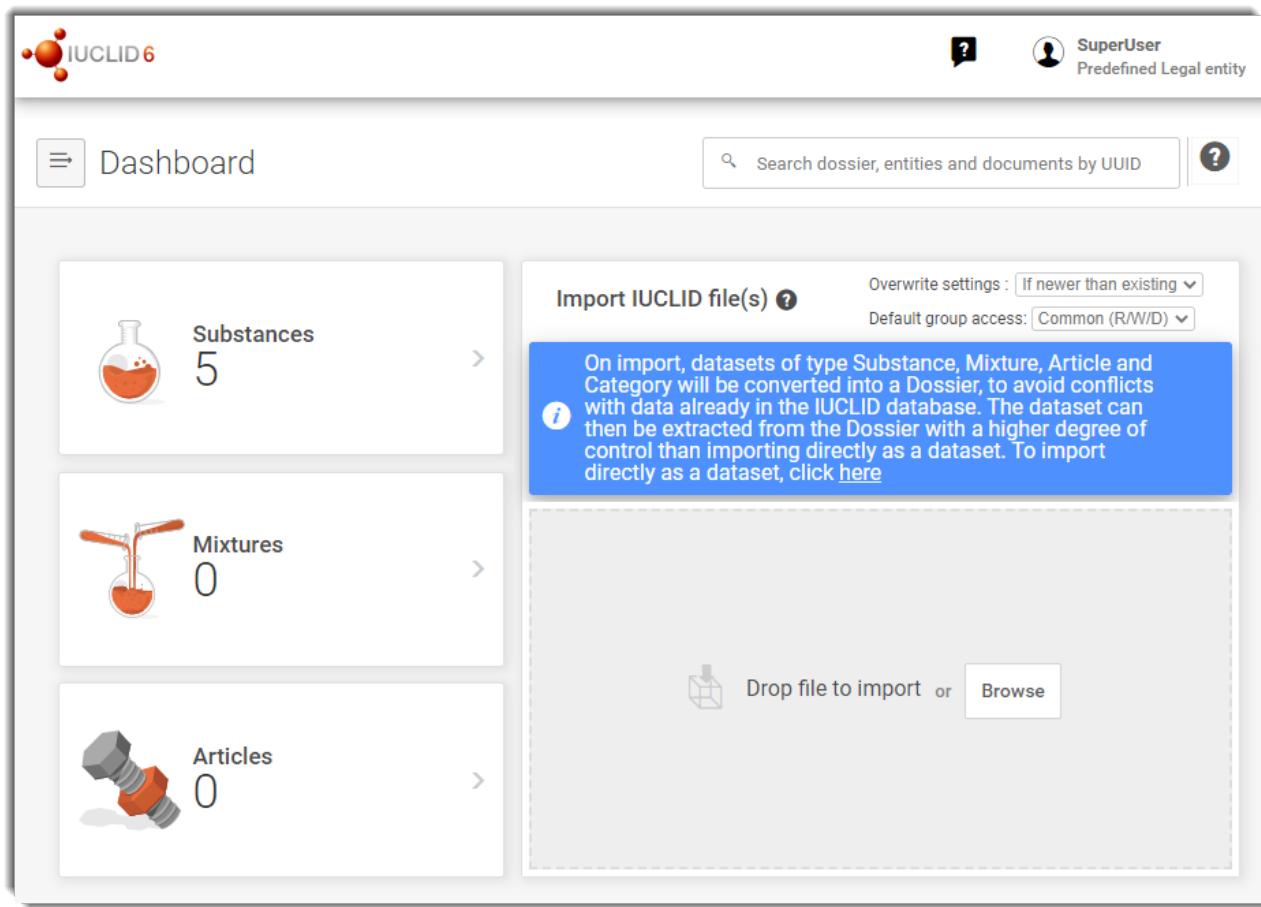
If you have not used the older type of IUCLID interface, referred to as the client, or the *classic* interface, go straight to section 3 *Overview of the web interface*.

The purpose of this chapter is to help users who are already familiar with the client, to learn how to use the web interface. If you know the client well, reading through all this chapter will save you time compared to clicking around in the web interface unaided.

### 2.1. Overview of the Home page / Dashboard

In the client, the home page is the page displayed when the interface is started, or a user logs in. A user can return to the home page from anywhere in the interface by clicking on the house icon.

The equivalent to that in the web interface is the *Dashboard*. A user can return to the *Dashboard* from anywhere in the interface by clicking on the IUCLID 6 icon at the top left of the interface. An example of the web interface with the *Dashboard* displayed is shown below.

**Figure 1:** Dashboard

Only the most used functionalities are presented on the *Dashboard*. The functionalities retained from the home page of the client are: *Substance*, *Mixture/Product*, *Search by UUID*, *Help*, and *Import*. All types of entity have a list page from where they can be created or edited. In addition, they can be edited and created from the point in an entity or dataset that refers to them.

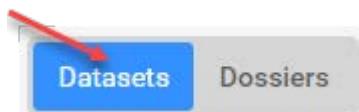
There is a new type of entity named *Article*.

*Import* allows IUCLID files to be dragged and dropped into an import area. *Advanced import* allows individual entities and documents to be excluded from the import. The exclusion does not work with *Dossiers* because they are read-only, and their integrity must be maintained.

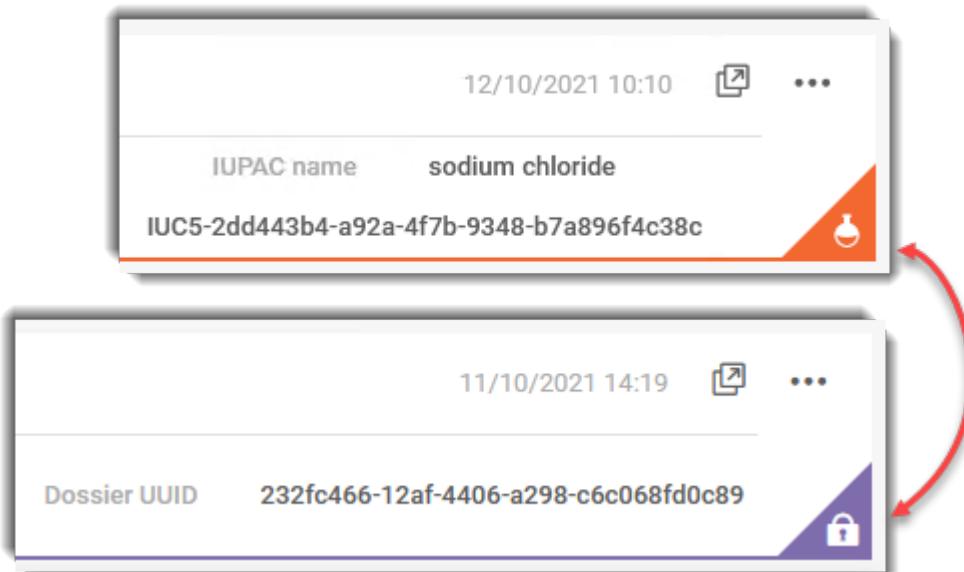
Search by UUID is available, limited to Dossiers and entities.

## 2.2. The listings for Substance and Mixture/Product

The icons for *Substance* and *Mixture/Product* lead to lists of entities, just as they do from the homepage of the client. However, and importantly, there is no longer an icon for *Dossier*, because access to *Dossiers* has been 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 2:** 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 3:** 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 4:** View the Dossiers for a Substance

The screenshot shows the IUCLID web interface. At the top, there's a header with buttons for 'View Dossiers', 'Validate', 'Create dossier', and other navigation options. Below the header, a substance is identified by its UUID: IUC5-2dd443b4-a92a-4f7b-9348-b7a896f4c38c. A red arrow points from the 'Substance name\*' field ('table\_salt') in the main header to the 'Dossier versions' button in the modal.

**Dossier versions**

TS Dossier 3 10-100 tpa		Date	Actions			
Subject name	table_salt / 231-598-3 / sodium chloride / 7647-14-5	Submission type	REACH Registration 10 - 100 tonnes	Dossier UUID	7117ae59-262f-4a52-b012-2eee071e1964	

TS Dossier 2 10-100 tpa		Date	Actions			
Subject name	table_salt / 231-598-3 / sodium chloride / 7647-14-5	Submission type	REACH Registration 10 - 100 tonnes	Dossier UUID	ac71bc63-22c0-4978-b126-f6e394454f04	

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

**Figure 5:** View the Substance dataset for a Dossier

The screenshot shows the 'View Dossiers' page. At the top, there are buttons for 'View Dossiers', 'Go to source' (with a circled arrow icon), 'Validate', and other actions. Below these are buttons for 'Hide empty fields' and navigation. The 'Go to source' button is highlighted with a red circle.

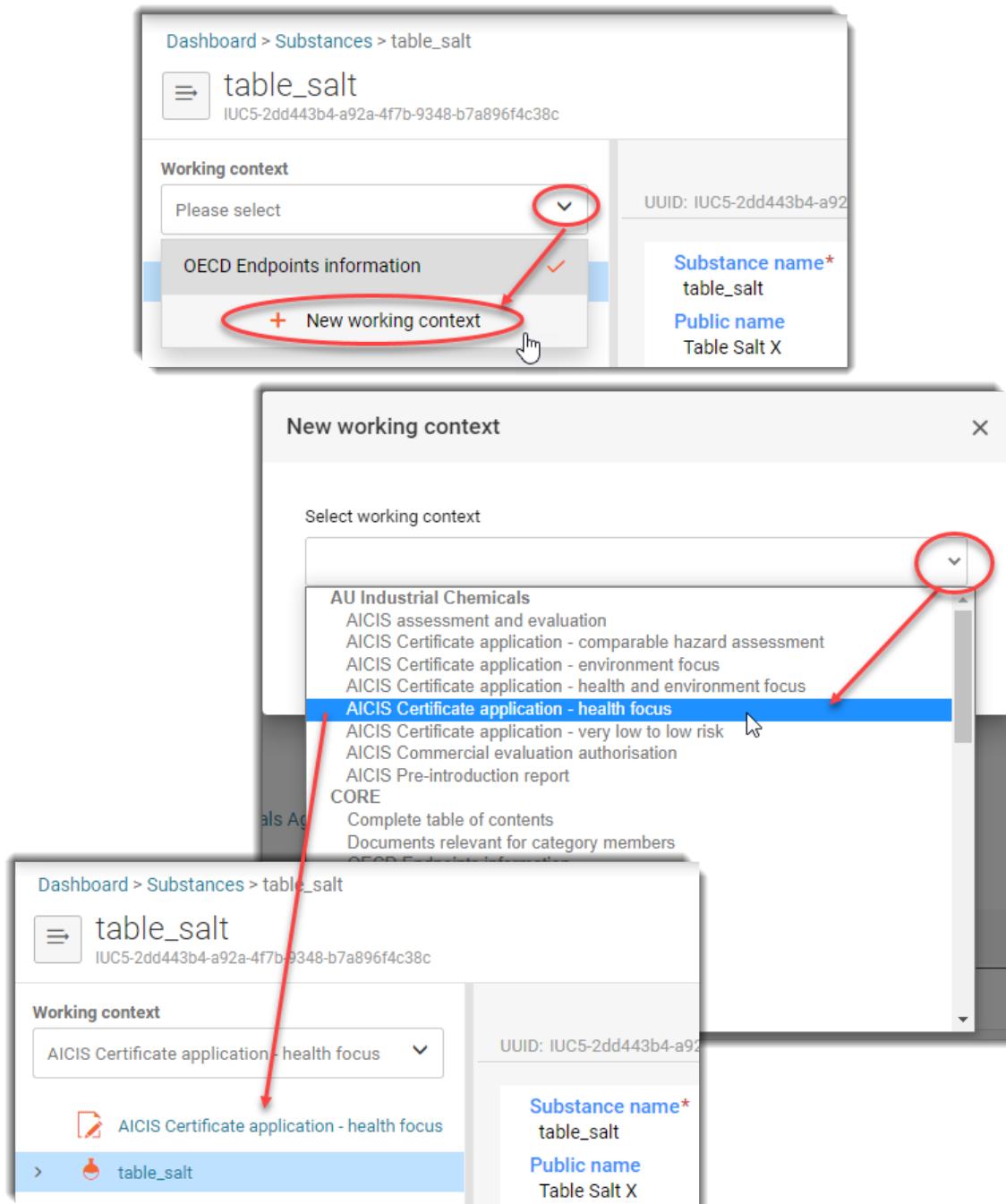
If *Go to source* is not visible, the source *Substance* or *Mixture/Product* dataset is not in the IUCLID database.

List pages grouped by type of entity are accessible via the *Main menu*, which is opened from the menu icon ( ) situated towards the upper left of the interface.

## 2.3. Dossier header

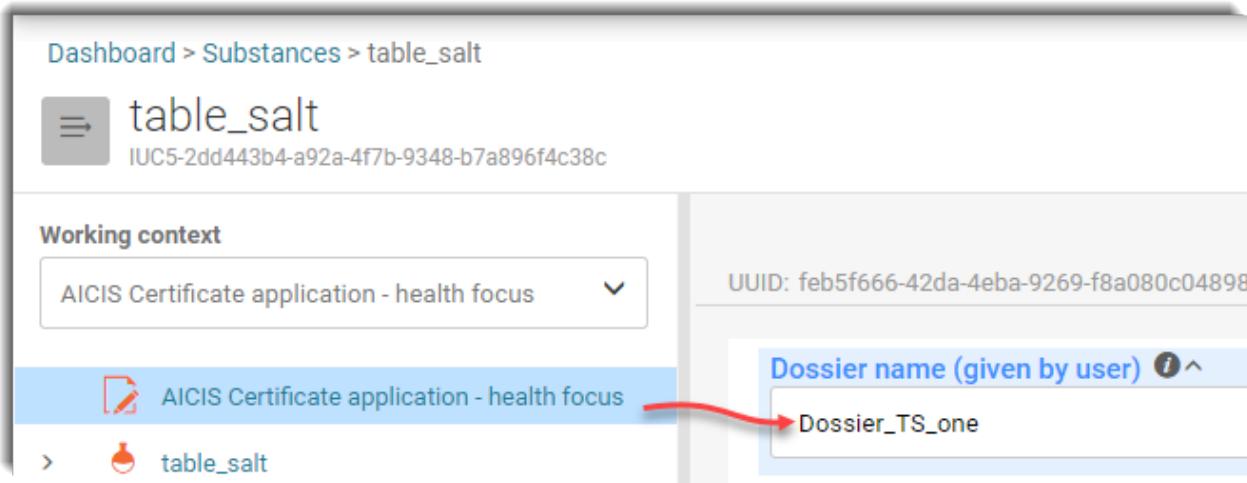
In the client, data is entered into a *Dossier* header only during the creation of a *Dossier*. In the web interface, each *Substance* or *Mixture/Product* dataset has a *Dossier* header associated with it which can be edited at any time. On *Dossier* creation it is written into a *Dossier*. Before a header is written into a dossier it is said to be in draft form. However, it can be accessed only after selecting a *working context* because this defines its format. *Working context* is a new concept that has been introduced in to IUCLID 6.5. It is effectively a new name for *Submission type*. An example of selecting a working context is given below in which the working context is changed from *OECD Endpoints information* to *AICIS Certificate application - health focus*.

Figure 6: Selecting a working context, formerly known as Submission type



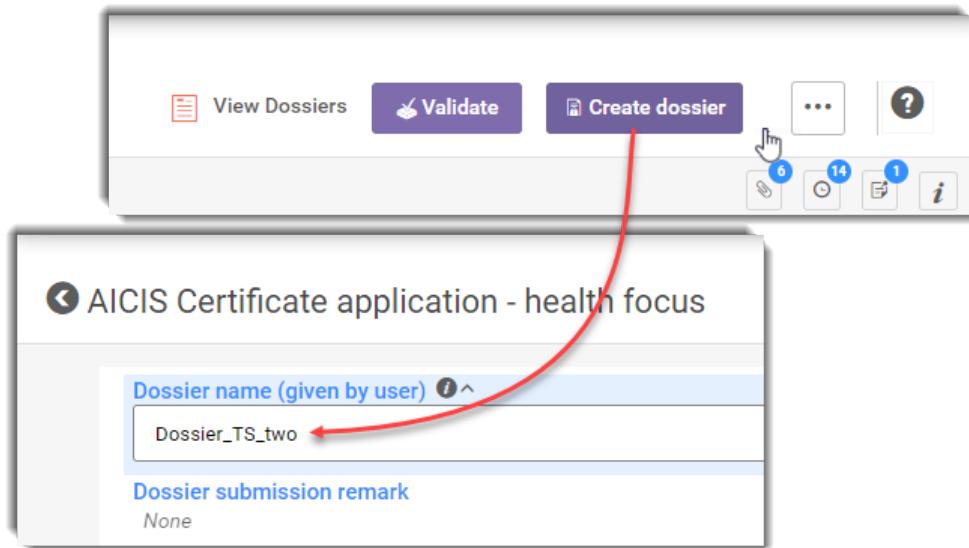
The *Dossier* header is accessed independently of *Dossier* creation via a link at the top of the table of contents on the left of the interface, as shown in the figure below.

**Figure 7: Editing the Draft dossier header before Dossier creation**



When a *Dossier* is created, the first step is to review and/or edit the *Dossier* header, as shown in the figure below.

**Figure 8: Editing the Dossier header at the start of Dossier creation**



## 2.4. Navigation, Information, and Data Panels

The panels *Navigation*, *Information*, and *Data* that are shown in the client have been replaced by a single central layout, in which data is presented in context. Where to find the new locations of functionalities is described below, per panel.

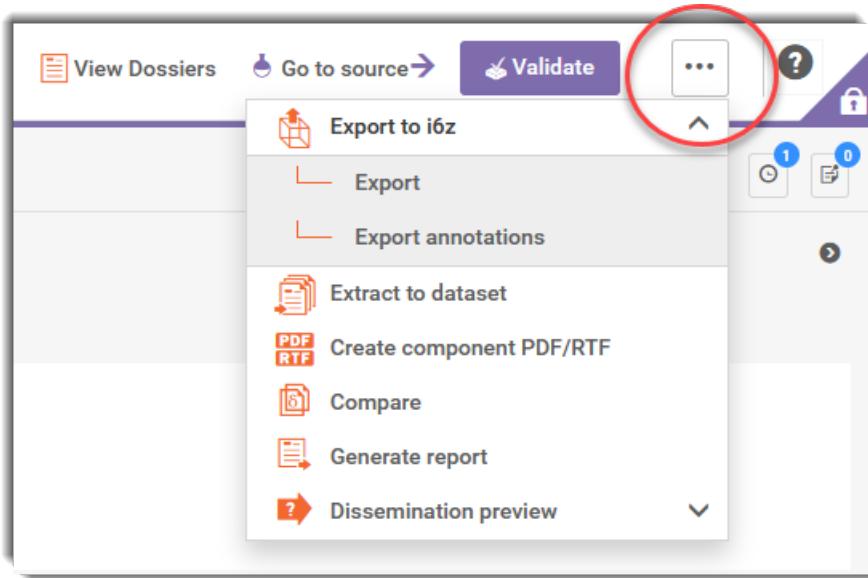
## 2.4.1. Navigation panel

A list of all the entities of a particular type is opened in the same way as in the client, that is, by clicking on the icon for that entity, either in the *Dashboard* or the main menu. The main difference is that the list of entities is shown centrally in the interface, rather than in a separate *Navigation* panel.

### 2.4.1.1. Right-click in the list of entities

In the client, there are various functionalities that are accessible per entity by right-clicking on the record of the entity in the list shown in the *Navigation* panel. Examples include *Export* and *Compare*. In the web interface these functionalities are accessed by first opening the record of the entity, and then selecting the functionality from the menu under the three-dot icon in the application bar. An example of the menu for *Dossier* is shown below.

Figure 9: Functionalities that can be applied to a specific Dossier



### 2.4.1.2. Search for entity

In the web interface, each list page of entities has its own simple search feature. In addition, more advanced searches are available for all types of entity. For more details, see section 3.10 *Search in a list of entities*.

### 2.4.1.3. Table of contents (TOC) and creating/deleting documents

The *Table of contents* (TOC) for a *Substance* or *Mixture/Product* is used to access documents and to manage them. Data values are edited in the data window on the right of the interface. A summary of the features is given below.

**Figure 10:** Navigating at the TOC at the section level, and managing documents via the data window

The screenshot illustrates the IUCLID web interface for managing substance datasets. On the left, the Table of Contents (TOC) lists various sections and their sub-documents. On the right, a detailed view of a selected document is shown, including its administrative data and study information.

**Left Panel (Table of Contents):**

- Dashboard > Substances > table\_salt
- IUC5-2dd443b4-a92a-4f7b-9348-b7a896f4c38c
- 1** 7 Toxicological information\*
- 7.1 Toxicokinetics, metabolism and distribution\* **2** 10
  - 3** 7.1.1 Basic toxicokinetics\*
    - Basic toxicokinetics.001
    - 4** Basic toxicokinetics\_123
    - Basic toxicokinetics\_abc
    - Data\_re-used\_using\_a\_template\_1
    - Data\_in\_template\_2
  - 7.1.2 Dermal absorption
- 7.2 Acute Toxicity\* 3

**Right Panel (Document Details):**

**Basic toxicokinetics\_123**  
UUID: cb61013c-4d61-4bb0-a2d4-df3fa0ea1bc5  
None None

**Administrative data**  
Endpoint: basic toxicokinetics in vitro / ex vivo  
Type of information: None  
Adequacy of study: key study

**Legend for Figure 10:**

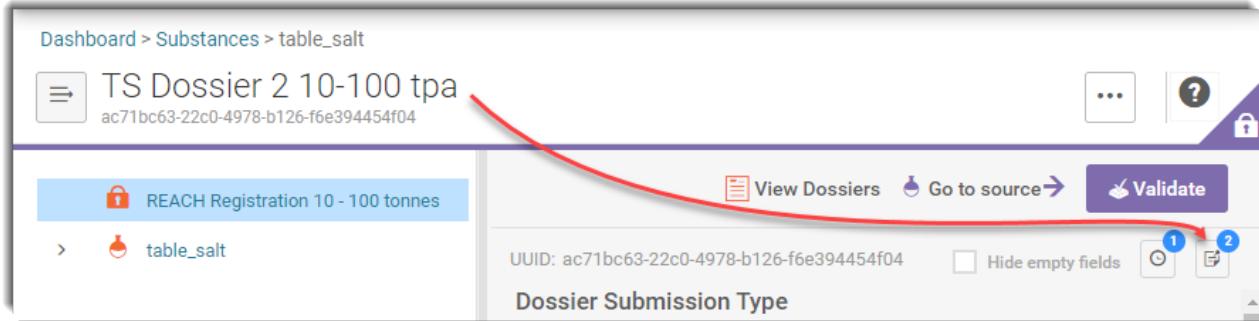
1. The *Table of contents* shown on the left is navigated by clicking on the arrowhead icons;
2. The number of documents in a section is shown to the right of the section. Empty sections have no icon;
3. To open a document, click on its name. This opens the document for viewing/editing in the data window on the right.
4. To create a document, hover over the section header, then click on the orange plus icon;
5. To delete a document, hover over its name, then click on the dustbin icon;

**2.4.1.4. Annotations**

There is no global management of *Annotations* like that presented in the *Navigation* window of the client. Instead, an *Annotation* is accessible from only the record of the document with which it is associated. An *Annotation* connected to a whole *Substance* dataset is accessible only from the section *Identification*. An *Annotation* connected to a whole *Mixture/Product* dataset is accessible from the first section under the identity of the mixture.

The link to *Annotations* for a document is at the top right of the record of the document, as indicated by the red ring in the figure below. Clicking on this icon opens a menu from which *Annotations* can be managed, as described in section 6 *Annotation*.

**Figure 11: Where to find Annotations**



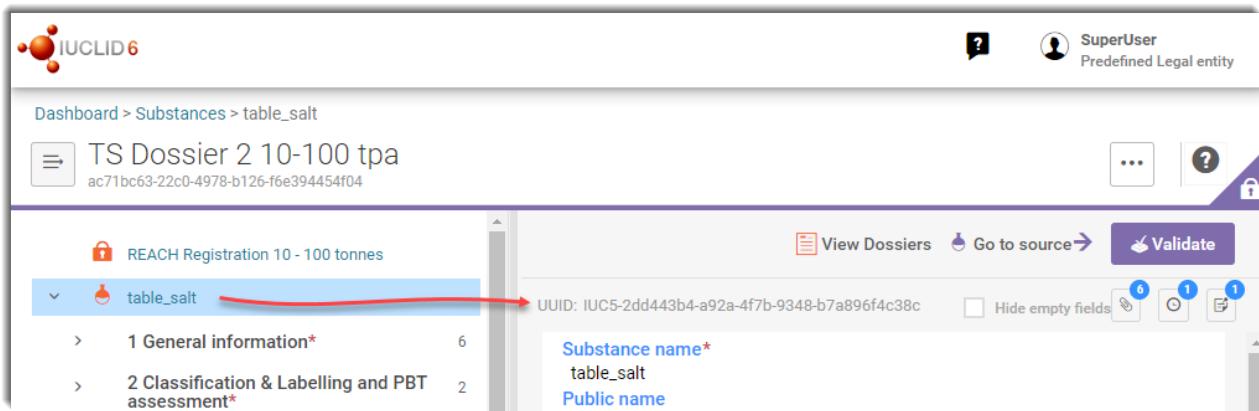
## 2.4.2. Information Panel

The Information and functionality available from the *Information panel* in the client are accessible as described below.

### 2.4.2.1. Information

The UUID of an open entity is always displayed under its name at the top left. The UUID of an open entity or document is displayed at the top of its record in the data window. For example, to view the UUID of a *Substance* in a *Dossier*, select the *Substance* in the table of content as shown below.

**Figure 12: Viewing the UUIDs of a Dossier, and a Substance within it.**

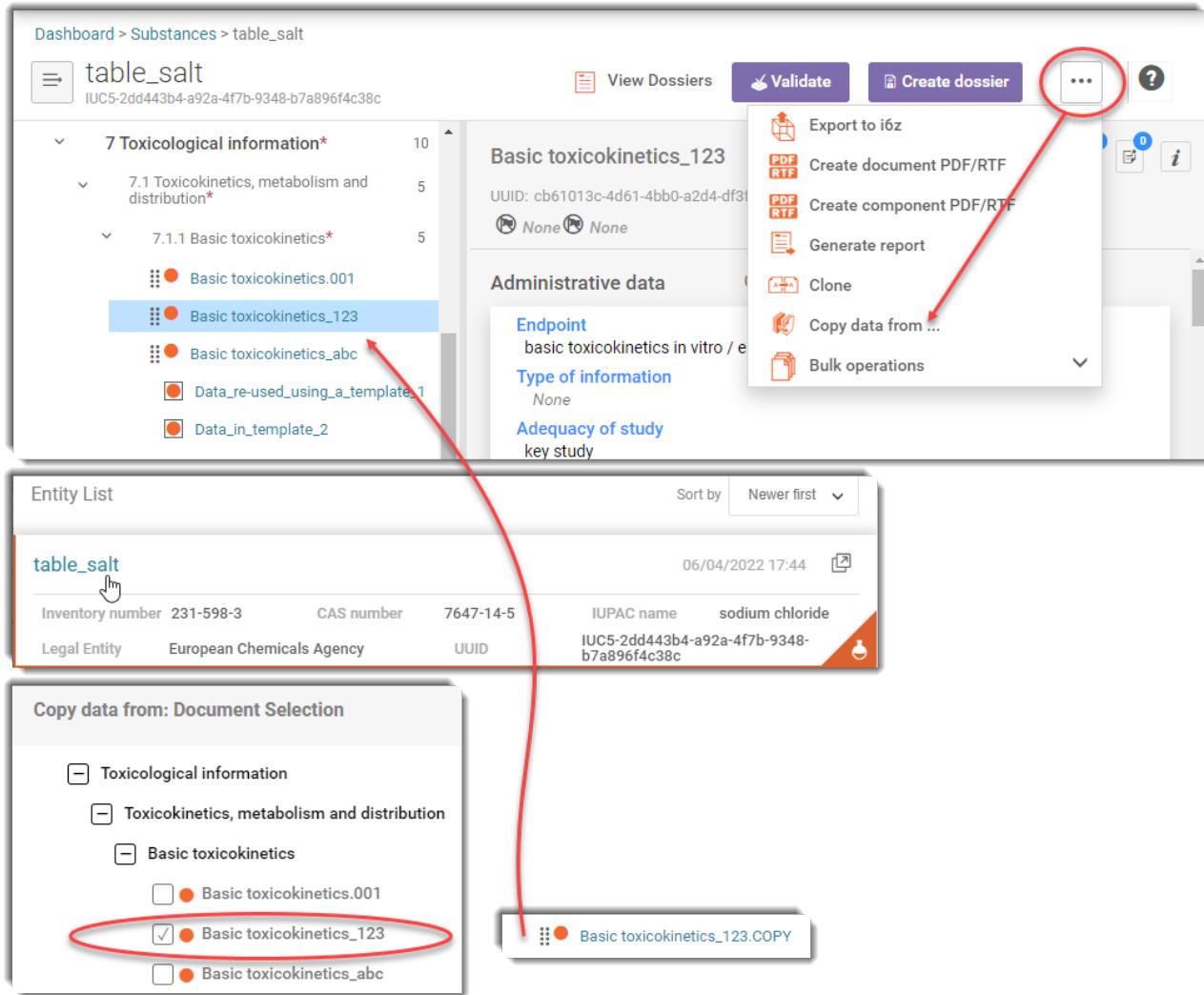


### 2.4.2.2. Clipboard manager

The functionalities in the *Clipboard* for copying documents are carried out using *Copy data from*. Documents can be copied from the same entity, or other entities and types of entities. After selecting *Copy data from*, the documents that can be copied are presented in a menu. Selecting an entity causes a window to open from which documents can be selected. An example is shown

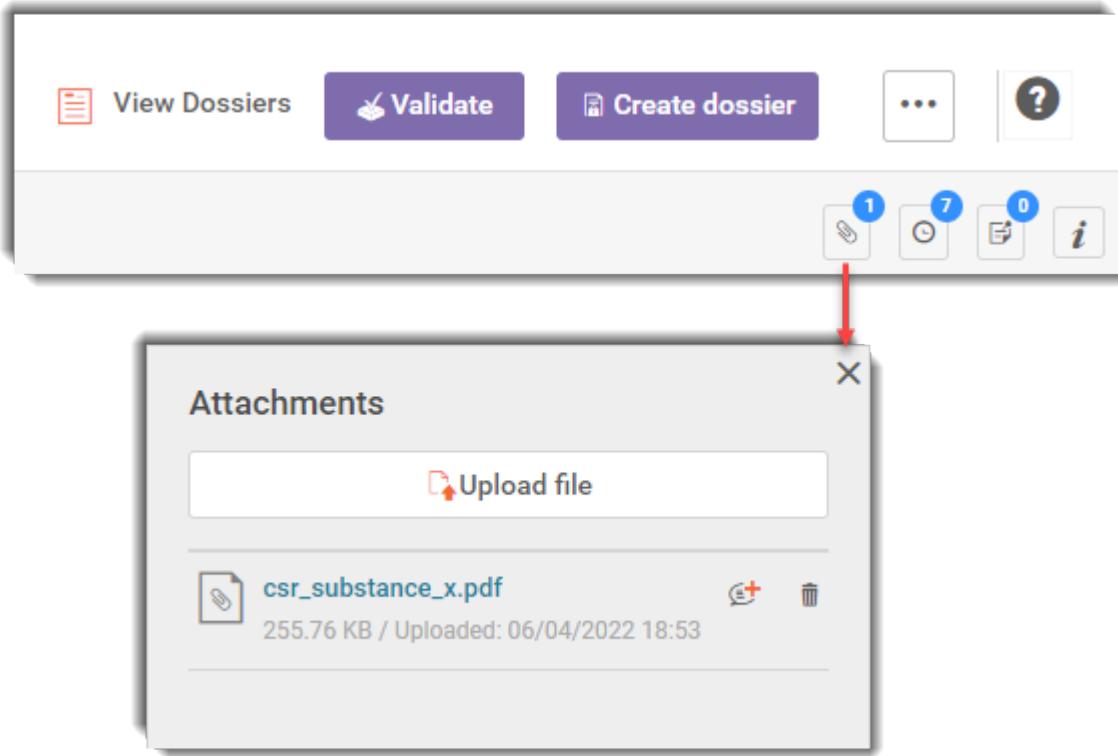
below in which a document in section 7.1.1 *Basic toxicokinetics* for REACH is going to be copied from the same *Substance* to create a duplicate, which can then be edited.

**Figure 13: Copy data from**



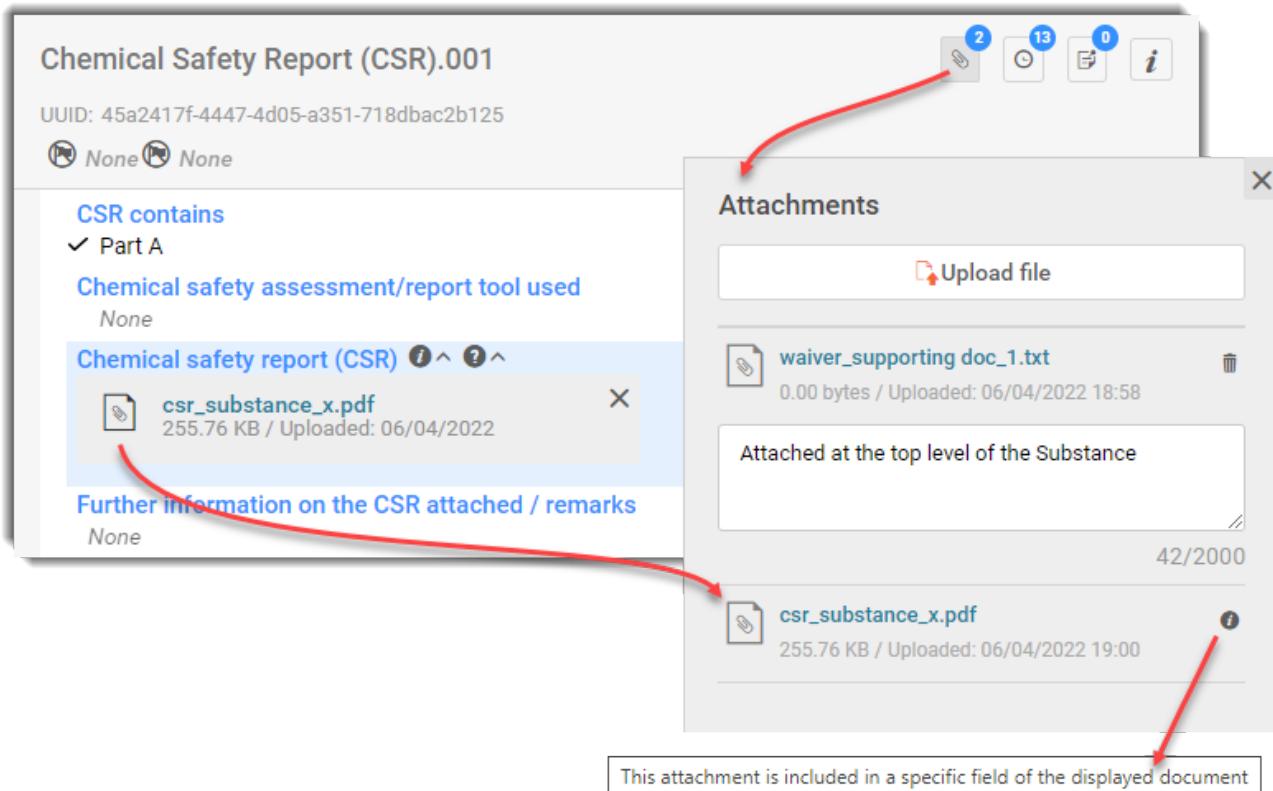
#### 2.4.2.3. Attachments

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 14: Open the attachments window**

Attachments at the entity and document level are managed from the attachments window. Attachments at the field level are managed from the field and indicated in the attachments window by an info icon to the right.

An example is given below for a document in section 13.1 *Chemical safety report* under REACH. The attachment `waiver_supporting_doc_1.txt` is attached to the whole document. The attachment `csr_substance_x.pdf` is attached only to the field *Chemical safety report CSR*.

**Figure 15: Where to find attachments**

The attachments window always shows all the files that are attached to the top-level entity, no matter where they are attached. However, attachments at the field level cannot be deleted via the attachments window. That can be done only from the field.

#### 2.4.2.4. *Modification history*

The modification history in the web interface is accessed from a button that is displayed at the top right of the data window. The button is visible only whilst the document is open in the data window. It contains the following fields from the classic interface: author, date, and remarks. For more information see section 3.7.16 *Modification History*.

#### 2.4.2.5. *Annotations*

See section 2.4.1.4 *Annotations*.

#### 2.4.2.6. *References*

To view the *Referenced documents*, see section 3.8 *Inbound references*.

### 2.4.3. **Data Panel**

The data panel is shown to the right of the table of contents. For a description of how data is entered and viewed, see the sections below on the structure of the interface.

#### 2.4.4. Function key F1 for help

The field specific help opened using the function key F1 in the client, is accessed from a question mark icon to the right of the field header, as shown in the example below:

Figure 16: Field specific help

Chemical Safety Report (CSR)

Type of CSR  
CSR (all uses)

CSR contains  
✓ Part A

Chemical safety assessment/report tool used  
None

Chemical safety report (CSR)    

This field serves as a container to attach a chemical safety report in the context of REACH.

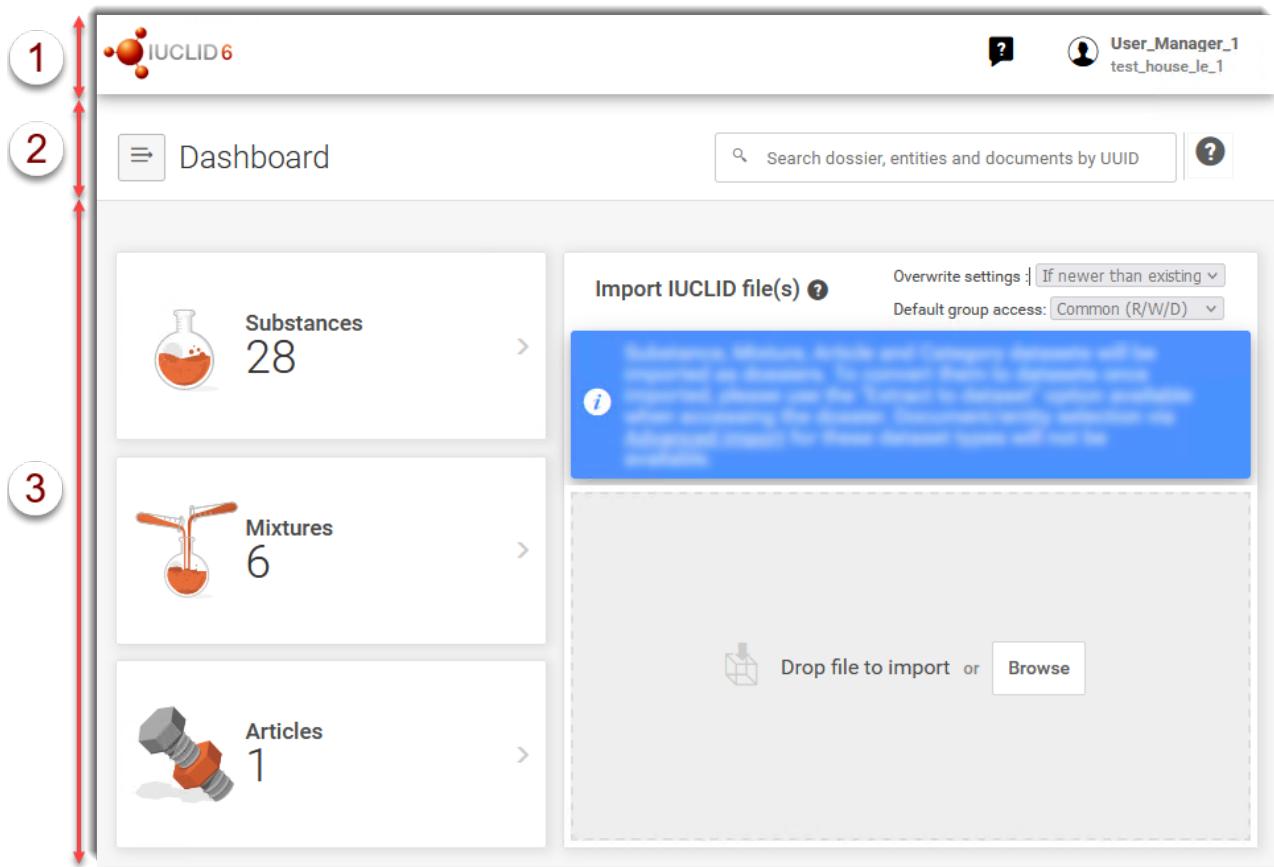
csr\_substance\_x.pdf

For other sources of help, see section 29 *Getting help*.

### 3. Overview of the web interface

The page shown on starting the web interface, or on logging in, is the *Dashboard*. The IUCLID icon at the top left of the screen links to it. The web interface of IUCLID has an area for data entry and navigation, with two horizontal bar areas above it. The overall structure of the interface is shown below.

Figure 17: The structure of the web interface of IUCLID - Dashboard



#### Legend for Figure 17:

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 of which 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 18: The structure of the web interface of IUCLID - List of Substances**

The screenshot shows the IUCLID 6 web interface. At the top, there is a navigation bar with the IUCLID 6 logo, a user icon labeled 'SuperUser Predefined Legal entity', and a search bar. Below the navigation bar is an application bar with a 'Dashboard' link, a 'Substances' link, a 'New substance' button, and a help icon. The main data area is titled 'Substances' and contains a search bar, an 'Advanced search' link, and a table of results. The table has three rows, each representing a substance: 'potassium chloride' and 'table\_salt'. Each row includes checkboxes, inventory numbers, CAS numbers, IUPAC names, and UUIDs. The 'potassium chloride' row is highlighted with a red border.

	Inventory number	CAS number	IUPAC name	UUID
<input type="checkbox"/> potassium chloride	231-211-8	7447-40-7	potassium chloride	b3ed489a-323e-4e8e-a752-5a8fdff2673e
<input type="checkbox"/> table_salt	231-598-3	7647-14-5	sodium chloride	IUC5-2dd443b4-a92a-4f7b-9348-b7a896f4c38c

**Legend for Figure 18:**

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*.

### 3.1. 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	<p>Entities in IUCLID are software objects that are used to store data that has a particular purpose, which depends on the type of entity. The types of entity are: <i>Dossier, Substance, Mixture/Product, Template, Annotation, Legal entity, Legal entity site, Reference substance, Test materials, Contact, Literature reference</i>.</p> <p>Entities can be viewed, printed, and deleted individually. They can also be exported and imported as individual files. With the exception of <i>Dossier</i>, entities are designed to be referred to by other entities. This reduces duplication of data sources and improves data consistency. On saving a change to an entity, the change is immediately seen in any other entity that refers to it. An exception to that is a <i>Dossier</i>, which is a read-only snapshot of data.</p>
Dataset	<p>A <i>dataset</i> is a collection of documents that relate to a particular chemical substance, or grouping of chemical substances. It can be of the following types: <i>Substance, Mixture/Product, Template</i>.</p> <p>For clarity and where appropriate, the type of the dataset should be stated, for example <i>Substance dataset</i>.</p>
Document	<p>A <i>document</i> is a page that contains functionality for creating, viewing, or modifying an <i>entity</i>, a <i>record</i>, or a <i>summary</i>. The term <i>document</i> is also used to mean a standardised set of data that exists in a dataset in a particular section.</p> <p>For example, in the OECD harmonised templates under the section named <i>Acute toxicity: oral</i>, there can be one or more documents that all have the same structure, but do not necessarily have the same name, or contain the same values.</p> <p>For more information about types of documents, see section 3.7.12 <i>Table of contents</i>.</p>
Fixed	<p>The term <i>fixed</i> means that a document is in a section that can contain only one document.</p>
Field	<p>A <i>field</i> is a location within an entity or document in which a specific piece of data is stored. The type of data is the same throughout an individual field, for example, the field could contain free text, a text value chosen from a drop-down menu, a number, or a date. There can be many fields in one document. An example of a field is <i>IUPAC name</i>.</p>

### 3.2. 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 User. To view the settings for the current *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 25 *User management*.

**Figure 19: User settings with Instance based security (IBS) active**

The screenshot shows the 'User settings' page with the following sections:

- 1 My Profile**: Displays basic user information: Username (Bobby\_12345), First name (Bobby), Last name (G), and Email. A 'Change password' link is also present.
- 2 Working Legal Entity**: Shows the current entity (European Chemical Agency) and a link to 'View & Change Working Legal Entity'.
- 3 Roles**: Shows 2 assigned roles.
- 4 Security groups**: Shows 3 assigned groups.
- 5 Default Group Access**: Shows a link to 'View & Change Default Group Access'.

#### Legend for Figure 19

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 25.4 *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 25.2.7 *Default group access for a User*.

### 3.3. 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 20: UUIDs of an entity and a document inside it**

Dashboard > Substances > table\_salt

table\_salt  
IUC5-2dd443b4-a92a-4f7b-9348-b7a896f4c38c

View Dossiers Validate

7 Toxicological information\*

- 7.1 Toxicokinetics, metabolism and distribution\*

  - 7.1.1 Basic toxicokinetics\*

    - Basic toxicokinetics.001
    - Basic toxicokinetics\_123**
    - Basic toxicokinetics\_abc
    - Basic toxicokinetics\_123.COPY

Basic toxicokinetics\_123

UUID: cb61013c-4d61-4bb0-a2d4-df3fa0ea1bc5

None None

Administrative data

Endpoint basic toxicokinetics in vitro / ex vivo

Type of information None

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

**Figure 21: UUID of an entity in a list of entities**

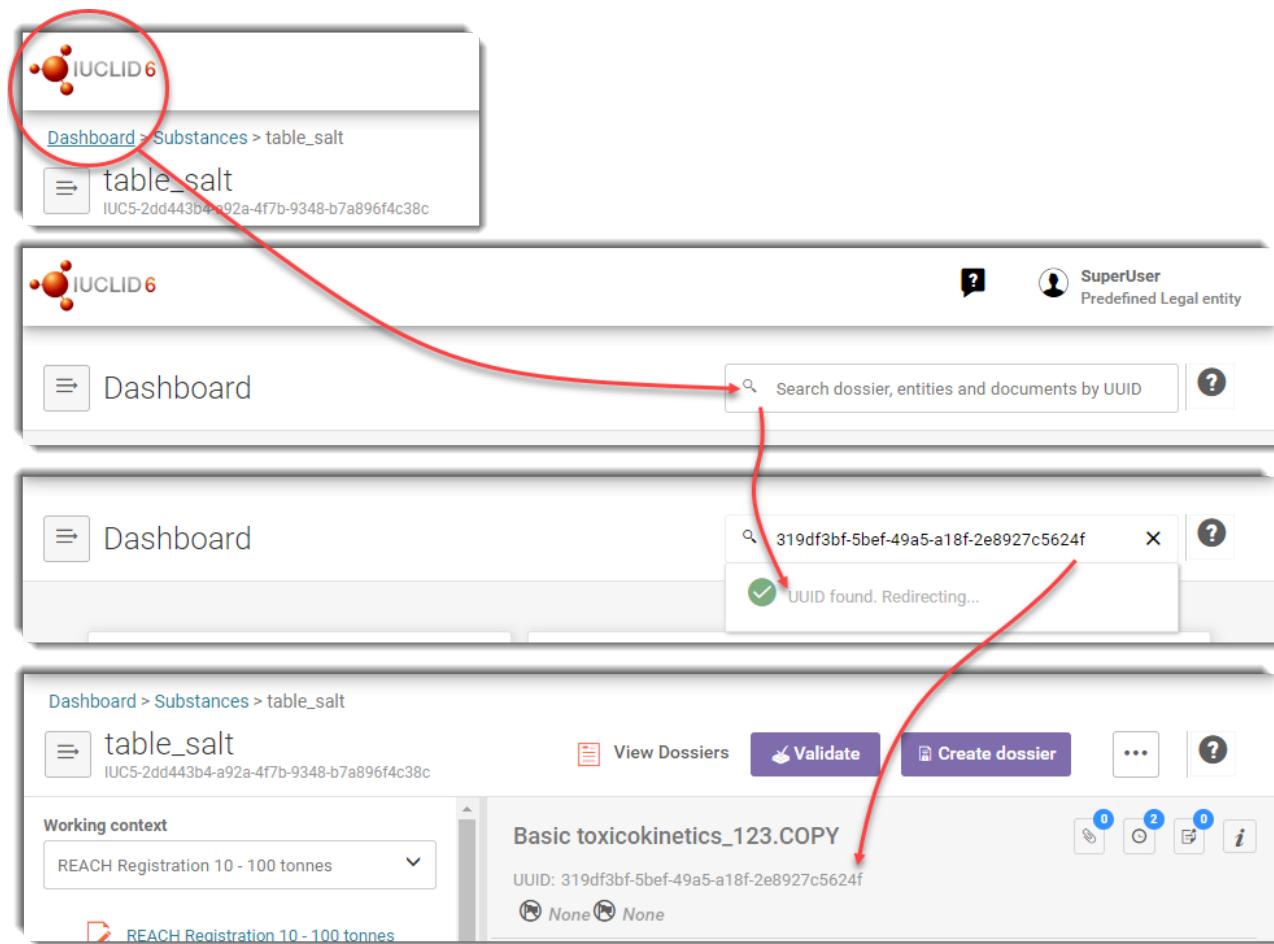
<input type="checkbox"/>	table_salt	06/04/2022 19:23	...
Inventory number	231-598-3	CAS number	7647-14-5
Legal Entity	European Chemicals Agency	IUPAC name	sodium chloride
		UUID	IUC5-2dd443b4-a92a-4f7b-9348-b7a896f4c38c

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

### 3.4. 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 22: Search by UUID across all entities and documents

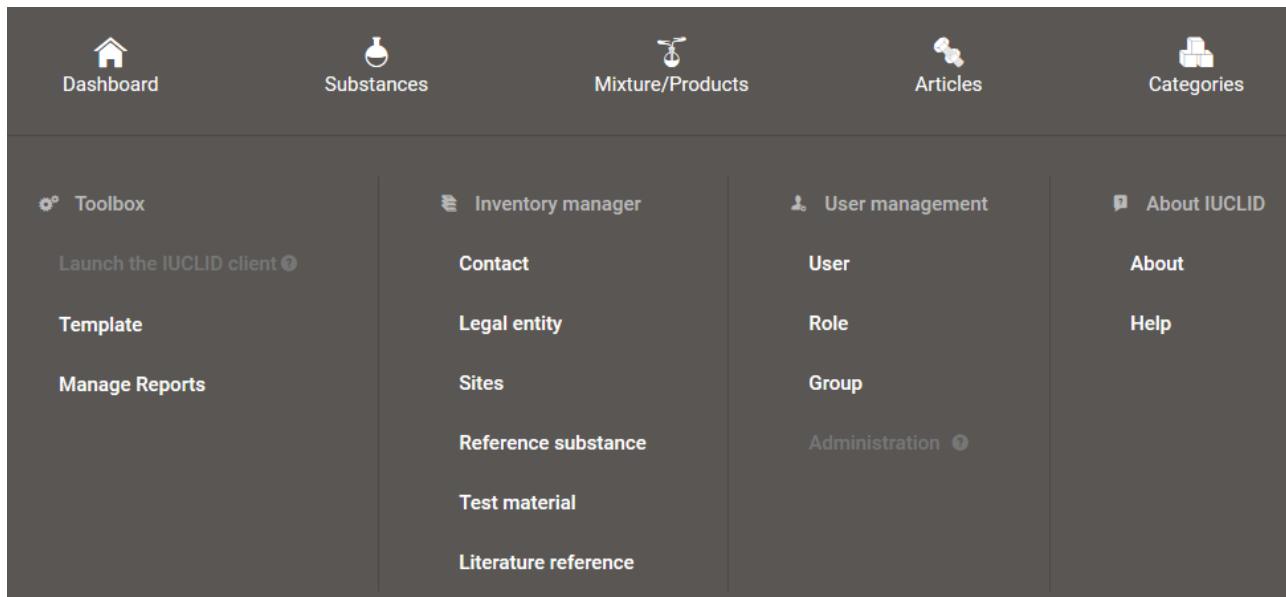


To search by UUID paste the UUID into the box. The search begins automatically. If a match is found for which there is only one instance in the database, the entity or document is opened automatically. If there is more than one match, a list is displayed from which an entity or document can be opened. 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.

### 3.5. 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.

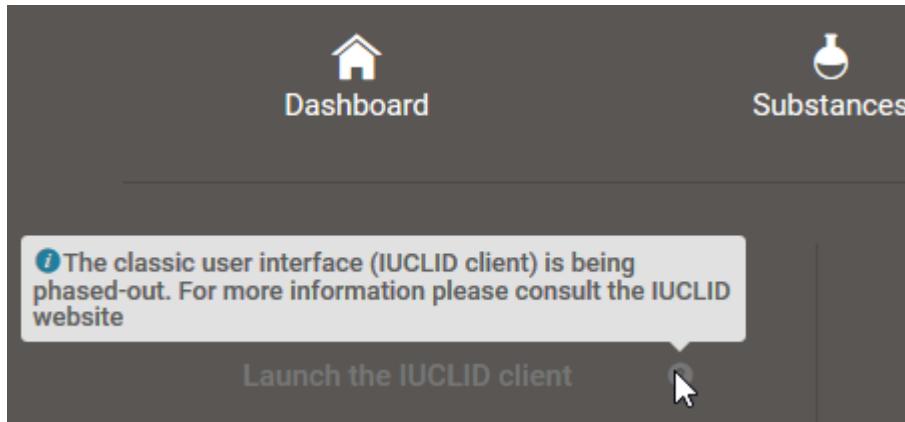
Figure 23: The main menu



#### 3.5.1. Launch the IUCLID client

This option is shown only when IUCLID is run on a remotely accessible server. Instructions on how to run the classic Java client interface are provided via the [IUCLID website](#).

Figure 24: Launch the IUCLID client



#### 3.5.2. About

*About* displays the version of the instance of IUCLID, and its components.

### 3.5.3. Help

*Help* contains a link to this manual.

## 3.6. Navigation using the keyboard

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

### 3.6.1. 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.

### 3.6.2. Enter

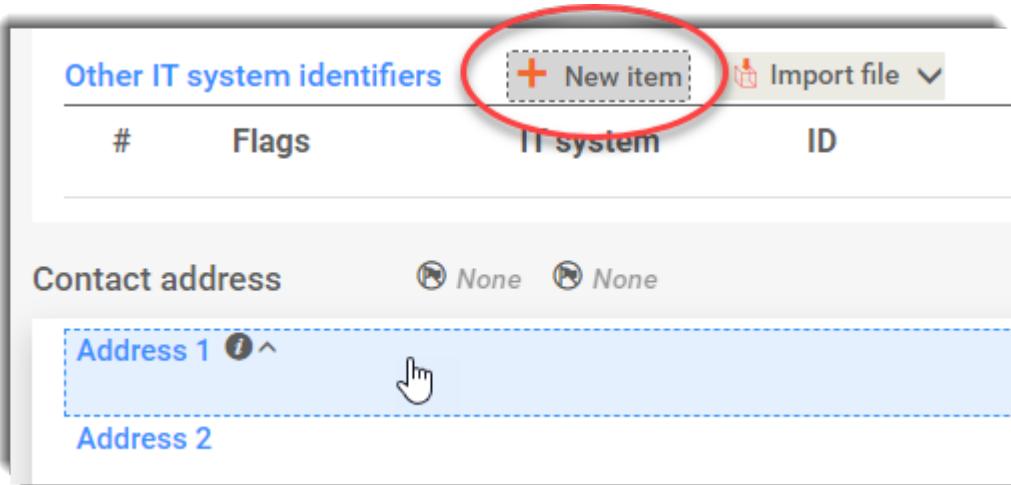
*Enter* is equivalent to a mouse click on an object that has been selected using *Tab*. Selection is indicated by a dashed border around the object. For example, the Save button can be selected using *Tab*, and then the data saved using *Enter*.

Figure 25: 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*.

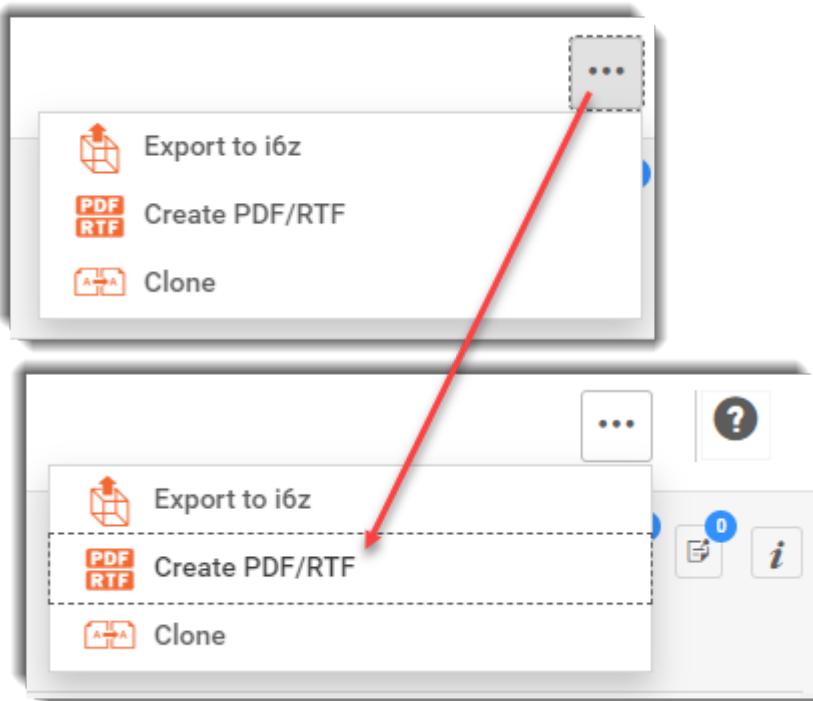
Figure 26: Enter acts on an object that has been selected using Tab, not the focus of the mouse



### 3.6.3. 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 27: Select an item from a three-dot menu without using the mouse:



### 3.6.4. Escape

Escape switches a field out of edit mode.

### 3.6.5. 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.

### 3.6.6. 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 28: Difference between highlighting by mouse hover, and selection using Tab**

Results and discussion										
Effect concentrations										
#	Key ...	Dura...	Dos...	Effe...	95% ...	Nom...	Con...	Basi...	Rem...	Actions
☰ 1	<input type="checkbox"/>	24 d	LC50	ca. 33	nominal	test mat.	abnormality equilibrium (fish)	not determinable	 	
☰ 2	<input type="checkbox"/>	48 d	LC50	ca. 33	nominal	test mat.	abnormality equilibrium (fish)	not determinable	 	

[Details on results](#)

## 3.7. Functionalities available in the data area

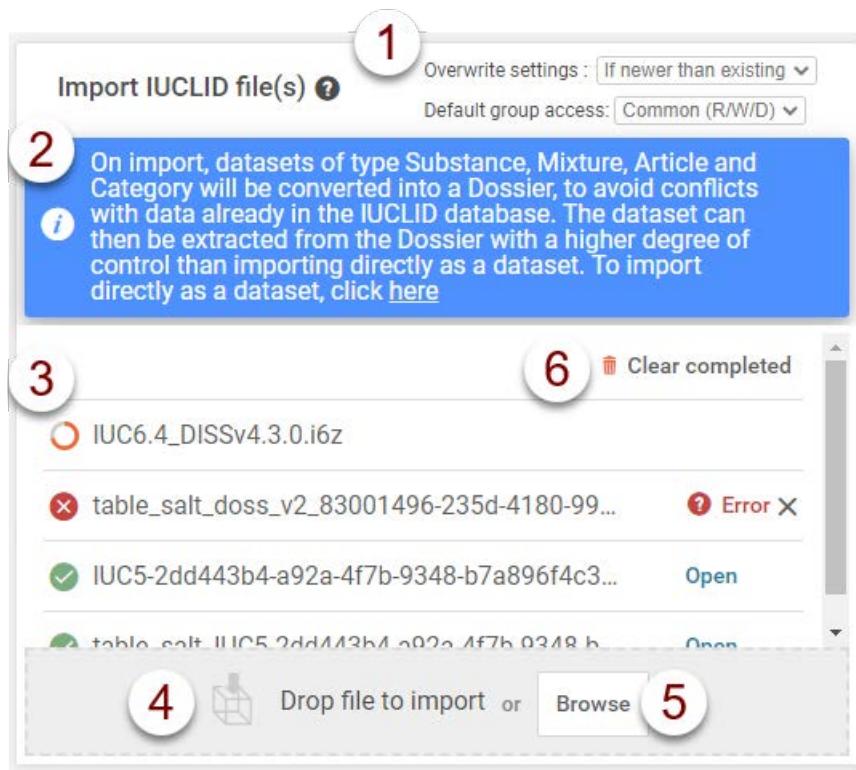
The following functionalities are used throughout the data area.

### 3.7.1. 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 8.4 *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.

**Figure 29: Import data in to IUCLID****Legend for Figure 29**

1. The Overwrite settings are described below in the next section.
2. By default, certain types of dataset 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 3.7.1.3 *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 particular 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*;

**3.7.1.1. 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

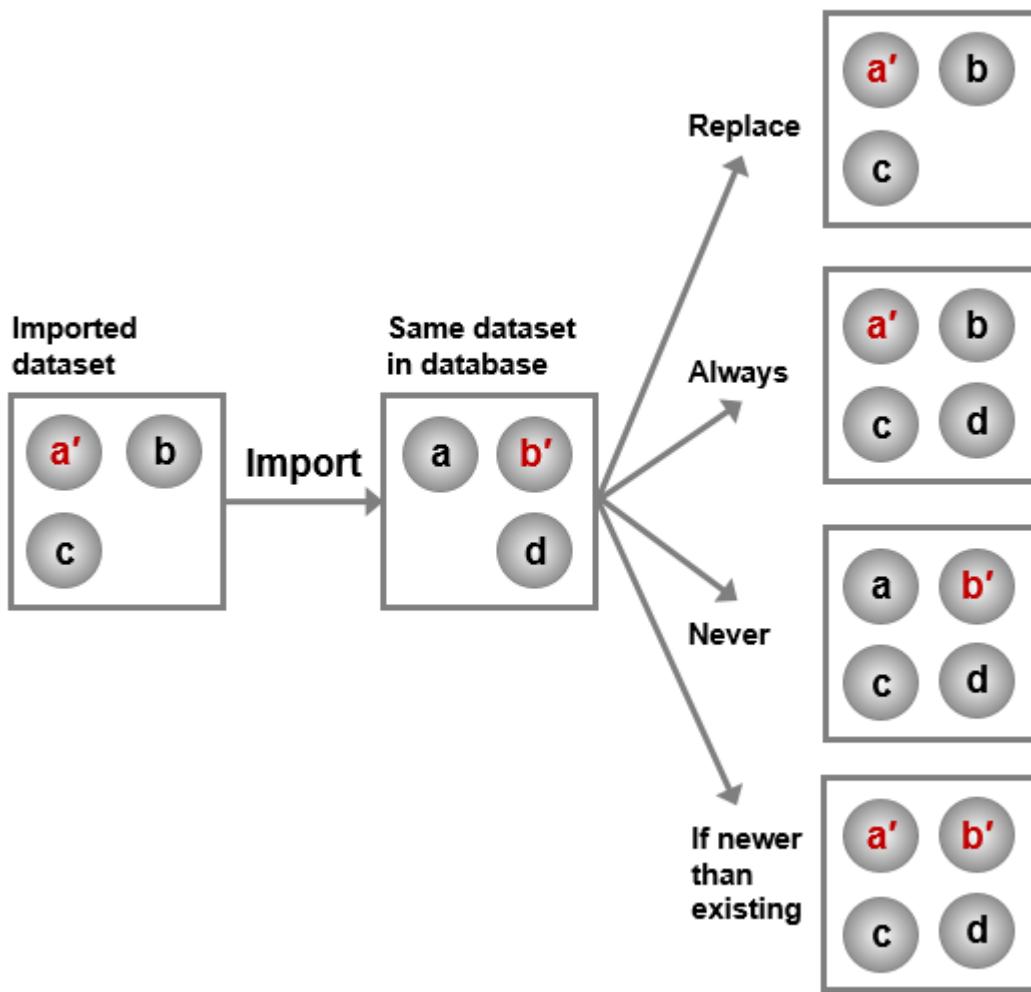
being imported. The name of the file does not matter. The import compares the UUIDs to what is already in the database, and then acts according to one of the four options listed below.

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 3.7.1.3 *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 30: Import in to IUCLID 6 where datasets and/or documents already exist in the database**



#### Legend for Figure 30:

**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.

#### 3.7.1.2. 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 25.2.7 *Default group access for a User* and 25.4 *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.

### 3.7.1.3. 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.

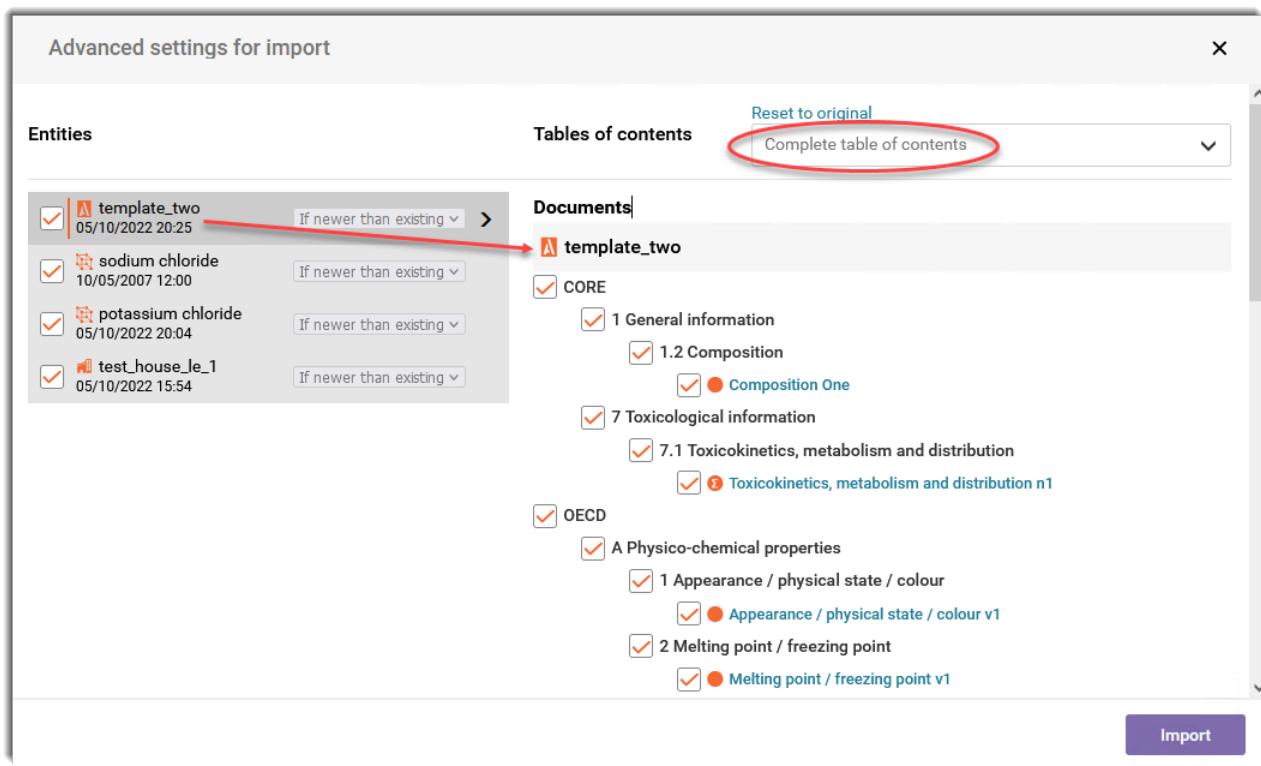
This does not apply to *Dossiers*, and datasets of type *Substance*, *Mixture*, *Article* and *Category*, for which document selection is not allowed. On import, by default, a dataset of one of those types is converted into a *Dossier*, which can then be converted into a dataset as explained in section 8.4 *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 31: 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 32: Advanced import: Change the working context**

**Tables of contents** [Reset to original](#)  
Complete table of contents ▾

**Documents**

**A template\_two**

CORE

- 1 General information
- 1.2 Composition
- Composition One

- 7 Toxicological information
- 7.1 Toxicokinetics, metabolism and distribution
- Σ Toxicokinetics, metabolism and distribution n1

OECD

- A Physico-chemical properties
- 1 Appearance / physical state / colour
- Appearance / physical state / colour v1

- 2 Melting point / freezing point
- Melting point / freezing point v1

**Tables of contents** [Reset to original](#)  
REACH Registration 10 - 100 tonnes ▾

**Documents**

**A template\_two**

1 General information

- 1.2 Composition
- Composition One

4 Physical and chemical properties

- 4.1 Appearance / physical state / colour
- Appearance / physical state / colour v1

- 4.2 Melting point / freezing point
- Melting point / freezing point v1

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 33: 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 3.7.1.1

**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 34: View the Last modification date**

### 3.7.1.4. Bulk import

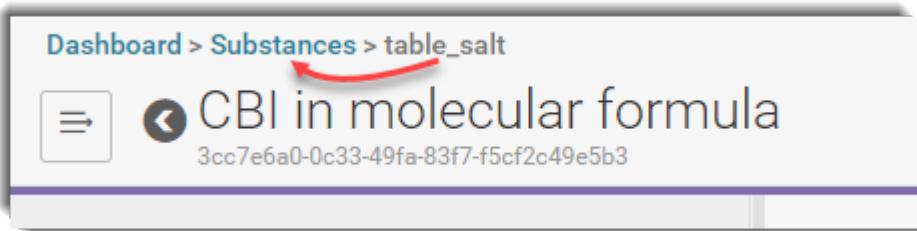
To import more than one entity from i6z files at once, place the i6z files in a zip archive, and then import the archive. A zip archive created using the bulk export feature of IUCLID can be imported. The number of files that can be imported at once using this method may be limited by system performance. 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.

### 3.7.2. 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 35: Navigation using breadcrumbs

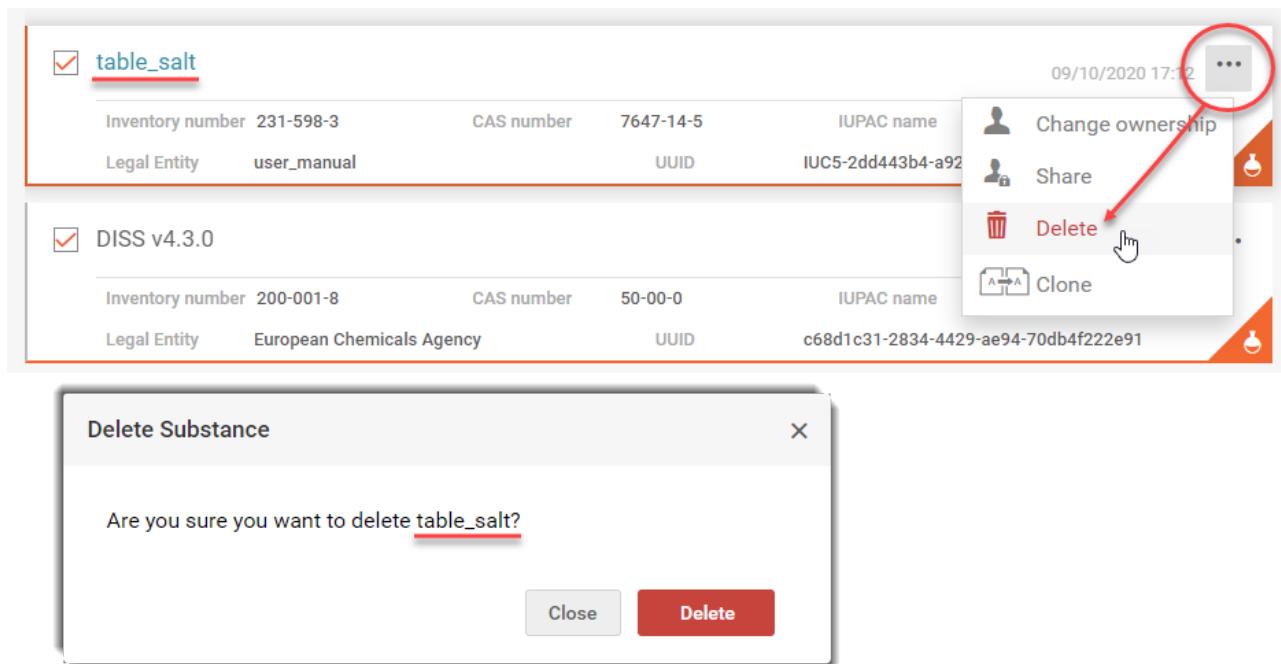


### 3.7.3. Individual versus bulk actions on entities

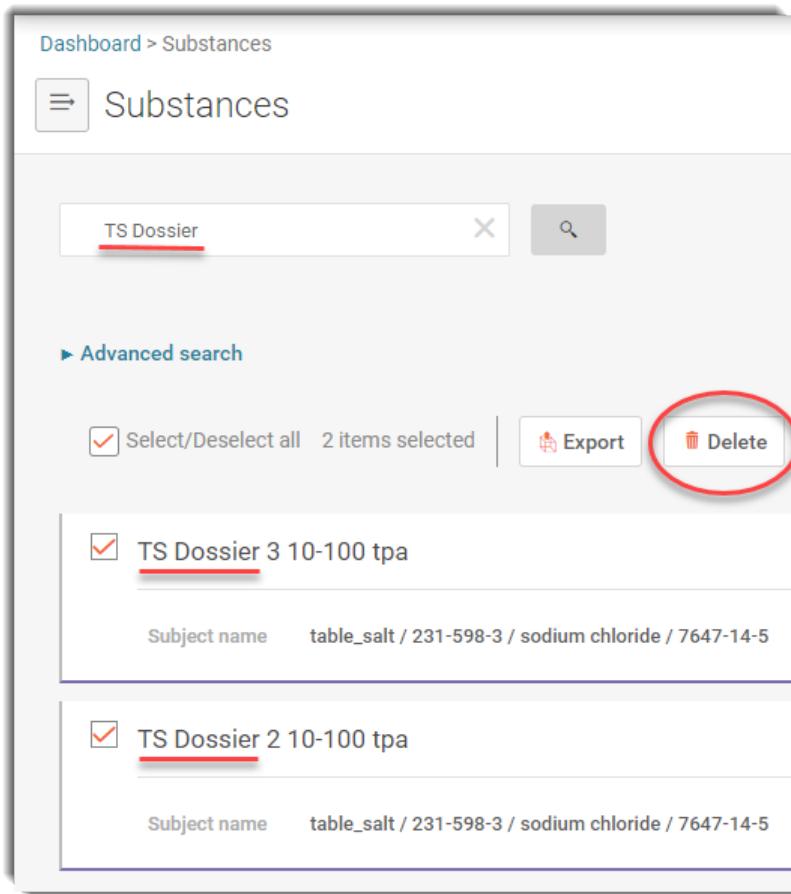
Each entry on a list page of entities has a tick box on the left, and a menu button on the right. The tick box is used to include an entity in a bulk action. The menu is used to perform a task on only that entity. The bulk actions are *Export* and *Delete*, as described in later sections.

### 3.7.4. Deleting entities

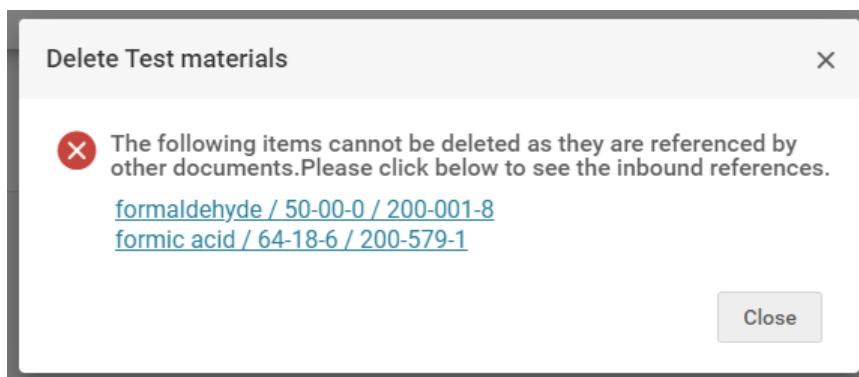
To delete a single entity from a list of entities, right-click on the menu button at the upper right of its list entry, and then select *Delete*. An example is shown below.

**Figure 36: 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.

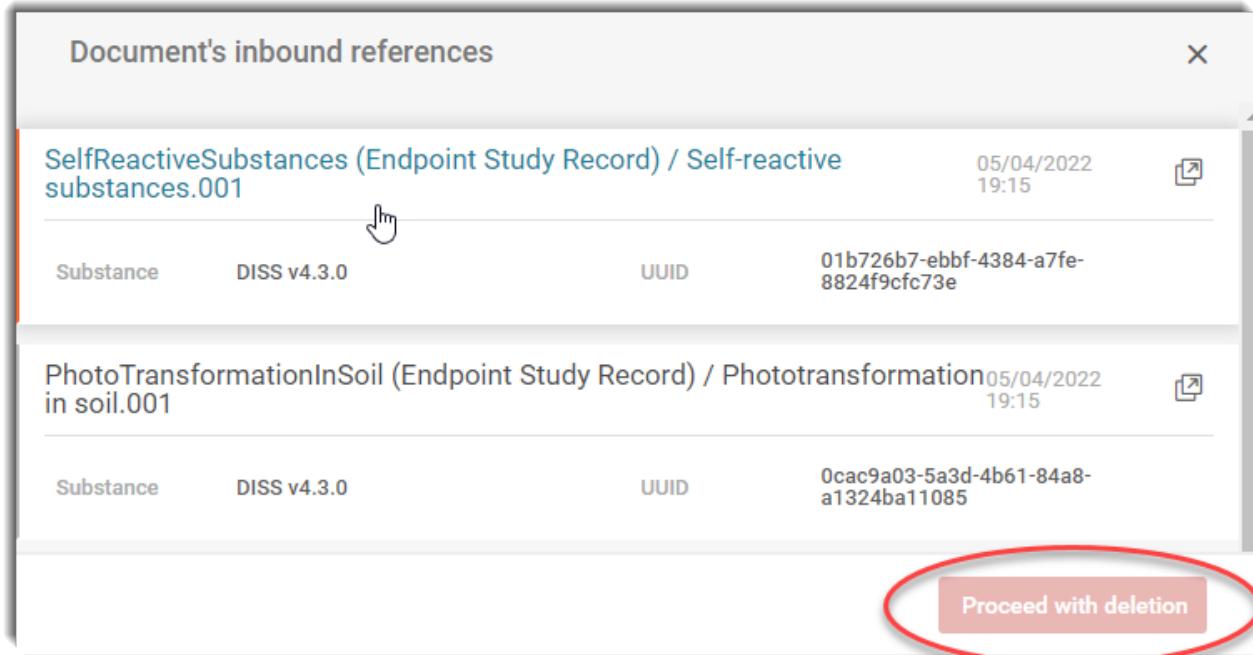
**Figure 37: Delete entities in bulk**

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 3.8. 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 38: Delete multiple entities that have inbound references**

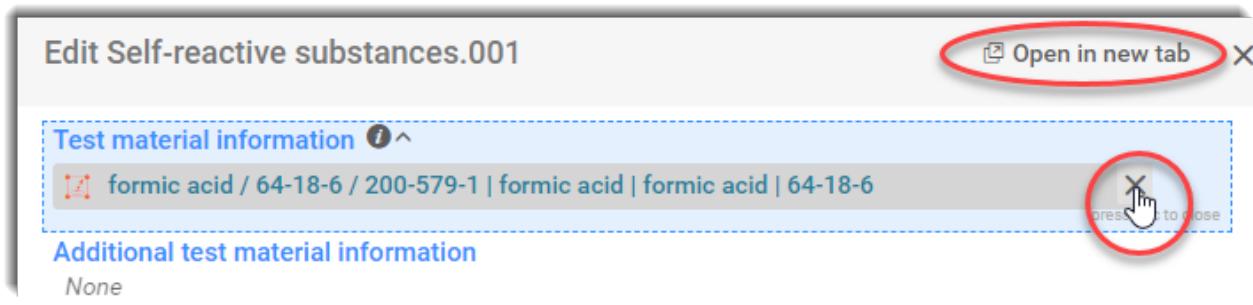
On clicking a link shown above, the inbound references are shown in a window with the delete button *Proceed with deletion* greyed out, as shown in the example below for the deletion of a *Test material* that is referred to by a *Substance*.

**Figure 39: Inbound references preventing deletion**

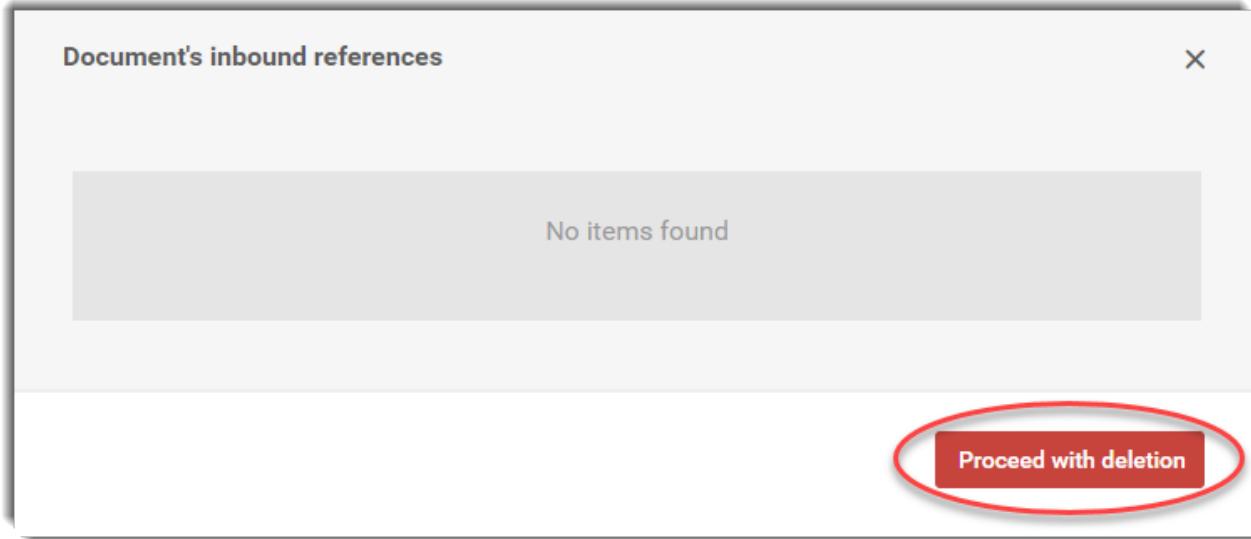


The referring entity or document can be opened for editing from the link provided. This can be done in a new tab, which can help to keep track of what you are doing if there are multiple references to remove. See below, in which a reference to the *Test material* is being deleted.

**Figure 40: An inbound reference being deleted**



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

**Figure 41: Proceed with deletion is active**

### 3.7.5. 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**

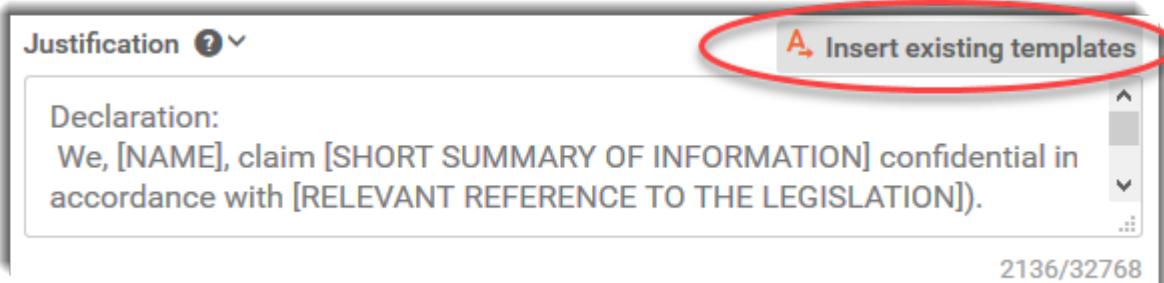
Header	Example value in the CSV file
Substance name	"1,2-dichloroethane"
Inventory number	203-458-1
CAS number	107-06-2
IUPAC name	
Legal Entity	Predefined Legal entity
UUID	3b8ab9b2-3b63-4fb0-8c70-f5cfaf021e51
Last modified date/time	2021-08-20T14:35:28.102Z
IUCLID entity URL	localhost:8080/iuclid6-web/?key=3b8ab9b2-3b63-4fb0-8c70-f5cfaf021e51/0

### 3.7.6. 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, A. 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 42: Free-text template**



### 3.7.7. 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 43: Flags applied individually to fields**

Substance name\*  
diethyl\_ether\_training

Public name  
diethyl ether for training at ECHA

Legal entity\* CBI EU: REACH  
 Training Company | Helsinki | Finland

Third party None None  
 None

None

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 44: Flags applied to all the fields in a section**

Typical Composition 2013  
UUID: a19b82c7-a4ca-34df-9dc5-402463b4c520

Characterisation of polymers

Polymer molecular weight CBI None

Number average molecular weight (NAMW)  
 None

Weight average molecular weight (WAMW)  
 None

Polydispersity index  
 None

Percentage of low molecular weight species (< 1,000 g/mol)  
 None

Percentage of low molecular weight species (< 500 g/mol)  
 None

Reactive functional groups CBI None

Polymer contains only low concern reactive functional groups  
Reactive functional groups - moderate concern

Reactive functional group New item Import file

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

**Figure 45: Flags applied individually to items in a table**

Typical Composition 2013		
UUID: a19b82c7-a4ca-34df-9dc5-402463b4c520		
Impurities		
#	Reference substance	
1	None EU: REACH	water   water   7732-18-5
2	None EU: REACH	butanone   butan-2-one   78-93-3
3	CBI EU: REACH	2-methylpropan-2-ol   2-methylpropan-2-ol   75-65-0

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 46: The extent of application of flags**

The screenshot shows the IUCLID web interface with several sections and numbered callouts:

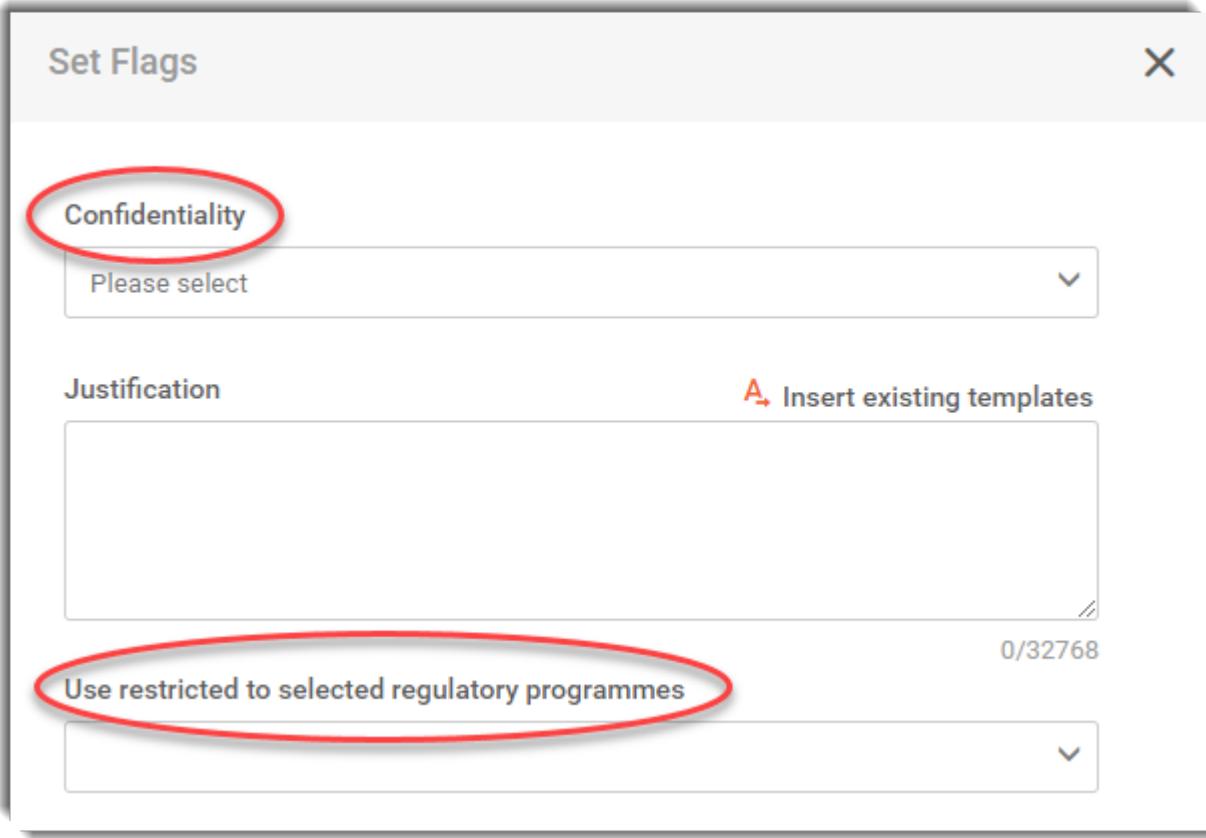
- Section 1 (Top Left):** Shows a document header with UUID: ECB5-10152c0c-31d1-4ed4-b52e-40ed218060ca. Below it, there are two flag icons: a blue circle with a white exclamation mark labeled "None" and a red flag icon labeled "EU: REACH".
- Section 2 (Main Content):** Contains substance details:
  - Reference substance name\***: butanone
  - IUPAC name**: butan-2-one
  - Description**: None
- Section 3 (Synonyms):** A table titled "Synonyms" with columns "#", "Identifier", and "New item" (button). It lists one row:
 

#	Identifier	New item
1	None	2 (highlighted with a red circle)
- Section 4 (Molecular and structural information):** Contains:
  - Molecular formula**: C4H8O
  - Molecular weight**: 72.1057

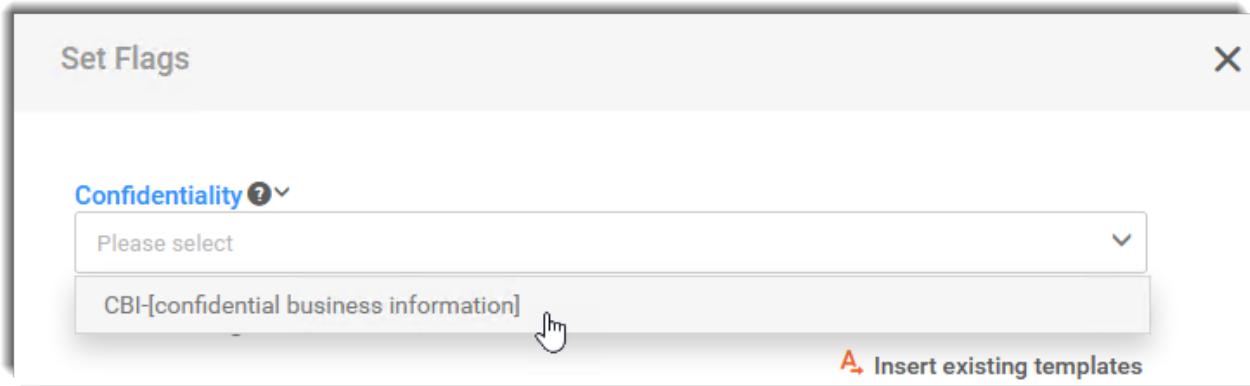
### Legend for

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 in this section. The flag set in (1) EU:REACH also applies.

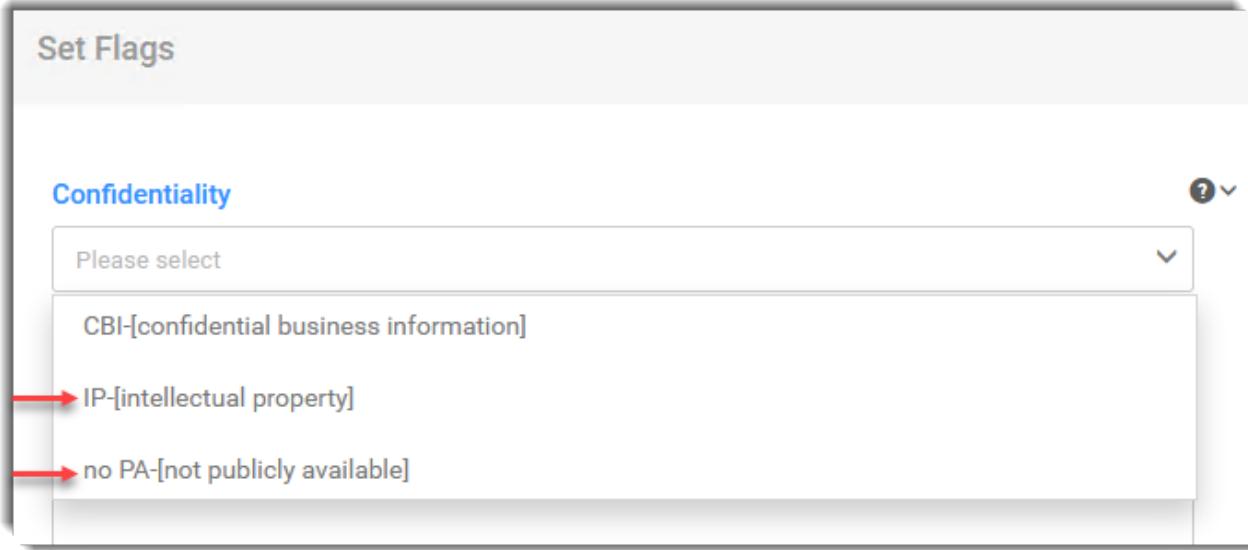
When a document is created, no flags are set. To edit a flag, click on either of the flag icons in its pair. The flag for confidentiality, and the flag for regulatory programme, are edited from the same page, as shown in the figure below:

**Figure 47: Setting flags for confidentiality, and/or regulatory programme**

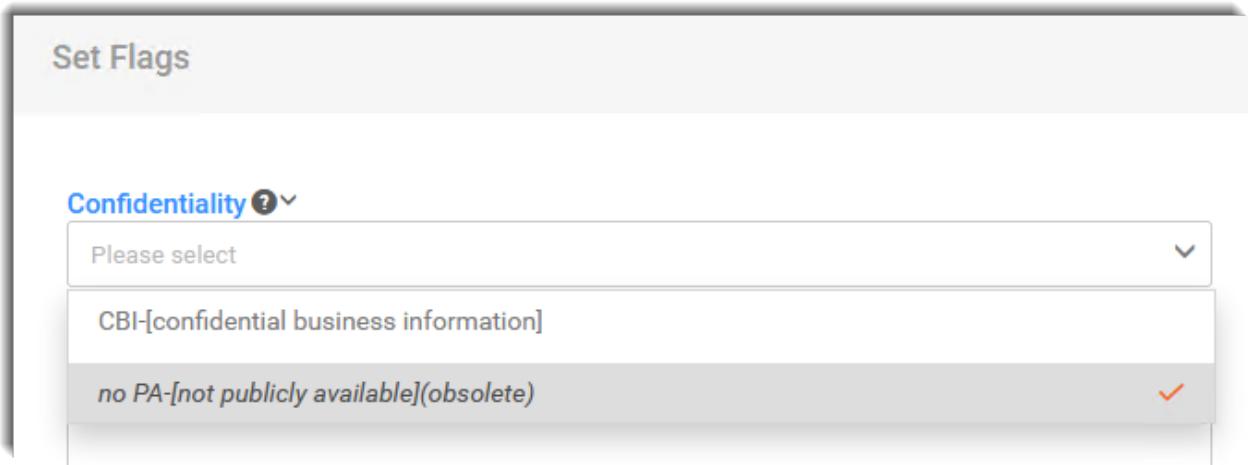
For confidentiality, select the type and then enter a justification. To ensure you select the correct type, read the help under the question mark icon. The type, *Confidential Business Information (CBI)* is being selected in the example shown below.

**Figure 48: Setting a confidentiality flag**

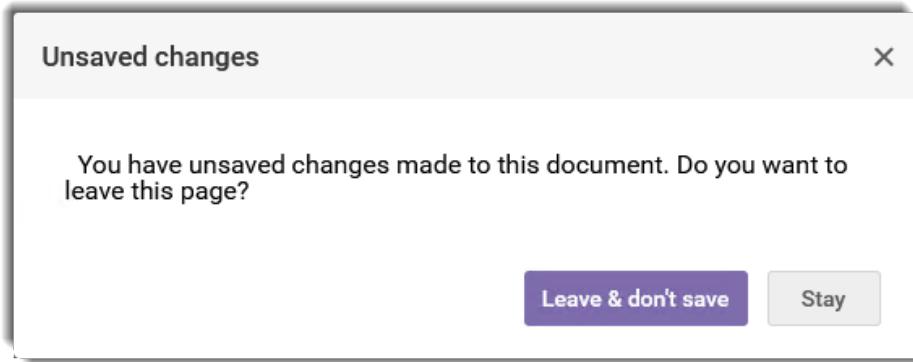
In this version of IUCLID the only option is CBI, but prior to IUCLID 6 version 6.0.0, there were two other options, as shown below.

**Figure 49: Types of flags that are obsolete**

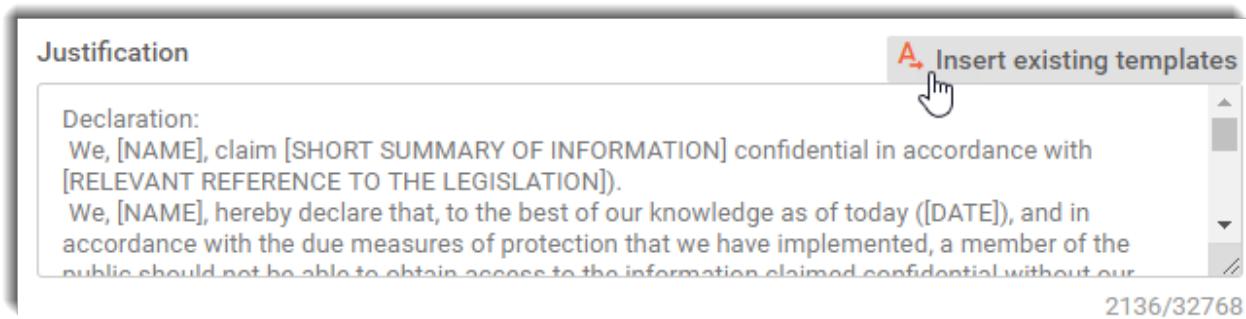
The options *IP-[intellectual property]* and *no PA-[not publicly available]* are obsolete. A flag set to either of those types, and then imported into the current version of IUCLID, is still visible, but it is read-only. An example of how obsolete flags appear is given below.

**Figure 50: An obsolete flag that was set in an earlier version of IUCLID**

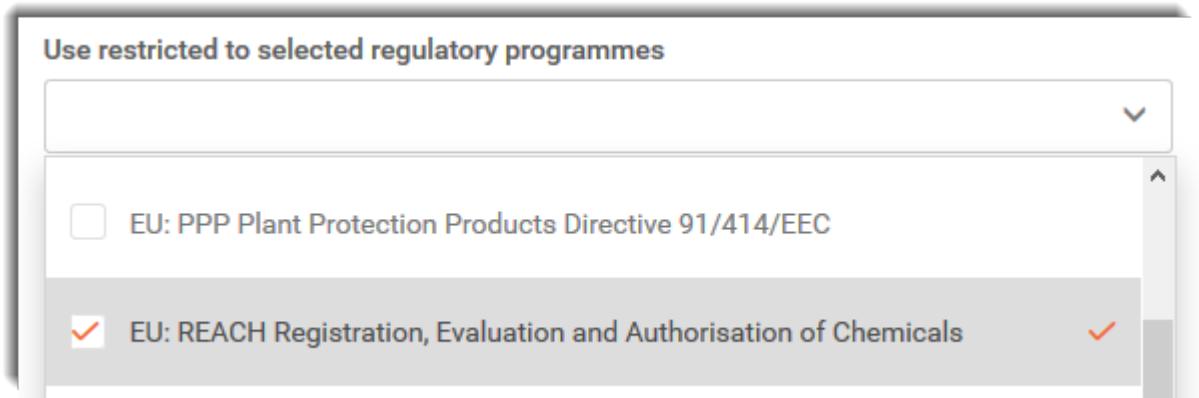
Note that selecting CBI from the menu, causes the obsolete value of the flag to disappear from the menu. If you do not want to change the value to CBI, close the window, navigate away from the documents without clicking on Save, and then select the option to not save the changes, as indicated below in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

**Figure 51: 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, A. 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 52: 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 53: 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 54: An example where the flags for Administrative data are set for the whole document automatically

The screenshot shows the 'Attached CSR' page. At the top, it displays the UUID: IUC5-d1c638bf-99d0-4452-b7f0-df65e555b0b4. Below the UUID, there are two sets of flags: 'CBI' (with a red icon) and 'None' (with a grey icon). A red arrow points from the 'CBI' icon in the 'Administrative data' section down to the 'CBI' icon in the 'None' section. The page title is 'Chemical Safety Report (CSR)'.

### 3.7.8. 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 55: Shortcuts to sections in a document

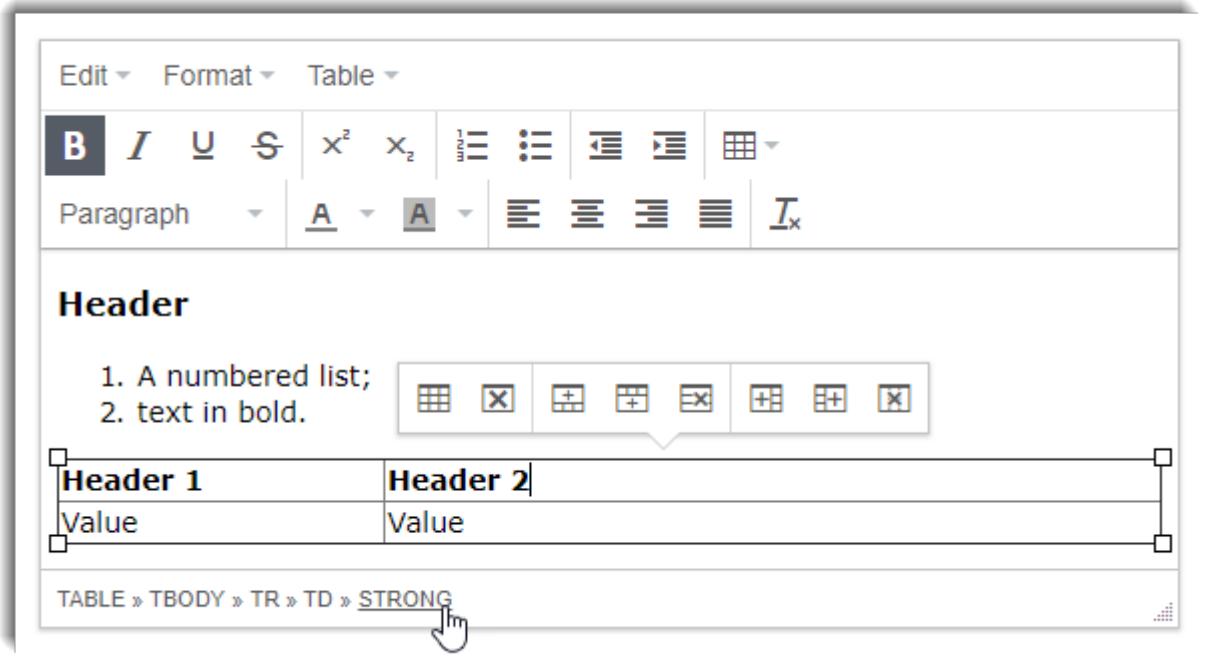
The screenshot shows the 'Repeated dose toxicity: dermal test 1' page. At the top, it displays the UUID: 0b4850a5-ac40-42df-b1ae-25c1844b9a9a. Below the UUID, there are two sets of flags: 'None' (red icon) and 'None' (grey icon). A red arrow points from the 'Materials and methods' section in the main content area up to the 'Materials and met...' button in the header. The 'Materials and met...' button is highlighted with a red oval and has a hand cursor icon over it. The page title is 'Materials and methods'. The header also includes buttons for 'Administrative data', 'Data source', 'Results and discu...', and 'Materials and methods'. Below the header, there is a table with columns: '#', 'Qualifier', 'Guideline', and 'Version / remarks'. The first row contains the text 'Principles of method if other than guideline'.

### 3.7.9. 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 56: A rich text field**



### 3.7.10. 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 57: Add a row to a table**

The screenshot shows two identical tables side-by-side. Both tables have columns for '#', 'Key result', 'Test no.', 'Toxicokinetic parameters', and 'Actions'. The top table has two rows: Row 1 (checkbox checked) with Test no. #1 and Toxicokinetic parameters 'half-life 1st: xxx123'; Row 2 (checkbox unchecked) with Test no. #2 and Toxicokinetic parameters 'half-life 2nd:'. The bottom table also has two rows: Row 1 (checkbox unchecked) with Test no. None and Toxicokinetic parameters None; Row 2 (checkbox checked) with Test no. #1 and Toxicokinetic parameters 'half-life 1st: xxx123'. A red arrow points from the 'New item' button in the top table to the same button in the bottom table.

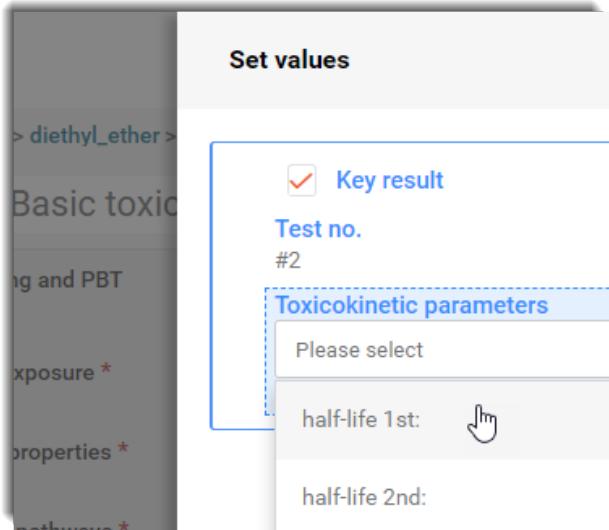
Toxicokinetic parameters		New item	Import file	
#	Key result	Test no.	Toxicokinetic parameters	Actions
# 1	<input checked="" type="checkbox"/>	#1	half-life 1st: xxx123	
# 2	<input type="checkbox"/>	#2	half-life 2nd:	

Metabolite characterisation studies		New item	Import file	
#	Key result	Test no.	Toxicokinetic parameters	Actions
# 1	<input type="checkbox"/>	None	None	
# 2	<input checked="" type="checkbox"/>	#1	half-life 1st: xxx123	
# 3	<input type="checkbox"/>	#2	half-life 2nd:	

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 58: 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 59: Clone or delete a row in a table**

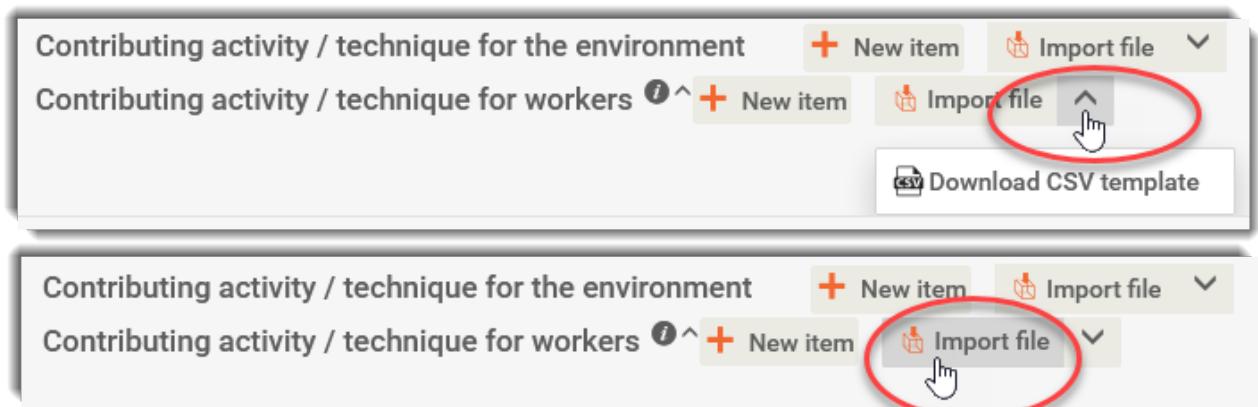
Toxicokinetic parameters		+ New item	Import file	Actions
#	Key result	Test no.	Toxicokinetic parameters	
# 1	<input checked="" type="checkbox"/>	#1	half-life 1st: xxx123	
# 2	<input type="checkbox"/>	#2	half-life 2nd:	
# 3	<input type="checkbox"/>	#3	half-life 3rd:	

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*.

### 3.7.10.1. 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 60: Import file - Download CSV template**

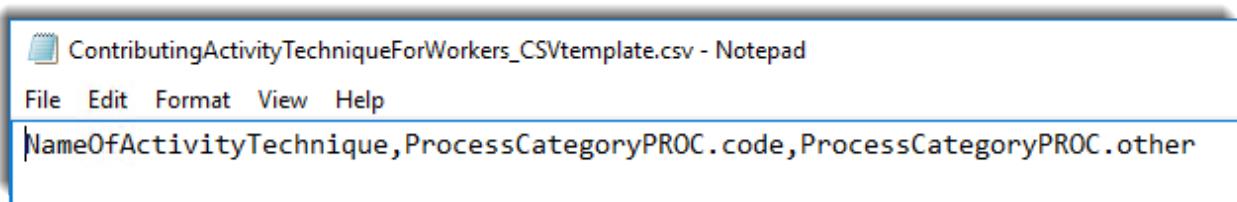
The import file is a table in text format, with each column separated by a comma (CSV). If a field can contain more than one phrase, the separator between the values is a semicolon “;”. If the multiple values can have fields for *other:* or *Remarks* associated with them, the values can be added in dedicated 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 61: 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 web 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 62: Example of the same CSV data file shown in Notepad and Excel**

	A	B	C
1	NameOfActivityTechnique	ProcessCategoryPROC.code	ProcessCategoryPROC.other
2	Activity_1	PROC 7: Industrial spraying;PROC 0: Other:;	;value in field 'other'
3			

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 63: Example of data that has been imported from a file into a table**

1	Name of activity / technique Activity_1	Process category (PROC) ✓ PROC 7: Industrial spraying ✓ PROC 0: Other: value in field 'other'
---	--	---

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 web interface.

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

**Figure 64: Entering boiling point data for a Key result with the data shown in Excel**

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

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*).

### 3.7.10.2. 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.

Toxicokinetic parameters				
Key result		Action		
#	Key result	↔ Test no.	Toxicokinetic parameters	Action

### 3.7.10.3. 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 65: Moving a row up or down in a table.

Cross-reference		New item	Import file	▼
#	Reason / purpose for cross-reference			
1	other: Value of column ReasonPurpose.other			
2	assessment report Value of column ReasonPurpose.remarks			
2	assessment report Value of column ReasonPurpose.remarks			
3	assessment report			

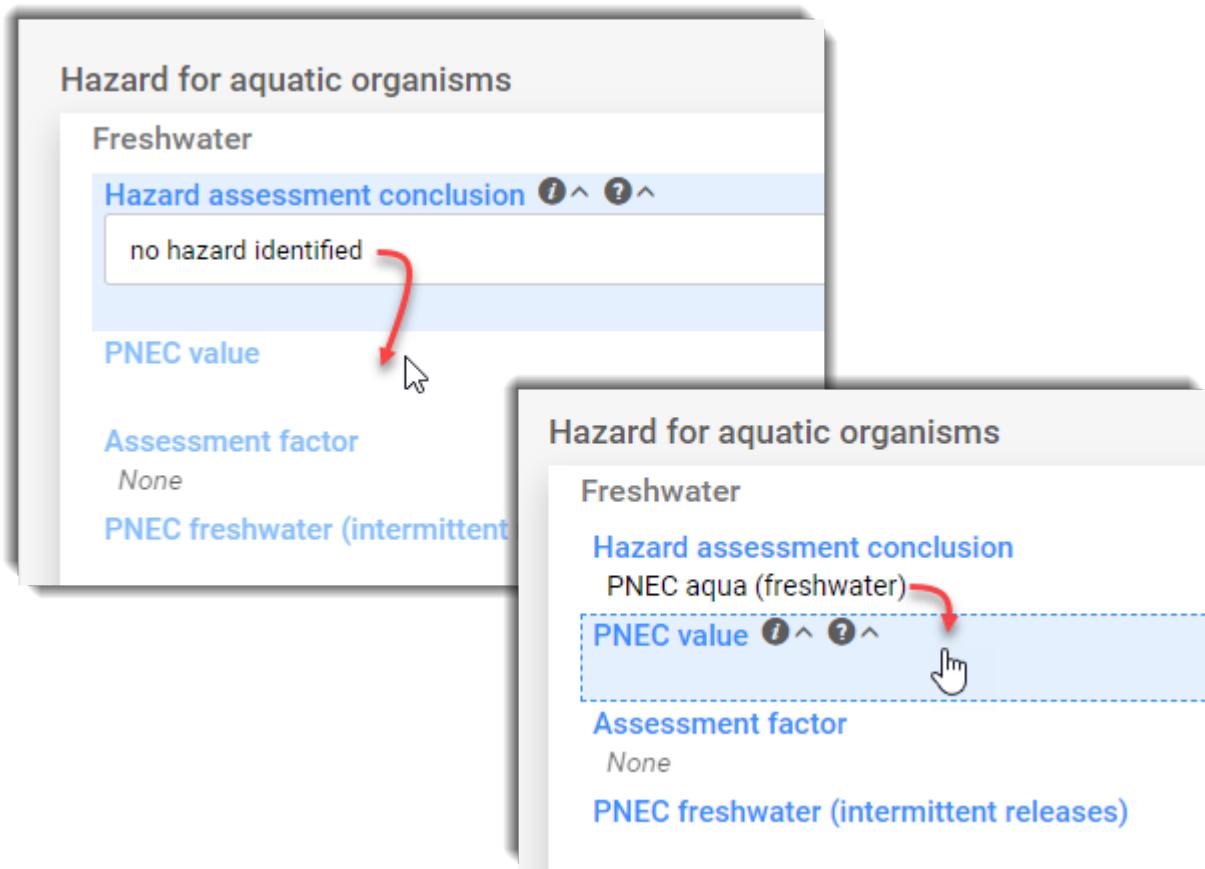
### 3.7.11. Dynamic content rules

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 66: 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 67: Effect of breaking a dynamic content rule**

The screenshot shows a form titled "Hazard for aquatic organisms" under the "Freshwater" section. The "Hazard assessment conclusion" field contains the text "insufficient hazard data available (further information necessary)". Below this, the "PNEC value" field is highlighted with a red dashed border and contains "23 µg/L". A red error message next to it says "✖ This field is expected to be empty". The "Assessment factor" field is set to "None" and the "Extrapolation method" field is also set to "None". The "PNEC freshwater (intermittent releases)" field is empty. At the bottom right, there is a red button with a question mark icon and a "Save" button. A red error message box is displayed above the buttons, stating "Error(s) blocked this document from being saved. Please correct them and try again." A cursor arrow points towards the question mark icon.

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 68: Dynamic content rules applied to imported migrated data**

**Endpoint**

acute toxicity: oral  
REMARKS\_ENDPOINT\_STUDY\_RECORD.AcuteToxicityOral.A

**Type of information**

other: No other  
REMARKS\_ENDPOINT\_STUDY\_RECORD.AcuteToxicityOral.T

**Adequacy of study**

key study ✖ This field is expected to be empty

Robust study summary

Used for classification

Used for SDS

**Study period**

ENDPOINT\_STUDY\_RECORD.AcuteToxicityOral.A

**Reliability**

other: No other

**Rationale for reliability incl. deficiencies**

other: No other  
REMARKS\_ENDPOINT\_STUDY\_RECORD.AcuteToxicityOral.R

**Data waiving**

study scientifically not necessary / other information ✖ This field is expected to be empty

the study does not need to be conducted because

**Endpoint**

acute toxicity: oral  
REMARKS\_ENDPOINT\_STUDY\_RECORD.AcuteToxicityOral.A

**Type of information**

other: No other  
REMARKS\_ENDPOINT\_STUDY\_RECORD.AcuteToxicityOral.T

**Adequacy of study**

key study

Robust study summary

Used for classification

Used for SDS

**Study period**

ENDPOINT\_STUDY\_RECORD.AcuteToxicityOral.A

**Reliability**

other: No other

**Rationale for reliability incl. deficiencies**

None

**Data waiving**

None

**Justification for data waiving**

None

5

3

Save

1

2

4

5

3

### 3.7.12. 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 69: Table of contents with the data window in editing or viewing mode**

The screenshot shows the IUCLID web interface with the following details:

- Working context:** REACH Registration 10 - 100 tonnes (highlighted with a red circle labeled 1).
- Table of contents (Tree View):**
  - REACH Registration 10 - 100 tonnes (highlighted with a red circle labeled 2)
  - table\_salt (highlighted with a red circle labeled 3)
    - 1 General information\* (6 documents)
    - 2 Classification & Labelling and PBT assessment\* (2 documents)
    - 3 Manufacture, use and exposure\* (18 documents)
    - 4 Physical and chemical properties\* (10 documents)
    - 5 Environmental fate and pathways\* (4 documents)
    - 6 Ecotoxicological information\* (6 documents)
      - Ecotoxicological information ESS1 (highlighted with a red circle labeled 4)
        - 6.1 Aquatic toxicity\* (3 documents)
          - Aquatic toxicity (highlighted with a red circle labeled 5)
          - Aquatic toxicity: A - template\_1
          - 6.1.1 Short-term toxicity to fish\* (3 documents)
            - Short-term toxicity to fish ESS1 (highlighted with a red circle labeled 6)
            - Short-term toxicity to fish ESR1
            - Short-term toxicity to fish.002
        - 6.1.2 Long-term toxicity to fish
- Data Window (Right Panel):** Short-term toxicity to fish ESR1
  - UUID: caf9b913-b5bf-437e-a1b4-e1537194f05
  - None None
  - Administrative data:** (None)
  - Endpoint:** short-term toxicity to fish
  - Type of information:** experimental study
  - Adequacy of study:** key study
  - Robust study summary:**
  - Used for classification:**
  - Used for SDS:**
  - Study period:** 3 m
  - Reliability:** 2 (reliable with restrictions)
  - Rationale for reliability incl. deficiencies:** None
  - Data waiving:** None
  - Justification for data waiving:** None
  - Justification for type of information:** None

**Legend for Figure 69**

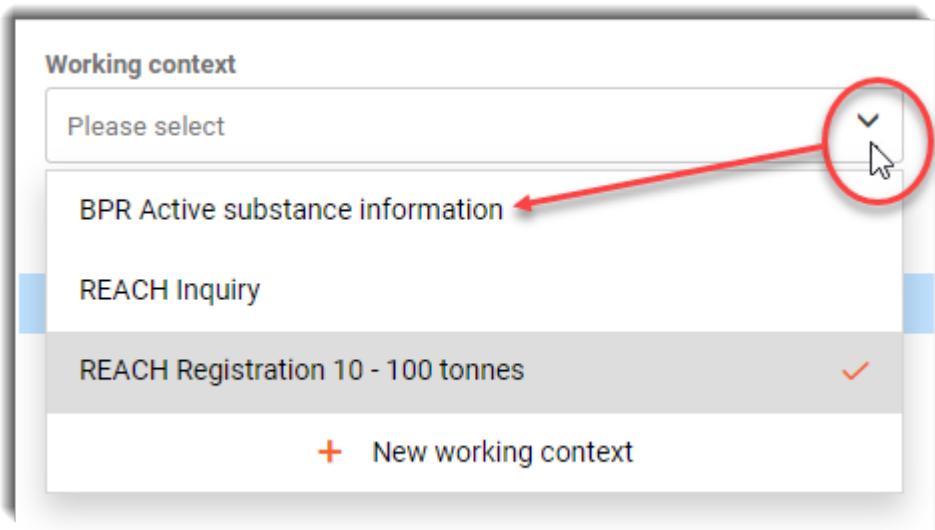
1. A working context of *REACH Registration 10 -100 tonnes* has been selected;
2. The first row gives access to the draft dossier header of a raw substance dataset, as indicated by the icon
3. The number of documents in a section;
4. On hovering over a section header, an orange cross (+) appears which 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 (trash bin) 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;

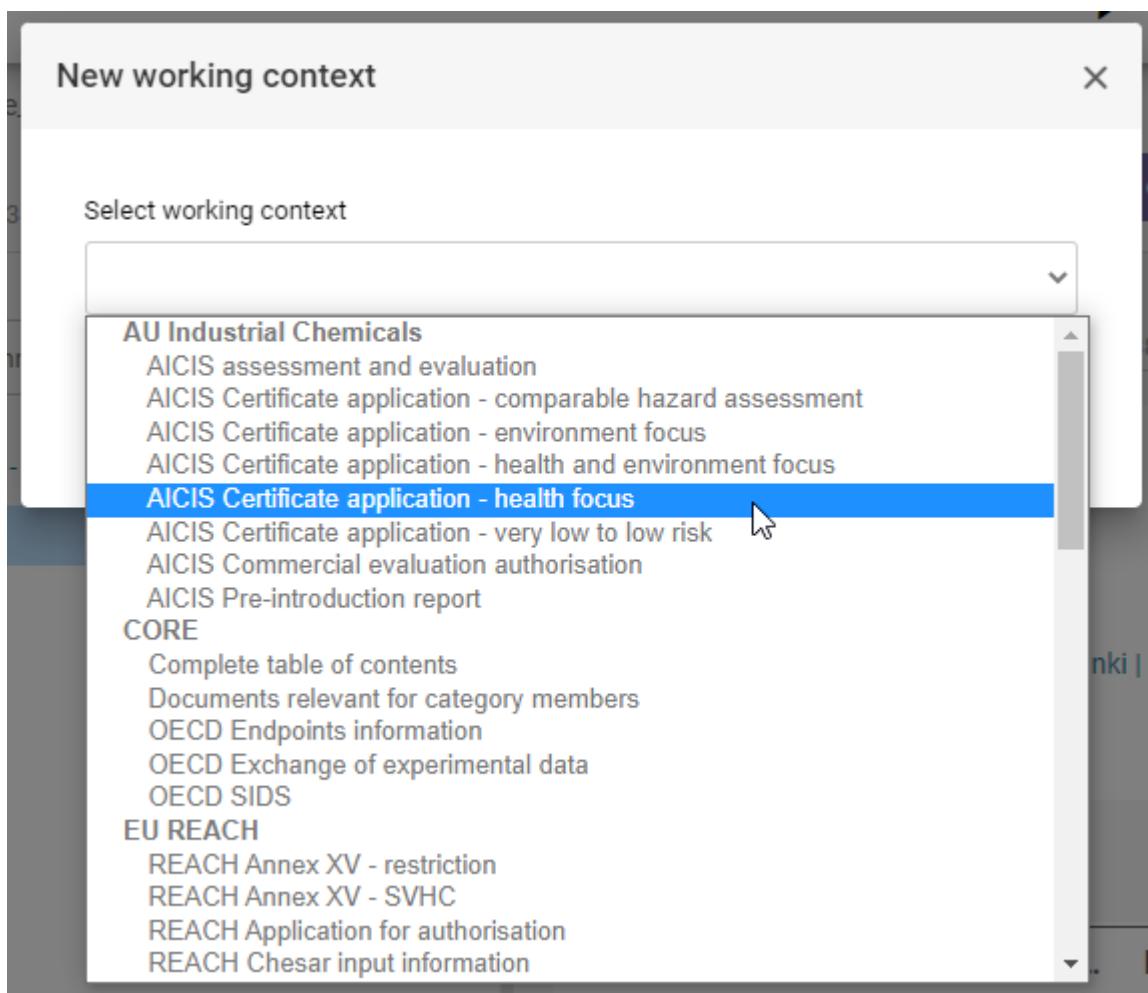
The working context is selected from a drop-down menu of options that have been pre-selected by the user to form a personalised list. An example menu is shown below, where the button to open it is ringed in red.

**Figure 70: 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, *A/CS Certificate application – health focus* is being added to the menu.

**Figure 71: 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*.

### 3.7.12.1. 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 72: Complete table of contents**

The screenshot shows the IUCLID web interface for a Substance dataset named 'table\_salt'. The left panel displays a 'Working context' sidebar with a dropdown menu set to 'Complete table of contents'. This menu is circled in red. Below it is a tree view of document categories and their counts: CORE (50), OECD (28), AU Industrial Chemicals, EU BPR, EU CLP, DOMAIN (1), and REACH (7). Under 'DOMAIN', the 'table\_salt' document is selected and highlighted with a blue bar. The right panel shows detailed substance information: Substance name\* (table\_salt), Public name (Table Salt from IUCLID 5.6.0.2), Legal entity\* (European Chemicals Agency | Helsinki | No other), and Third party (None). It also includes sections for Other substance identifiers, Contact persons (one person listed), Identification of substance (Reference substance: sodium chloride | sodium chloride | 7647-14-5), and Type of substance.

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

Working context

REACH Registration 10 - 100 tonnes

- REACH Registration 10 - 100 tonnes
- ▼ table\_salt
  - > 1 General information\* 6
  - > 2 Classification & Labelling and PBT assessment\* 2
  - > 3 Manufacture, use and exposure\* 18
  - > 4 Physical and chemical properties\* 10
  - > 5 Environmental fate and pathways\* 4
  - ▼ 6 Ecotoxicological information\* 4
    - Ecotoxicological information ESS1
      - ▼ 6.1 Aquatic toxicity\* 3
        - Aquatic toxicity
          - > 6.1.1 Short-term toxicity to fish\* 2
            - Short-term toxicity to fish ESS1
            - Short-term toxicity to fish ESR1
          - 6.1.2 Long-term toxicity to fish

**Figure 74: Example location in table of content: Short-term toxicity to fish under 'Complete table of contents'**

Working context	
Complete table of contents	
	table_salt
	CORE
	1 General information
	2 Classification & Labelling and PBT assessment
	3 Manufacture, use and exposure
	4 Physical and chemical properties
	5 Environmental fate and pathways
	6 Ecotoxicological information
	Ecotoxicological information ESS1
	6.1 Aquatic toxicity
	Aquatic toxicity
	6.1.1 Short-term toxicity to fish
	Short-term toxicity to fish ESS1
	6.1.2 Long-term toxicity to fish
	OECD
	A Physico-chemical properties
	B Degradation and accumulation
	C Effects on biotic systems
	41 Short-term toxicity to fish
	Short-term toxicity to fish ESR1
	42 Long-term toxicity to fish

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 75: Filtering a table of contents

Working context

REACH Registration above 1000 tonnes

skin

- REACH Registration above 1000 tonnes
- table\_salt
- 7 Toxicological information\*
  - 7.1 Toxicokinetics, metabolism and distribution\*
    - 7.1.2 Dermal absorption
      - Skin absorption tests from lab ABC
  - 7.3 Irritation / corrosion\*
    - 7.3.1 Skin irritation / corrosion\*
  - 7.4 Sensitisation\*
    - 7.4.1 Skin sensitisation\*
- Inherited templates

### 3.7.12.2. 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*.

### 3.7.12.3. 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.

#### 3.7.12.4. 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*.

#### 3.7.12.5. 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*.

#### 3.7.12.6. 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*.

#### 3.7.12.7. 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 76:** Opening a sub-tree in the table of contents

Dashboard > Mixtures / Products > Biocidal product 1

# Biocidal product 1

05fca313-ea0a-4dc0-bd56-e4f8787d34bb

## Working context

EU PPP Active substance application (product)

Type at least 3 characters

- EU PPP Active substance application (product)
- Biocidal product 1
  - 1 Identity of the plant protection product and applicant
    - 1.1 Identity of the plant protection product, trade name or proposed trade name, and applicant
    - 1.2 Producer of the plant protection product
    - 1.3 Producer's development code number if appropriate
    - 1.4 Detailed quantitative and qualitative information on the composition of the plant protection product
      - 1.4.1 (Cf. 1.4) Composition of the plant protection product
      - 1.4.2 (Cf. 1.4) Information on the active substances
      - 1.4.3 (Cf. 1.4) Information on safeners, synergists and co-formulants
    - 1.4.4 Information on metabolites
      - Information on metabolites.001
        - Metabolite One
        - Metabolite Two

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 77: Closing a sub-tree in the table of contents**

Dashboard > Mixtures / Products > Biocidal product 1

## Biocidal product 1

05fca313-ea0a-4dc0-bd56-e4f8787d34bb

Working context

EU PPP Active substance application (product)

Type at least 3 characters  X

Biocidal product 1  Information on metabolites.001

Metabolite One 

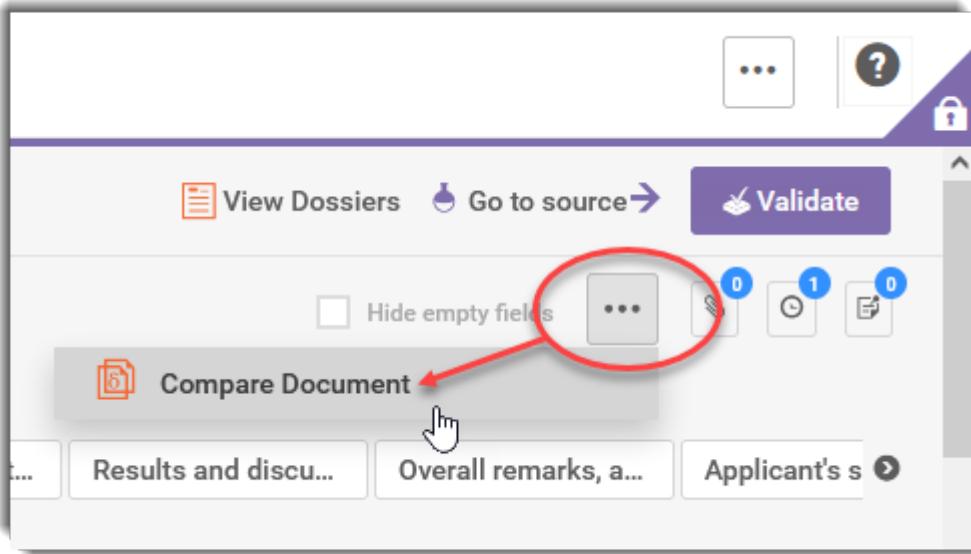
> 1 Identity of the substance	1
> 2 Physical and chemical properties of the substance	2
> 3 Further information on the substance	



### 3.7.13. Compare two documents

The output of *Compare Document* is an HTML file that can be viewed in a web browser, for example by opening it in a tab alongside the web interface of IUCLID. To compare two *Dossiers*, start by viewing the record of the source *document* against which the comparison will be made, and then select *Compare Document*, from the three-dot menu, at the top righthand corner of the data window, as shown below.

Figure 78: Open the feature that compares two documents



Select the entity that contains the other document.

**Figure 79: Select the entity that contains the other document to be compared**

The screenshot shows a dialog titled "Compare with: Entity Selection". At the top, there is a search bar and a dropdown menu for "Entity Type" with options: Substance (selected), Mixture, Templates, and Dossiers. Below the search bar, a message says "6 results found". The results are listed in a table with columns: Name, Date, and various metadata fields (Inventory number, CAS number, IUPAC name, Legal Entity, Predefined Legal entity, Submission type, UUID). Two entries are highlighted with orange borders: "table\_salt" (Inventory number 231-598-3) and "Metabolite One" (Inventory number 200-580-7). A cursor arrow points to the "Metabolite One" entry.

Name	Date	Inventory number	CAS number	IUPAC name	Legal Entity	Predefined Legal entity	Submission type	UUID
table_salt	21/09/2022 19:51	231-598-3	7647-14-5	sodium chloride			REACH Registration 10 - 100 tonnes	IUC5-2dd443b4-a92a-4f7b-9348-b7a896f4c38c
Metabolite One	20/09/2022 19:10	200-580-7						8445e42a-1c05-4514-bd00-ce266e851186

Select a document. Only documents in the same section of the table of contents, and of the same type are offered for selection. In the example shown below an endpoint study record in the section *Water solubility* is the source document. There is an endpoint study summary in that section, but it is not offered for comparison.

**Figure 80: Select a document to be compared**

The screenshot shows a dialog titled "Compare with: Document Selection". It displays a list of documents under the heading "REACH Registration 10 - 100 tonnes". The first item is "Physical and chemical properties". Below that is a section titled "Water solubility" containing three items: "ws\_record\_1", "ws\_record\_2", and "ws\_record\_3". The "ws\_record\_2" item is highlighted with a red oval, and a cursor arrow points to it.

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, which is described in section 8.5 *Compare Dossiers*.

**Figure 81: A document comparison report**

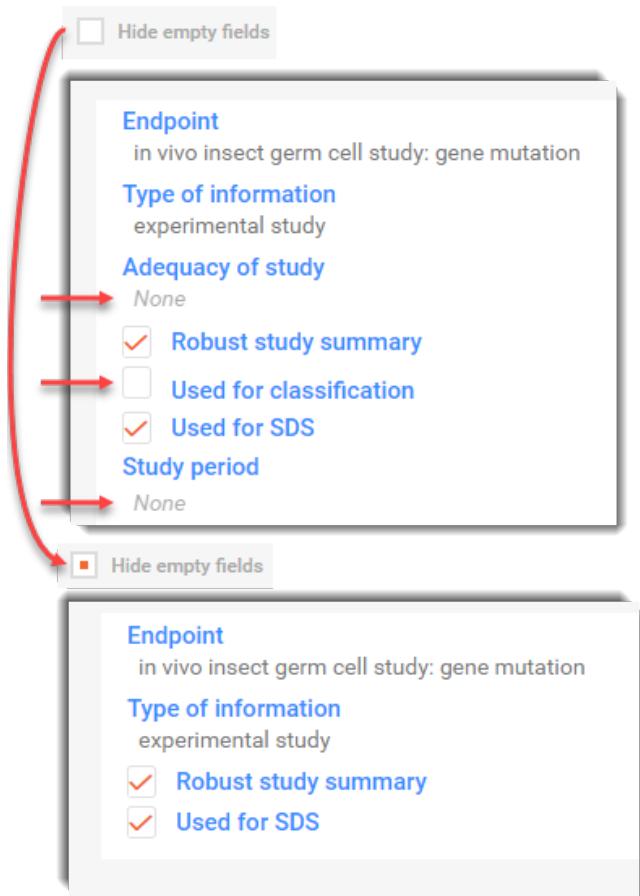
The screenshot shows a 'Document Comparison Report' for two study records, ws\_record\_1 and ws\_record\_2. The table has three columns: Field, Source, and Target.

Field	Source	Target
<b>Attachments</b>		• migrated_TMI-d78e7bb0-1cfa-3700-897f-d6c828d708ce.txt 176 text/plain
<b>Document name</b>	ws_record_1	ws_record_2
<b>Type of information</b> i Water solubility > Administrative data	(Q)SAR default Remark in second Dossier	
<b>Adequacy of study</b> i Water solubility > Administrative data	key study	other information
<b>Robust study summary</b> i Water solubility > Administrative data	true	false
<b>Reliability</b> i Water solubility > Administrative data	2 (reliable with restrictions)	
<b>Reliability</b> i ENDPOINT_STUDY_RECORD.WaterSolubility.AdministrativeData.Reliability	2 (reliable with restrictions)	

### 3.7.14. Hide empty fields

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

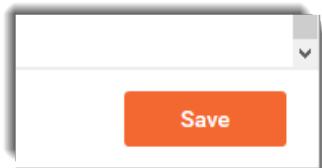
Figure 82: Hide empty fields



### 3.7.15. Save

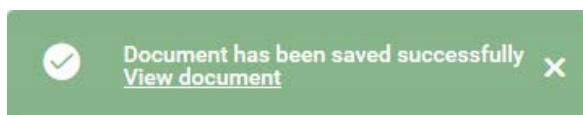
After editing a document, click on the **Save** button at the bottom right of the interface:

Figure 83: 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.

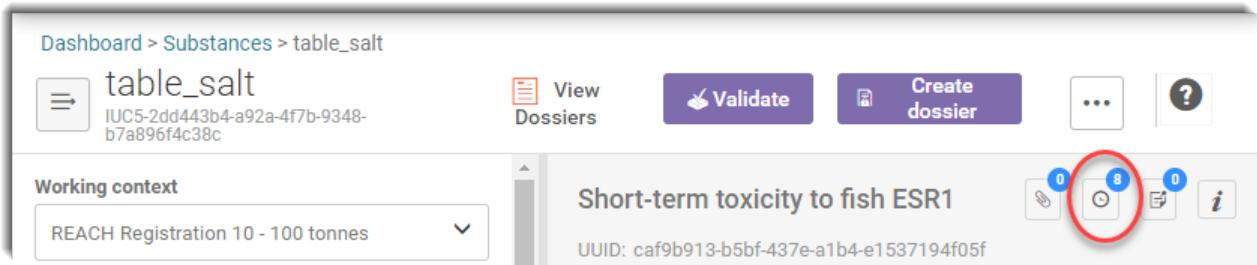
Figure 84: Option to view a document that has just been saved



### 3.7.16. Modification History

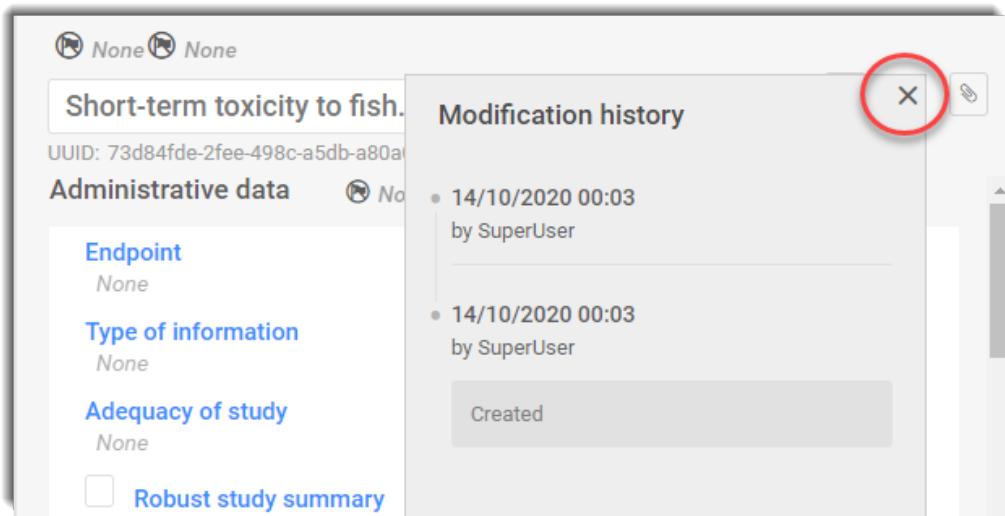
The modification history for a document is available whilst the document is open in the data window. It is accessed via a button at the top right of the data window, as shown in the example below. The number of items in the history is indicated in a superscript:

**Figure 85: Access to the modification history**



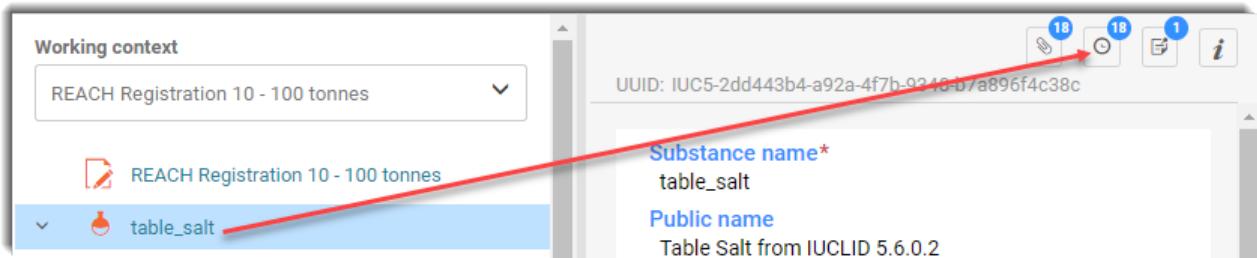
For each event, the history shows a timestamp, the IUCLID User that carried out the action, and for some cases, a description of the event. The example below shows the modification history of an *Endpoint study record* immediately after it has been created. Note that the document is open in the data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

**Figure 86: 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 87: Access to the modification history of a Substance**



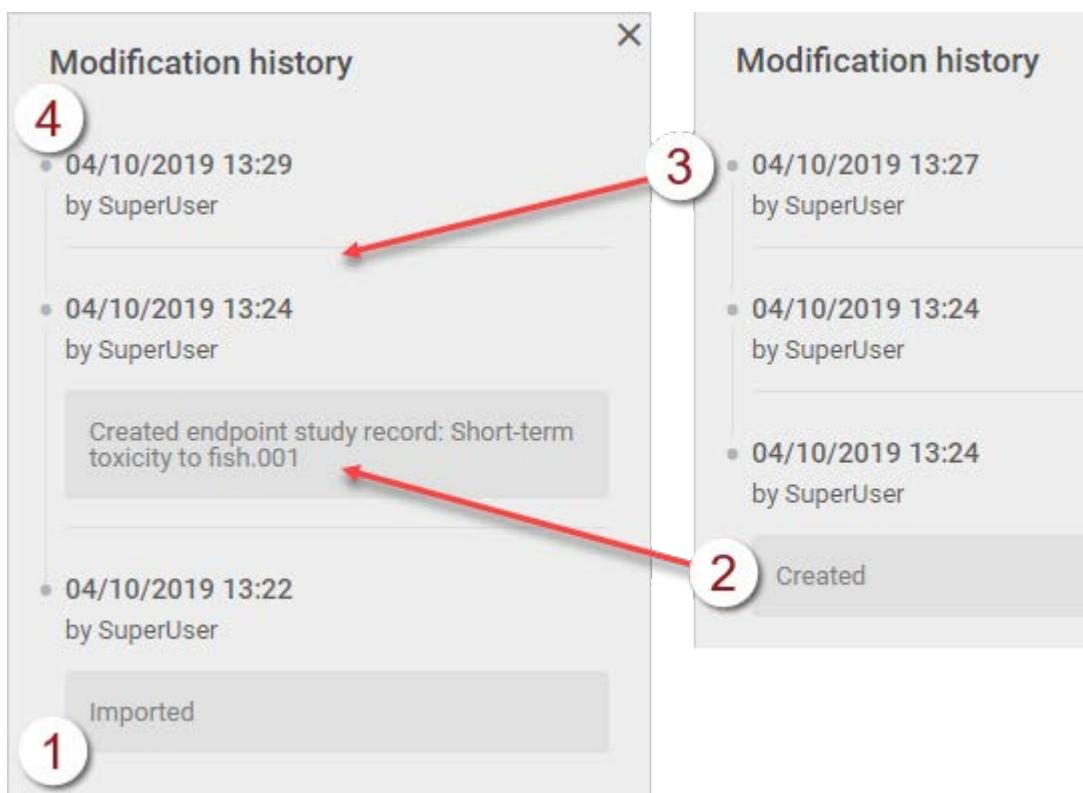
When the content inside a IUCLID document is edited, the edit does not appear in the modification history of a IUCLID document or entity that refers to it. For example, when the value of a field is changed inside an *Endpoint study record*, the event does not appear in the modification history of a *Substance* 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 88: Example modification histories for a Substance and an Endpoint study record inside it**



#### Legend for Figure 88

- 13:22 *Substance* was imported from an i6z file;
- 13:24 An *Endpoint study record* was created with the default name, *Short-term toxicity to fish.001*;
- 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*;

### 3.7.17. Bookmarks, hyperlinks, and the sharing of entities and documents

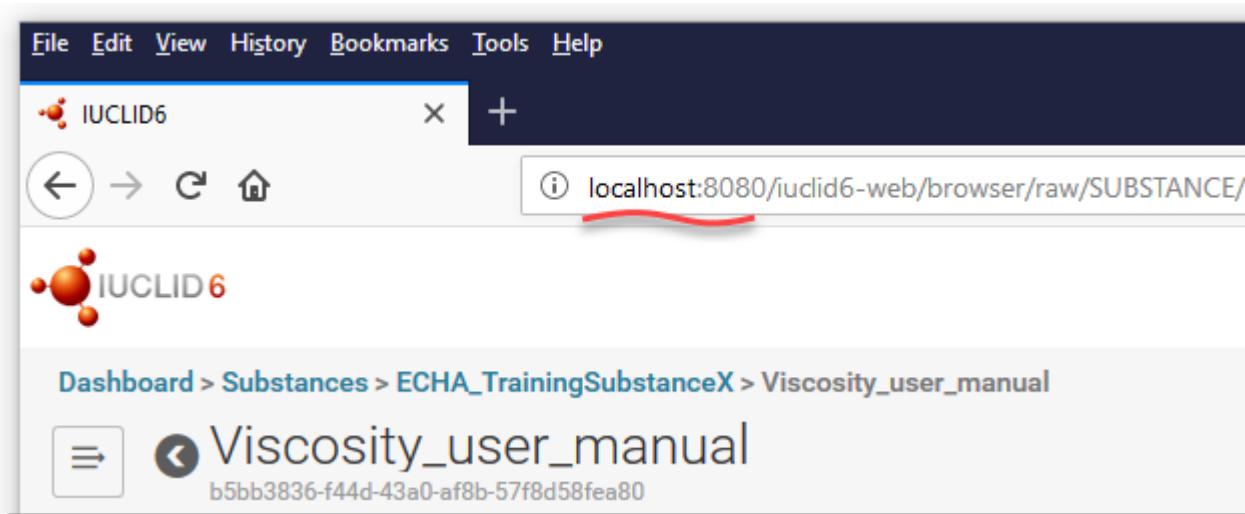
The web technology behind the interface means that it is possible to create a hyperlink that points to any document or entity. Such links can be saved as bookmarks, and then shared between colleagues. To create a bookmark that links to an entity, view the entity, and then create a bookmark in the browser. 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 89: 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.

The screenshot shows the IUCLID web interface. At the top, the URL is 'Dashboard > Substances > 1,2-dichloroethane'. Below this, there's a card for '1,2-dichloroethane\_R\_10\_100' with the UUID '0d1d896a-38bb-450f-bdcb-562bba785a02'. A red arrow points from the dossier name to its UUID. To the right, there are buttons for 'View Dossiers', 'Go to source', and 'Validate'. Below the UUID, the 'Dossier Submission Type' section is shown, containing the 'Dossier name (given by user)' '1,2-dichloroethane\_R\_10\_100'.

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>

### 3.7.18. 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 90: Open in new tab from a list page

The screenshot shows a substance record for formaldehyde. The record includes fields for DISS v4.3.0, Inventory number (200-001-8), CAS number (50-00-0), IUPAC name (formaldehyde), Legal Entity (European Chemicals Agency), and UUID (c68d1c31-2834-4429-ae94-70db4f222e91). A red circle highlights the 'Open in new tab' icon (a square with a plus sign) in the top right corner of the record card.

### 3.7.19. 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 91:** Re-order repeatable blocks in a numbered list

Contact persons + New item

1 Person  
User, Manual; ECHA | User | Manual | ECHA

2 Person  
Tester, T; Not available | Tester | T | Not available | Fenton

3 Person  
Substance-manager; ECHA | Substance-manager | ECHA

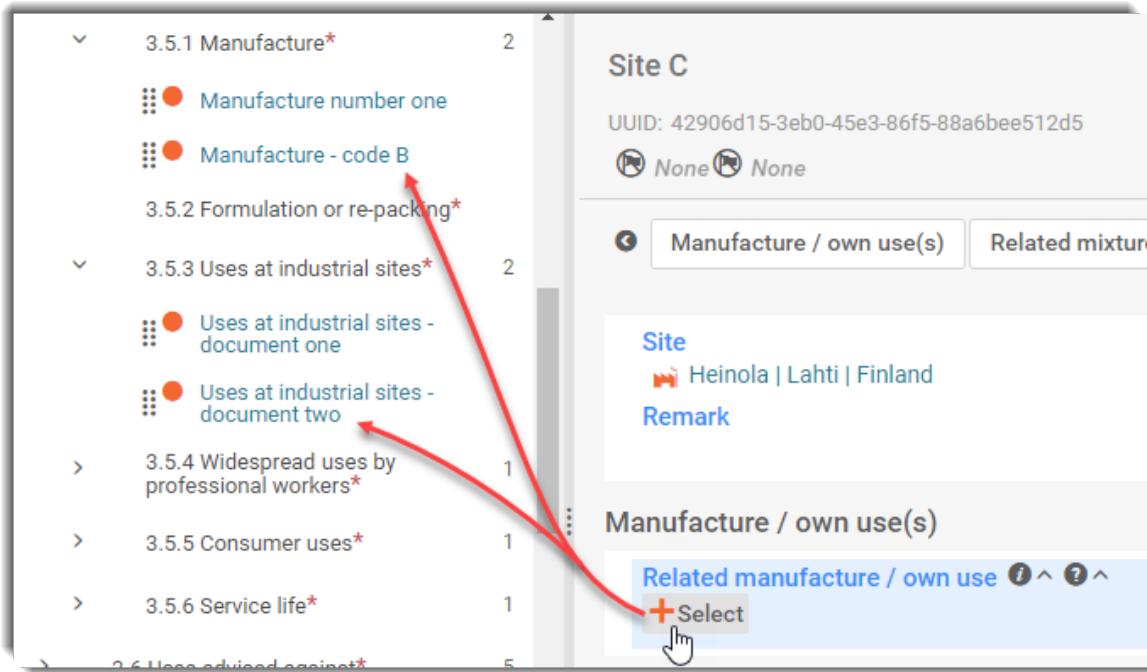
In the example below, a numbered table row has been moved from position one to three.

**Figure 92:** Re-order numbered table rows

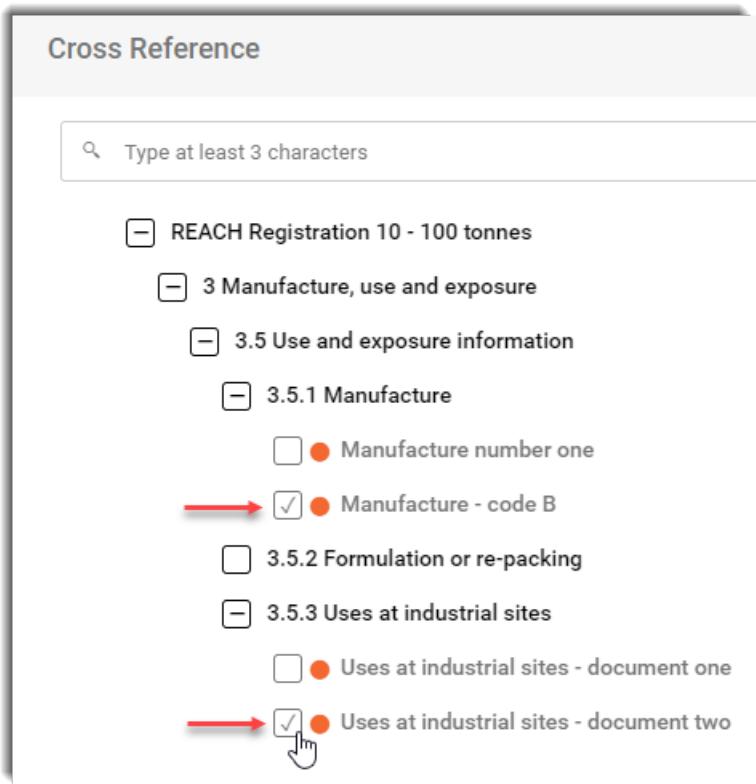
Other substance identifiers		+ New item	Import file	▼
#	Flags	Identifier	Identity	Country
2	(P) None (P) None	common name	Coal	None
3	(P) None (P) None	common name	Carbon	None
1	(P) None (P) None (P) None (P) None	common name common name	coking coal coking coal	None

### 3.7.20. 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*.

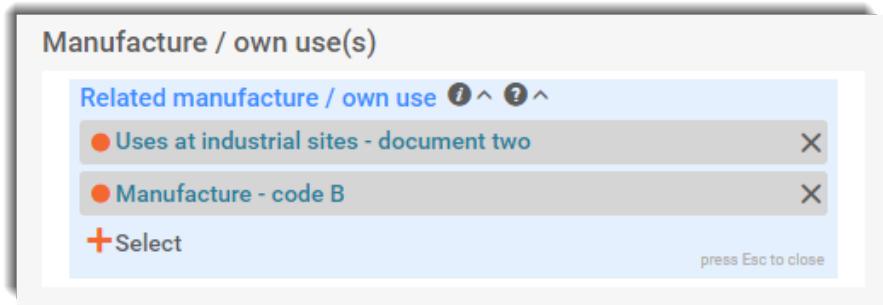
**Figure 93: Creating references between documents**

A document is selected from the tree by ticking its box. There can be multiple selections.

**Figure 94: The Cross Reference window**

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

**Figure 95: Cross references between documents**



### 3.8. 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 96: Example of an inbound reference**

The screenshot displays two separate windows for "Composition X" and "Composition Y". Both windows have a red circle around their respective titles ("Composition X" and "Composition Y").

**Composition X:**  
UUID: 287d3366-a13e-356b-abaf-42a9737b67ef  
Constituents

#	Reference substance
1	(P) None (P) None  sodium chloride   sodium chloride   7647-14-5

**Composition Y:**  
UUID: f7c04edb-b52d-4511-856e-8c99ffaa4ab9  
Constituents

#	Reference substance
1	(P) None (P) None  sodium chloride   sodium chloride   7647-14-5

A red arrow points from the "sodium chloride" entry in Composition X to the same entry in Composition Y, indicating a shared reference.

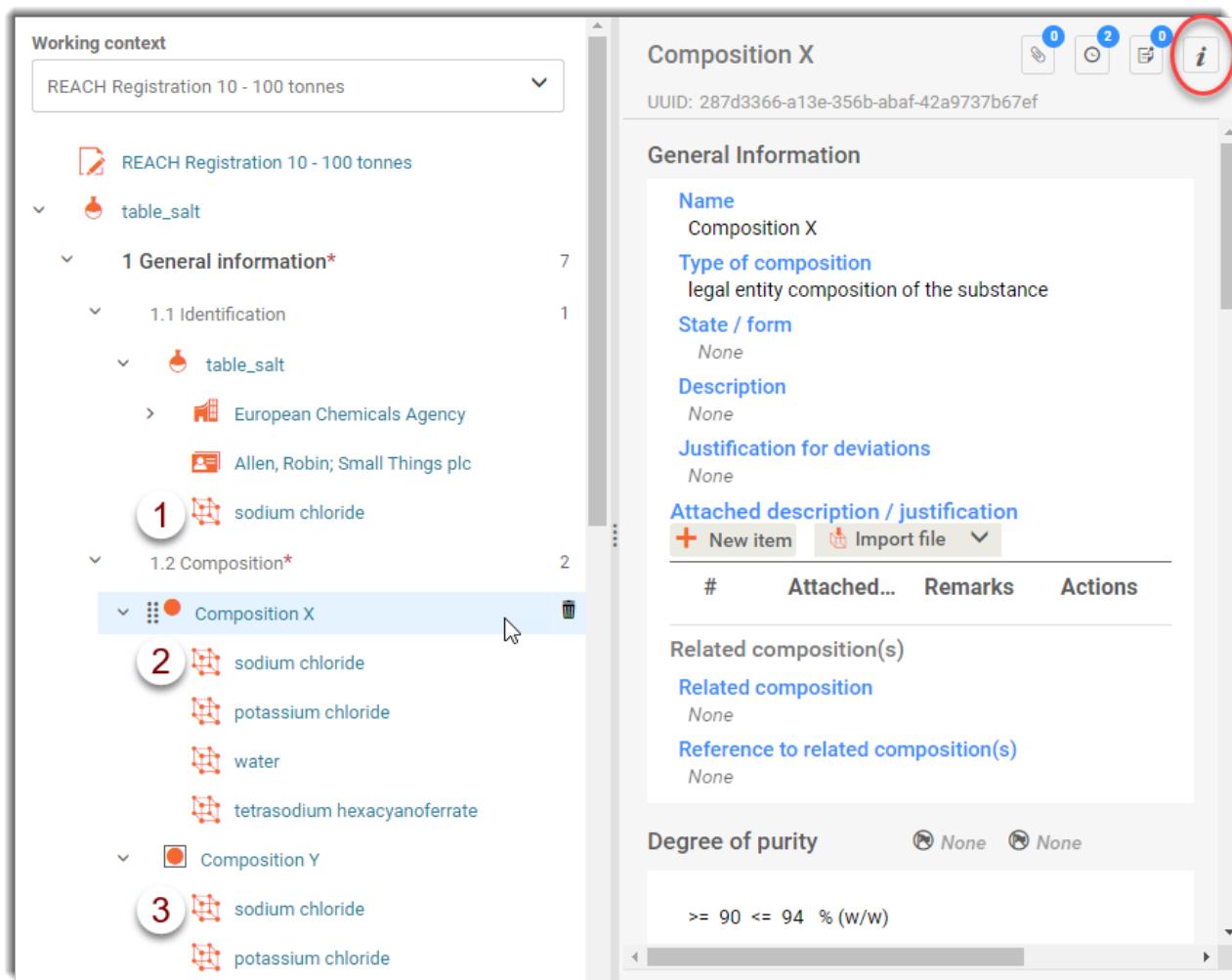
An entity that is directly linked to or referred to as shown in the example above is said to have an *inbound reference*.

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  , 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 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 97: An example of inbound links to a Reference substance from a Composition and a Substance**



The screenshot illustrates the IUCLID web interface. On the left, the 'Working context' panel shows a 'REACH Registration 10 - 100 tonnes' entry. The main area displays 'Composition X' details, including its UUID: 287d3366-a13e-356b-abaf-42a9737b67ef. The 'General Information' section includes fields for Name (Composition X), Type of composition (legal entity composition of the substance), State / form (None), Description (None), and Justification for deviations (None). The 'Attached description / justification' section allows for new items or importing files. Below this is a table for Related composition(s) with columns for # (Count), Attached... (Attachment status), Remarks, and Actions. The table shows one entry: 'Related composition' (None) and 'Reference to related composition(s)' (None). At the bottom, there's a 'Degree of purity' section with two radio buttons set to 'None' and a text input field containing '>= 90 <= 94 % (w/w)'. On the far right of the composition window, a circled 'i' icon is highlighted, indicating the presence of inbound references. The left sidebar lists three instances of sodium chloride: 1) in the REACH registration, 2) directly in the composition, and 3) in a template.

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 98: The inbound links for the Reference substance shown in the example above**

Document's inbound references

2 SubstanceComposition (Flexible Record) / Composition X 05/04/2022 19:19

Substance	table_salt	UUID	287d3366-a13e-356b-abaf-42a9737b67ef
-----------	------------	------	--------------------------------------

test\_material\_one\_13\_14\_0 05/04/2022 19:19

UUID	713b1a23-b7f1-4fb1-bce5-0164d892856d
------	--------------------------------------

1 table\_salt 06/04/2022 22:56

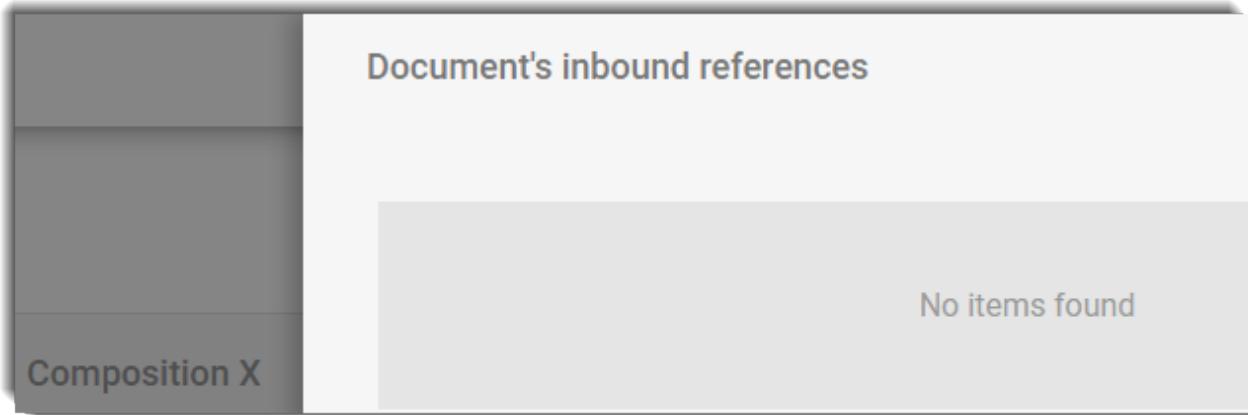
Inventory number	231-598-3	CAS number	7647-14-5	IUPAC name	sodium chloride
Legal Entity	European Chemicals Agency	UUID	IUC5-2dd443b4-a92a-4f7b-9348-b7a896f4c38c		

3 SubstanceComposition (Flexible Record) / Composition Y 06/04/2022 22:57

Template	Composition Y	UUID	f7c04edb-b52d-4511-856e-8c99ffaa4ab9
----------	---------------	------	--------------------------------------

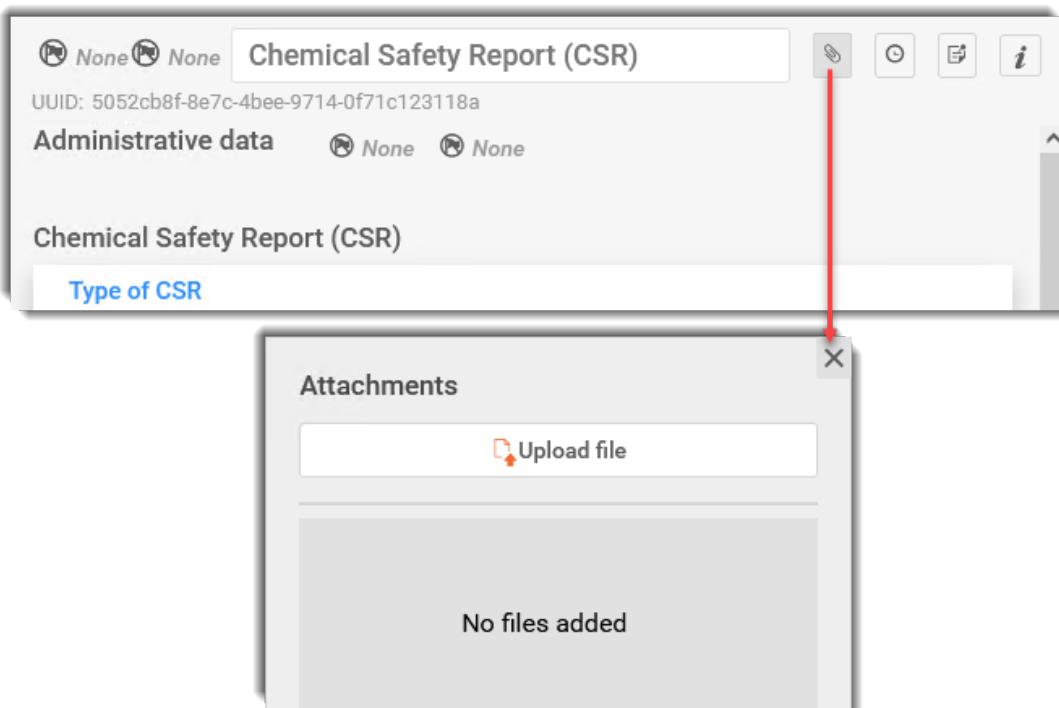
The referring entity or document can be opened in a new browser tab from the arrow icon .

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 99: Documents with no inbound references**

### 3.9. 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.

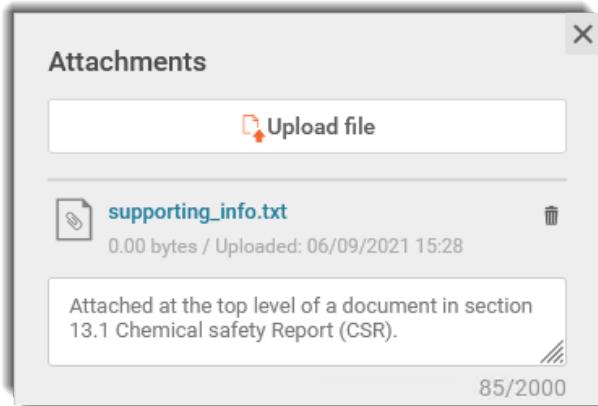
**Figure 100: Open the attachments window**

### 3.9.1. 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 101: Attaching an attachment to a whole document**

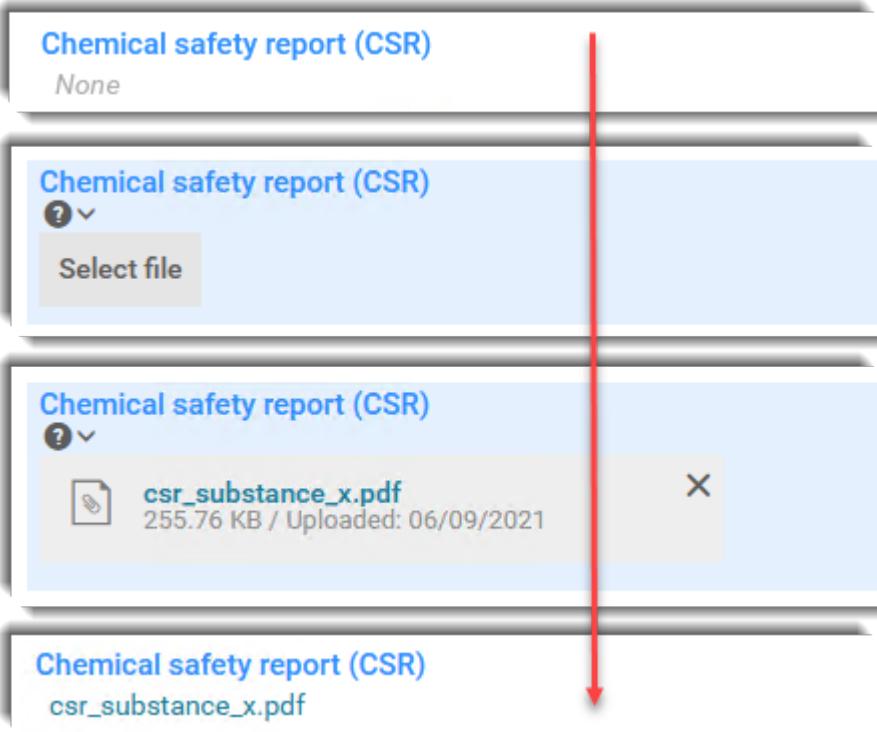


The draft dossier header and whole datasets behave as their own separate documents. Files can be attached at their top level, and they are accessible only from there, in the attachments window. Note that a file attached to a whole *Substance* dataset is accessible from the section *Identification*, and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

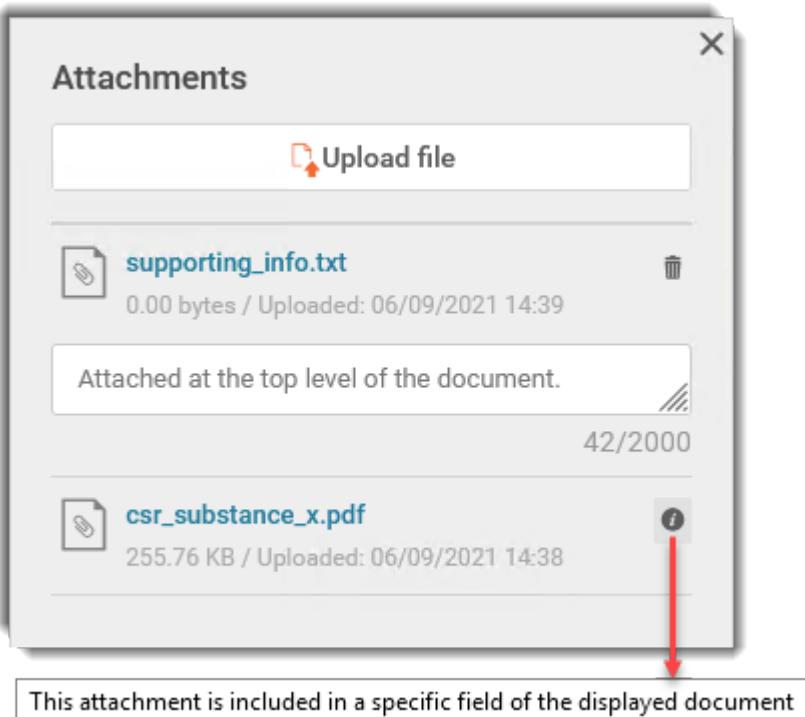
### 3.9.2. Attachments at the field level

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 102: 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 103: 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.

### 3.9.3. 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
```

## 3.10. 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*.

### 3.10.1. 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 104: Search for an entity**

The screenshot shows the 'Reference substances' list page. A red circle highlights the search input field containing 'sodium'. A red arrow points from this circle down to the 'Advanced search' link. Below the search bar, there are buttons for 'Select/Deselect all', '3 results found', 'Export', and 'Delete'. The search results are listed in three items:

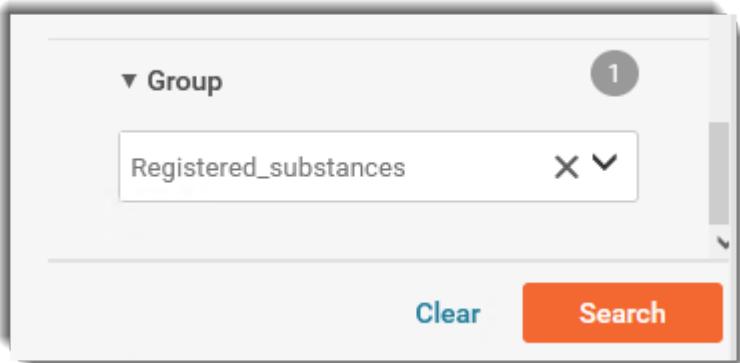
- sodium bromide  
CAS number 7647-15-6  
Inventory number 231-599-9
- sodium iodide  
CAS number 7681-82-5  
Inventory number 231-679-3
- sodium chloride  
CAS number 7647-14-5  
Inventory number 231-598-3

### 3.10.2. 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 25.4) 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 105: Search by security group**

An example search for *Substances* is shown below.

**Figure 106: Advanced search for entities in a list page - Example for Substances**

The screenshot shows an advanced search interface for substances. The search term 'table\_salt' is entered in the 'Name' field. Under 'Reference Substance', 'sodium chloride' is selected. In the 'Impurity Reference Substance' section, 'potassium bromide' and 'potassium chloride' are selected and circled in red. The results list shows two entries:

Entity	Inventory number	CAS
table_salt	231-598-3	CAS
table_salt_no_KCL_impurity	231-598-3	CAS

A red arrow points from the circled 'potassium chloride' to the second result entry.

### Example above

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

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

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*.

## 4. 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 3.7.12 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.

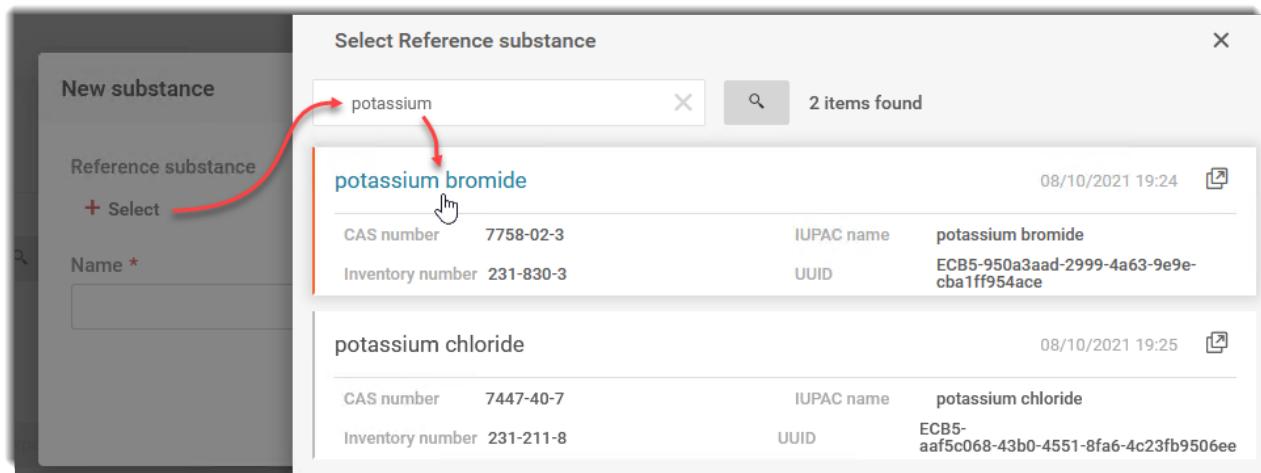
<http://echa.europa.eu/manuals>

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 8.3 *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 11 *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 107: 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 108: Location of the identifying Reference substance of a Substance where no working context is set**

The screenshot shows the IUCLID web interface for managing substances. At the top, it displays the URL 'Dashboard > Substances > 1,2-dichloroethane' and the substance name '1,2-dichloroethane' with its UUID: 3b8ab9b2-3b63-4fb0-8c70-f5cfaf021e51.

**Working context:** A dropdown menu labeled 'Please select' is shown. To its right, a tree view of working contexts is displayed, with '1,2-dichloroethane' selected. Other contexts listed include CORE, OECD, AU Industrial Chemicals, EU BPR, EU CLP, and DOMAIN. The 'DOMAIN' node is circled in red, and a red arrow points from this circle to the 'Identification of substance' section on the right.

**UUID:** 3b8ab9b2-3b63-4fb0-8c70-f5cfaf021e51

**Substance name\***: 1,2-dichloroethane

**Public name**: None

**Legal entity\***: Predefined Legal entity | Helsinki  
Third party  
None

**Other substance identifiers**

#	Flags	Identifier
Contact persons	+ New	
<b>Identification of substance</b>		
Reference substance		1,2-dichloroethane   107-06-2
Type of substance		

## 4.1. 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 109: Assessment entities in the table of contents**

Working context  
REACH Substance Evaluation

REACH Substance Evaluation	
table_salt	
1 General information*	11
1.1 Identification	1
1.2 Composition*	1
1.3 Identifiers	
1.4 Analytical Information*	1
1.7 Suppliers	1
1.10 Assessment approach (assessment entities)	7
Assessment approach	
Registered substance as such	1
Registered substance as such.001	
Specific composition / form of the registered substance	1
Specific composition / form of the registered substance.001	
(group of) constituent in the registered substance	3
(group of) constituent in the registered substance.001	
(group of) constituent in the registered substance.002	
(group of) constituent in the registered substance.003	
Transformation of the registered substance	1
Transformation of the registered substance.001	
2 Classification & Labelling and PBT assessment*	2

#### 4.1.1. 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.

##### 4.1.1.1. 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*.

##### 4.1.1.2. Approach to fate/hazard assessment - public information

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

#### 4.1.2. 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*.

##### 4.1.2.1. 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 3.7.7 *Flag*.

##### 4.1.2.2. 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.

##### 4.1.2.3. Relation to the registered substance

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

##### 4.1.2.4. 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*]

#### 4.1.2.5. 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*.

#### 4.1.2.6. 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.

#### 4.1.2.7. 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.

#### 4.1.2.8. Reaction schema

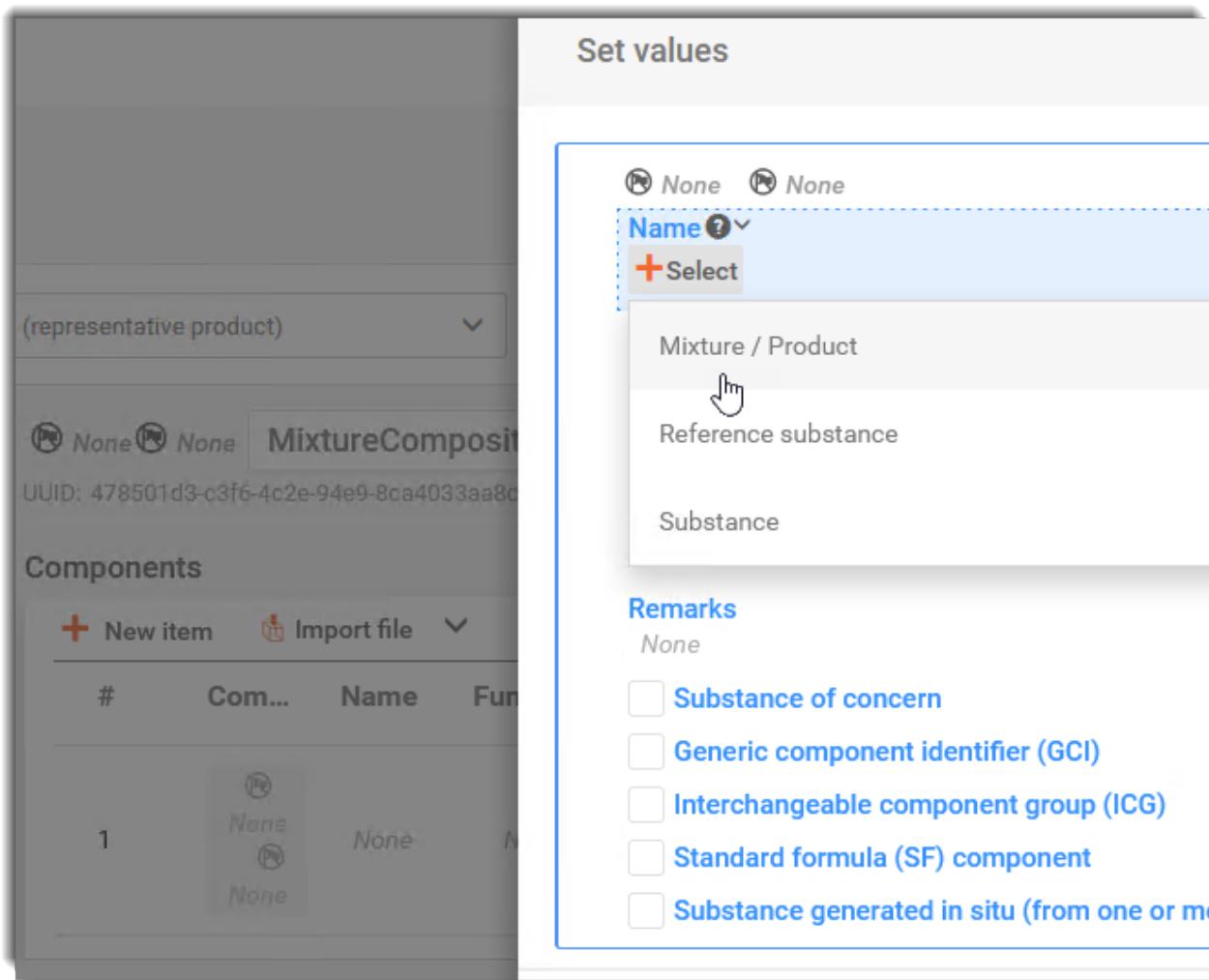
Upload the image of the reaction schema when needed [for *Transformation of the registered substance*].

## 5. 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 110: 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, whilst 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 111: Mixture/Product component - create a Substance based on a Reference substance**

Create new Substance

**Substance name\***  
potassium chloride

**Public name**  
None

**Legal entity\***

Predefined Legal entity

Third party  
None

**Other substance identifiers** + New item Import file ▾

#	Flags	Identifier	Identity	Country
Contact persons <span style="float: right;">+ New item</span>				
Identification of substance <span style="float: right;">(None) (None)</span>				
<b>Reference substance</b> <span style="float: right;">? ▾</span>				
potassium chloride   potassium chloride   7447-40-7				

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 112: Components in a Mixture/Product**

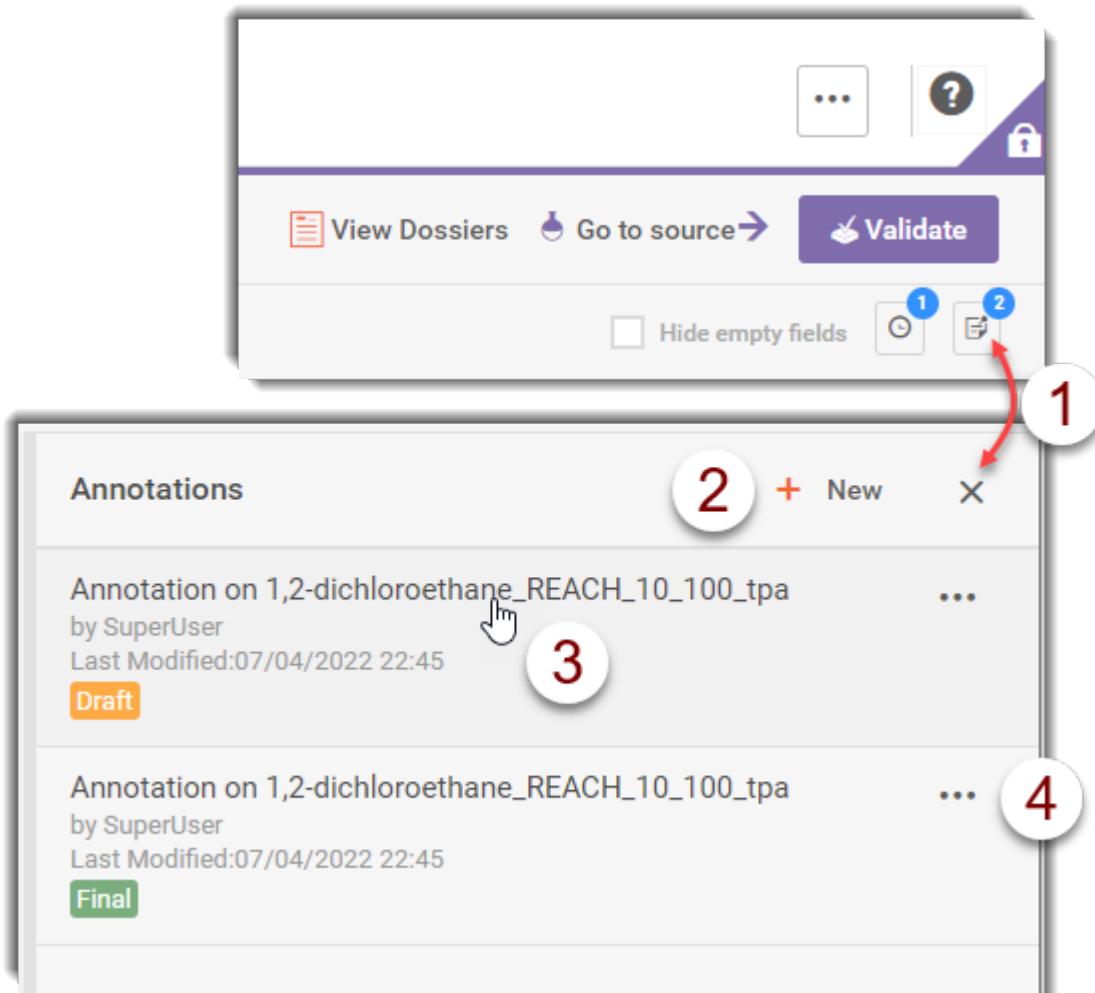
Components		
#	Component flag	Name
1	(P) None (B) None	 testene   testene
2	(P) None (B) None	 potassium bromide   potassium bromide   7758-02-3
3	(P) None (B) None	 potassium chloride   potassium chloride   7447-40-7

*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 8.3 *Viewing Dossiers and Substances or Mixture/Products*.

## 6. Annotation

An *Annotation* is a type of entity in IUCLID 6 that is used as a container for information that relates to the evaluation of data in a particular regulatory context, for example, by a regulatory body. It 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 113: Viewing and managing the Annotations applied to a document**

#### Legend for Figure 113

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.

#### 6.1. 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*.

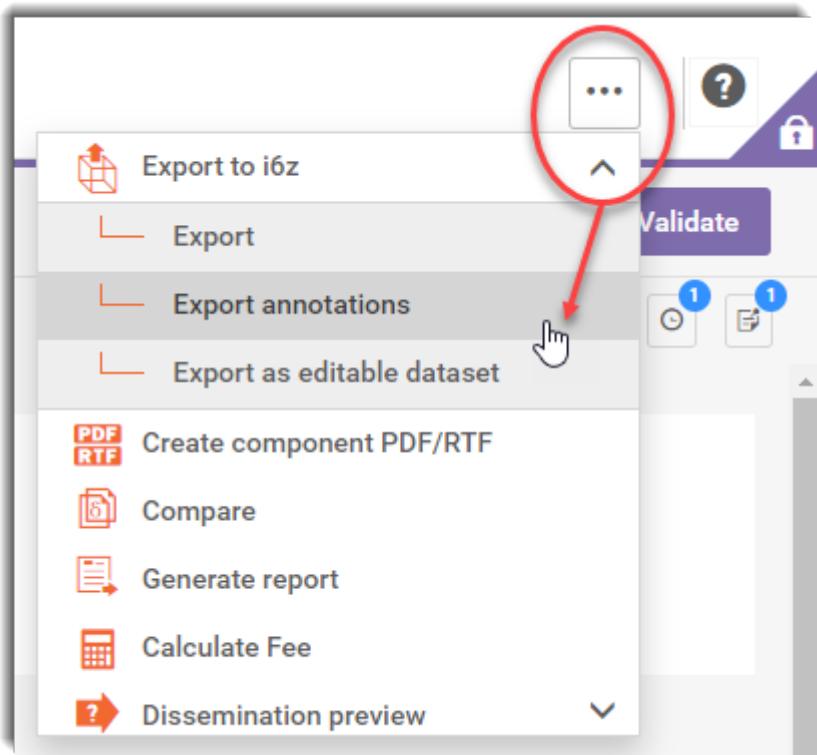
## 6.2. Annotation - Dataset data

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, A. 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.

## 6.3. 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 is on the menu shown in the application bar whilst viewing the record of the *Dossier*.

Figure 114: Export the Annotations from a specific Dossier



## 7. 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.

### 7.1. 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*.

### 7.2. 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 24 *Copy data from ...*.

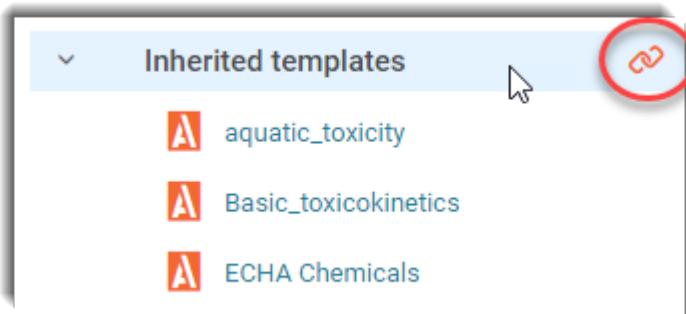
A document copied in this way can be modified in the *Substance* or *Mixture/Product* to which it was copied. Changes to the data in the *Template* do not affect the *Substance* or *Mixture/Product* to which it was copied. If a *Template* is copied more than once to the same *Substance* or *Mixture/Product*, 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.

### 7.3. 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 115: 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 116: A document from an inherited Template in the table of contents**

The screenshot shows a hierarchical table of contents. At the top level, there is a section titled "6 Ecotoxicological information" with a count of 7 items. Underneath it, there are two entries: "Ecotoxicological information ESS1" and "Ecotoxicological information.002". The next level down is a section titled "6.1 Aquatic toxicity" with a count of 5 items. Underneath it, there are three entries: "Aquatic toxicity", "Aquatic toxicity: A - template\_1" (which is highlighted with a blue background and has a red border around its icon), and "6.1.1 Short-term toxicity to fish" with a count of 3 items.

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:

**! This IUCLID information is part of a Template. Note that any modification will impact all datasets making reference to this Template. ×**

## 8. 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*.

### 8.1. 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 117: Editing the Dossier header independently of Dossier creation**

The screenshot shows the IUCLID web interface with the following details:

- Header:** Dashboard > Substances > table\_salt
- Title:** table\_salt  
IUC5-2dd443b4-a92a-4f7b-9348-b7a896f4c38c
- Working context:** REACH Registration 10 - 100 tonnes
- Content Area:**
  - REACH Registration 10 - 100 tonnes** (highlighted with a red arrow pointing to the 'Dossier name (given by user)' field)
  - table\_salt**
  - 1 General information\*** (12 items)
  - 2 Classification & Labelling and PBT assessment\*** (2 items)
- Dossier Header Fields (highlighted with a dashed blue box):**
  - Dossier name (given by user)**: Dossier TS v2
  - Dossier submission remark**: None
  - Type of submission**

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 118: View the read-only Dossier header in a completed Dossier**

The screenshot shows the IUCLID web interface for a dossier titled "Dossier TS v2". The URL in the address bar is "Dashboard > Substances > table\_salt". The main content area displays the dossier header information:

- REACH Registration 10 - 100 tonnes**
- table\_salt**
- UUID:** 22d2b741-b6a2-4946-ab46-877f8e51dace
- Dossier Submission Type**
  - Dossier name (given by user)**: Dossier TS v2
  - Version**: reach 7.0
  - Submission Type**: REACH Registration 10 - 100 tonnes
- Buttons:** View Dossiers, Go to source, Validate, Hide empty fields, and two circular icons with numbers 1 and 0.

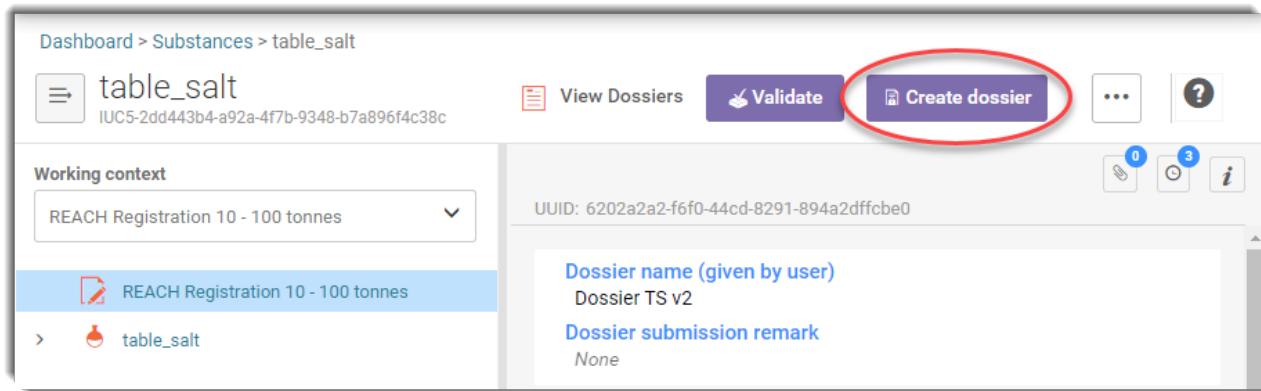
The values to be entered into the *Dossier* header depend on the specific circumstances under which data is to be submitted to a regulatory authority. For example, for advice on how to fill out the header under the REACH regulation, see the manual *How to prepare registration and PPORD dossiers*, which 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>

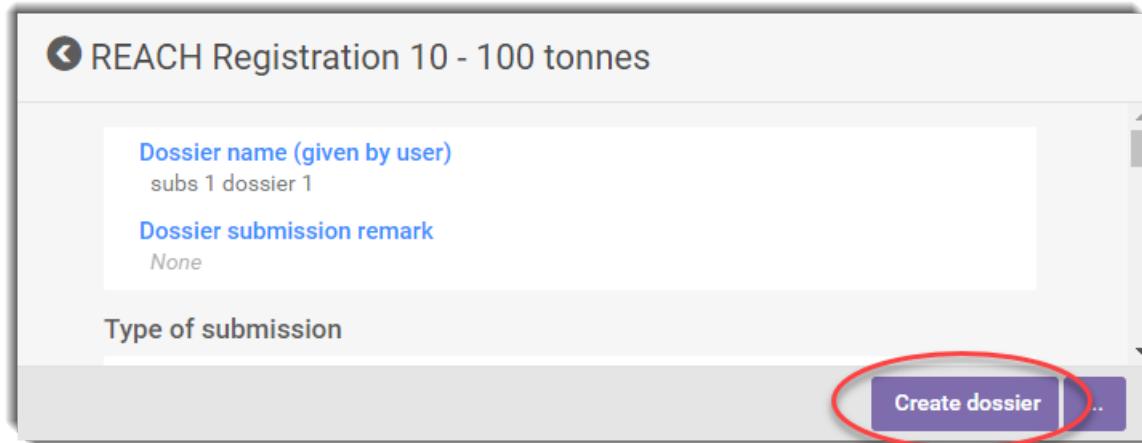
## 8.2. Creating a Dossier

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 8.1 *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 119: 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 120: Enter values into the Dossier header during creation of a Dossier**

### 8.2.1. Advanced settings for excluding and including data from the Dossier

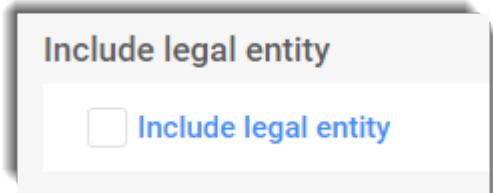
The filtering rules that are set in the following fields are applied cumulatively such that if any rule excludes a type of document or a field, it is excluded from the *Dossier*. To use advanced settings, click on the button labelled with three dots, as ringed in red in the screenshot below.

**Figure 121: Enter values into the Dossier header during Dossier creation**

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

#### 8.2.1.1. *Include legal entity*

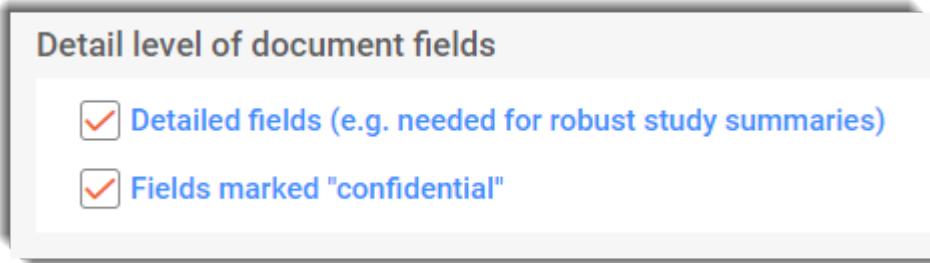
Either exclude or include the *Legal entity* that is attached to the *Substance* or *Mixture/Product*. Unlike the other fields, the default is to **exclude**, which is the setting shown in the screenshot below.

**Figure 122: Include/Exclude legal entity from a Dossier**

#### 8.2.1.2. *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 123: 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 124: Example of a field marked as confidential but with no flag**

Test material

Test material information

test\_material\_one\_13\_14\_0 | sodium chloride | sodium chloride | 7647-14-5

Additional test material information

test\_material\_xyz | sodium chloride | sodium chloride | 7647-14-5

Specific details on test material used for the study

SOURCE OF TEST MATERIAL

...

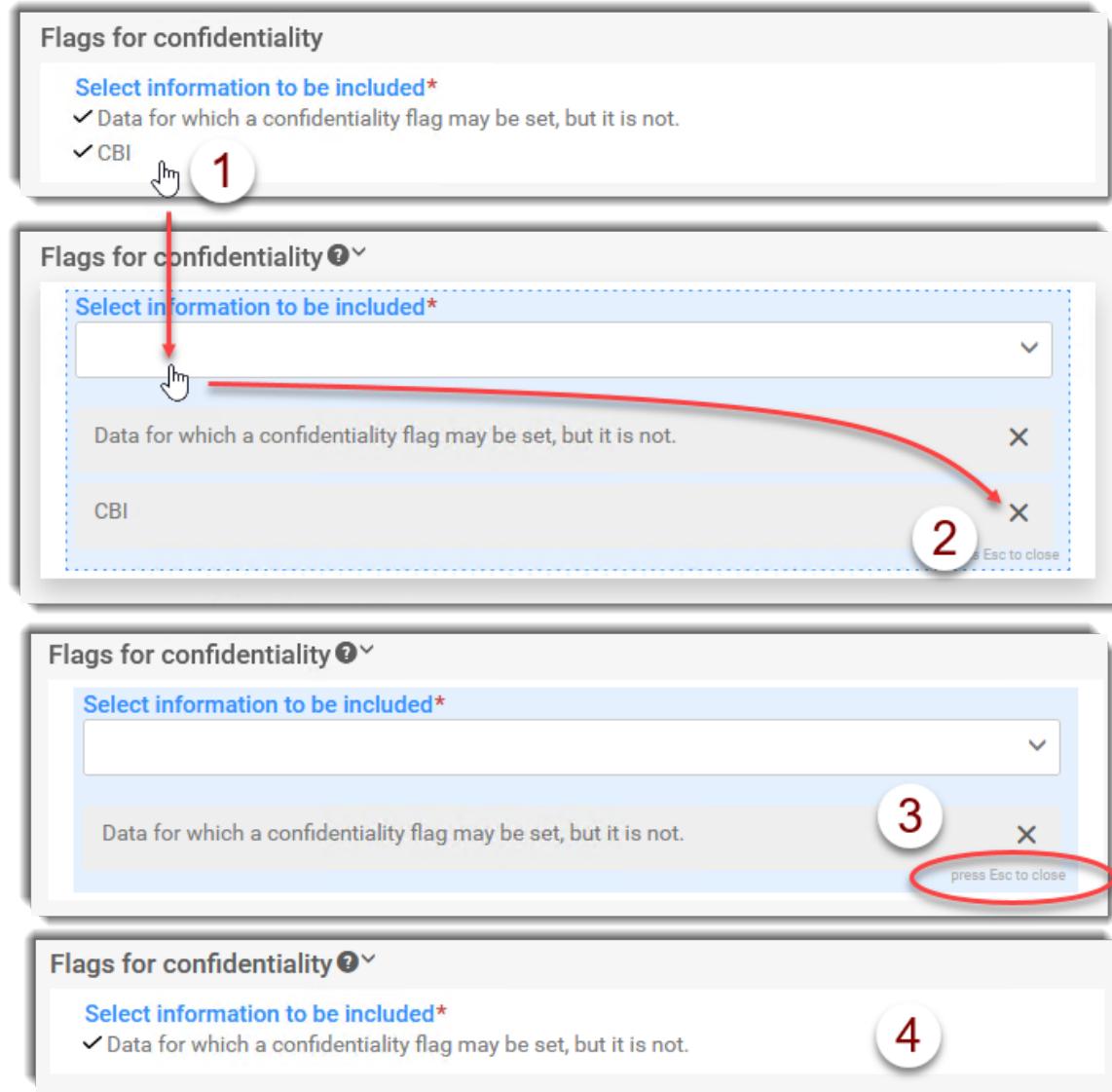
Specific details on test material used for the study (confidential) ▲

SOURCE OF TEST MATERIAL

...

#### 8.2.1.3. Flags for confidentiality

*Flags for confidentiality* relates to flags, which are described in section 3.7.7 *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 125: Example of excluding data flagged as confidential business information (CBI) from a Dossier**

### Legend for Figure 125

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.

#### 8.2.1.4. Flags for regulatory programme

*Flags for regulatory programme* relates to flags, which are described in section 3.7.7 *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 126: Flags for regulatory programme**

**Flags for regulatory programme**

Select information to be included

EU: PPP X

EU: REACH X

CA: CEPA X

CA: PCPA X

JP: CSCL X

OECD: CoCAP X

US: EPA HPVC X

US: FIFRA X

US: TSCA X

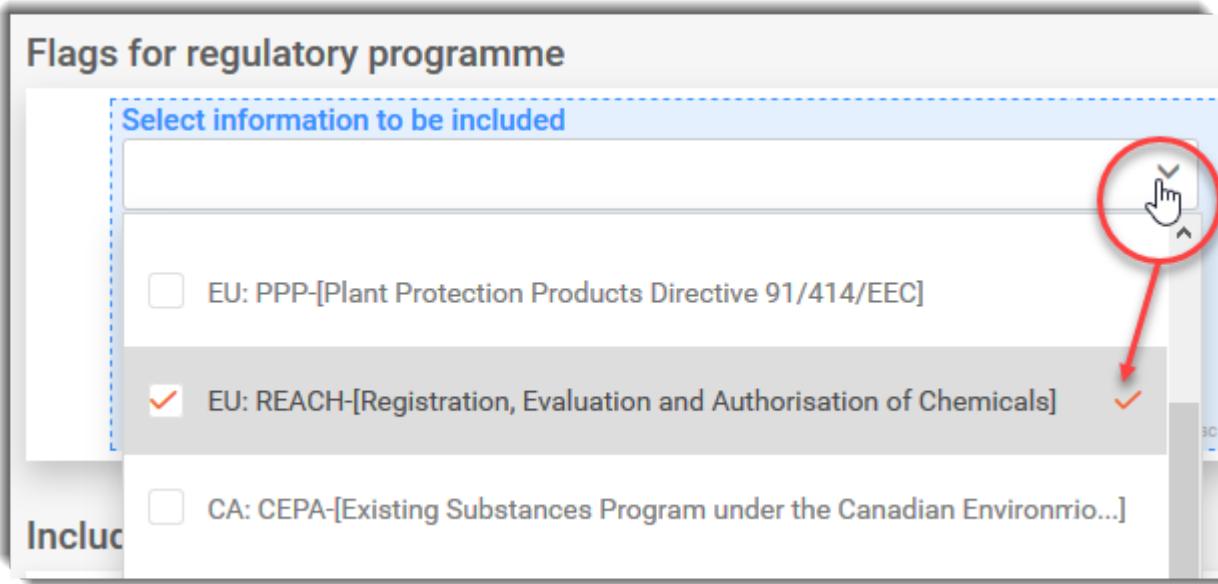
other: X

Some other value, as entered by the user.

41/255

The screenshot shows a list of regulatory programs selected for inclusion. Each item is a horizontal bar with the code name on the left and a close ('X') button on the right. Below this is a section for 'other' entries, which contains a text input field with placeholder text and a character limit indicator (41/255).

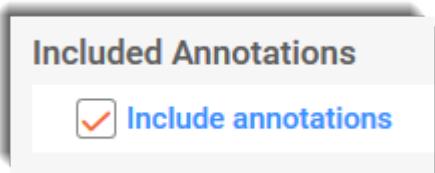
To add an option that is not shown on the list, open the drop-down menu, and then click on the item, as shown in the example below.

**Figure 127: 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.

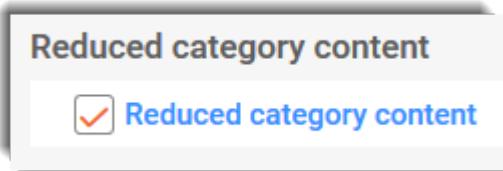
#### 8.2.1.5. *Included Annotations*

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

**Figure 128: Exclusion of Annotation entities**

#### 8.2.1.6. *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 129: 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 130: Reduced category content for a Substance in a Dossier**

The screenshot shows a sidebar menu for a dossier entry. At the top, there are two main categories: 'potassium chloride' (with a flask icon) and 'alkali\_metal\_halides' (with a flame icon). Below these are several sections, each with a small icon and a title. Some sections have a dropdown arrow, indicating they can be expanded. The sections listed are:

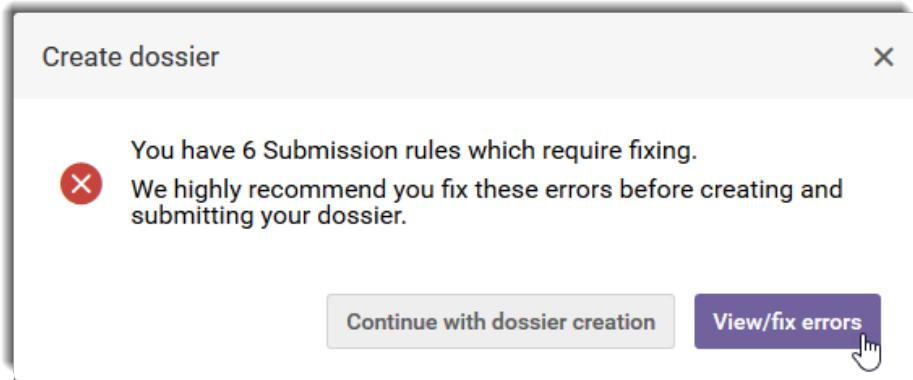
- table\_salt
  - 1 General information 2
  - 4 Physical and chemical properties 10
  - 5 Environmental fate and pathways 4
  - 6 Ecotoxicological information 2
  - 7 Toxicological information 6
  - 9 Residues in food and feedingstuffs
  - 10 Effectiveness against target organisms
  - 12 Literature search 1
- 13 Assessment reports 1
  - 13.2 Other assessment reports 1
- Inherited templates 1

At the bottom of the sidebar, there is a red square icon with a white letter 'A' and the text 'Template\_in\_table\_Salt'.

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

### 8.2.2. Validation during creation of a Dossier

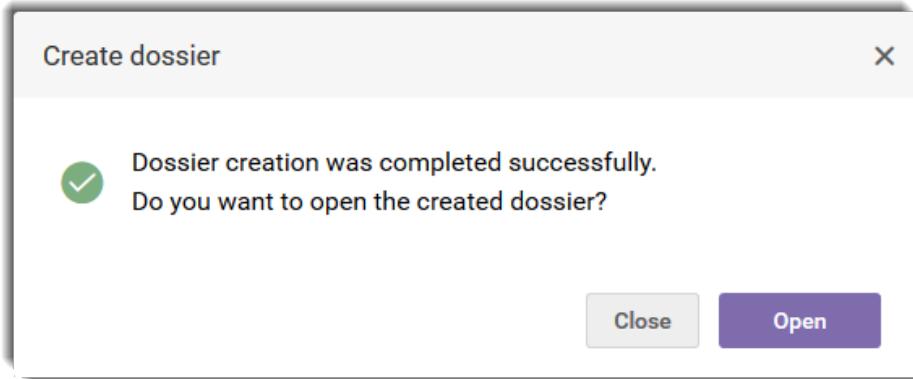
Next, the *Validation assistant* is run automatically in the background. If any *Submission checks* fail that would prevent the *Dossier* from being submitted to the relevant regulatory authority, an option is given to go straight into the *Validation assistant* to try to start fixing the problems in 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 131: 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 17 *Validation assistant*.

### 8.2.3. 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.

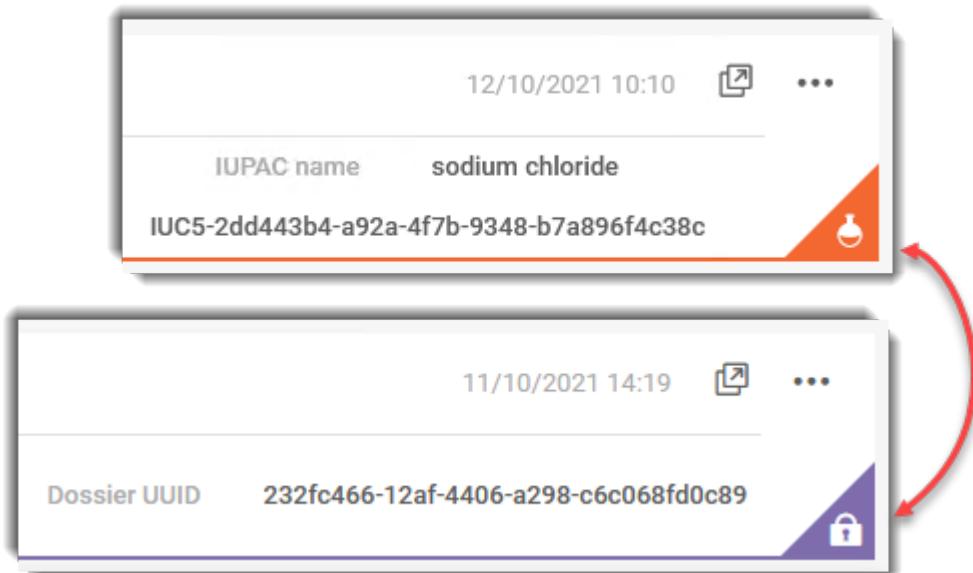
**Figure 132: Successful Dossier creation**

## 8.3. 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 133: 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 134: Substance versus Dossier**

There is a 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 135: View the Dossiers for a Substance**

The screenshot shows the IUCLID web interface. At the top, there is a toolbar with several buttons: 'View Dossiers' (highlighted with a red arrow), 'Validate', 'Create dossier', and others. Below the toolbar, the substance name 'table\_salt' is displayed. A red arrow points from the 'View Dossiers' button to a modal window titled 'Dossier versions'. This modal lists two dossier entries:

Dossier TS v2		08/04/2022 10:38		
Subject name	table_salt / 231-598-3 / sodium chloride / 7647-14-5	Submission type	REACH Registration 10 - 100 tonnes	Dossier UUID 22d2b741-b6a2-4946-ab46-877f8e51dace

TS Dossier 3 10-100 tpa		05/04/2022 19:39		
Subject name	table_salt / 231-598-3 / sodium chloride / 7647-14-5	Submission type	REACH Registration 10 - 100 tonnes	Dossier UUID 7117ae59-262f-4a52-b012-2eee071e1964

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 136: View the Substance dataset for a Dossier**

The screenshot shows the IUCLID web interface. At the top, there is a toolbar with buttons: 'View Dossiers', 'Go to source' (highlighted with a red oval), 'Validate', and others. Below the toolbar, the UUID '7117ae59-262f-4a52-b012-2eee071e1964' is displayed. A checkbox 'Hide empty fields' is checked. The main area shows 'Dossier Submission Type' with the following details:

**Dossier name (given by user)**  
TS Dossier 3 10-100 tpa

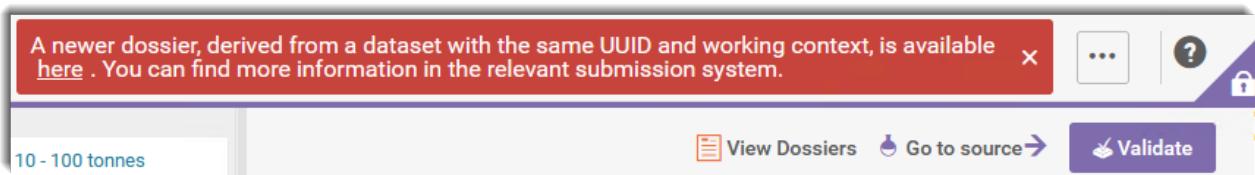
**Version**  
reach 7.0

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

### 8.3.1. 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 137: Waring message: “A newer dossier, derived from a dataset with the same UUID...”**



## 8.4. 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 138: The subject of a Dossier**

Dashboard > Substances > table\_salt

To demonstrate extraction to a dataset  
9db17ff8-80fd-4135-a899-d2cd413c890b

Type at least 3 characters

REACH Registration 10 - 100 tonnes

> table\_salt

UUID: 9db17ff8-80fd-4135-a899-d2cd413c890b  Hide empty fields (1) (0)

View Dossiers Go to source Validate

Dossier Submission Type Dossier Subject Type of submission

Dossier Submission Type

Dossier name (given by user)  
To demonstrate extraction to a dataset

Version  
reach 7.0

Submission Type  
REACH Registration 10 - 100 tonnes

Dossier Subject

Dossier Subject  
table\_salt | sodium chloride | sodium chloride | EC 231-598-3 | 7647-14-5

Submitting Legal Entity  
None

Dossier creation date/time  
2022-09-18T20:02:48.534

Dossier submission remarks  
Document in 7.1.1 excluded from dossier

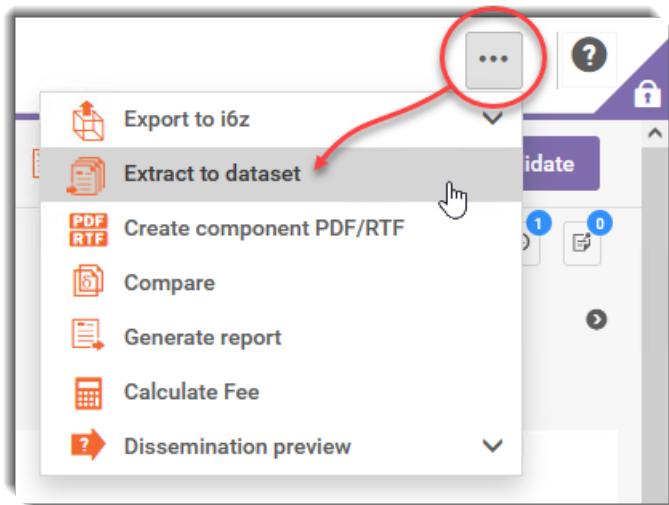
*Extract to Dataset* reads data from the subject of a *Dossier*, and then writes it to the raw dataset from which the *Dossier* was created. If the raw dataset is not present in the IUCLID database, an editable copy is created.

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, its entity 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.

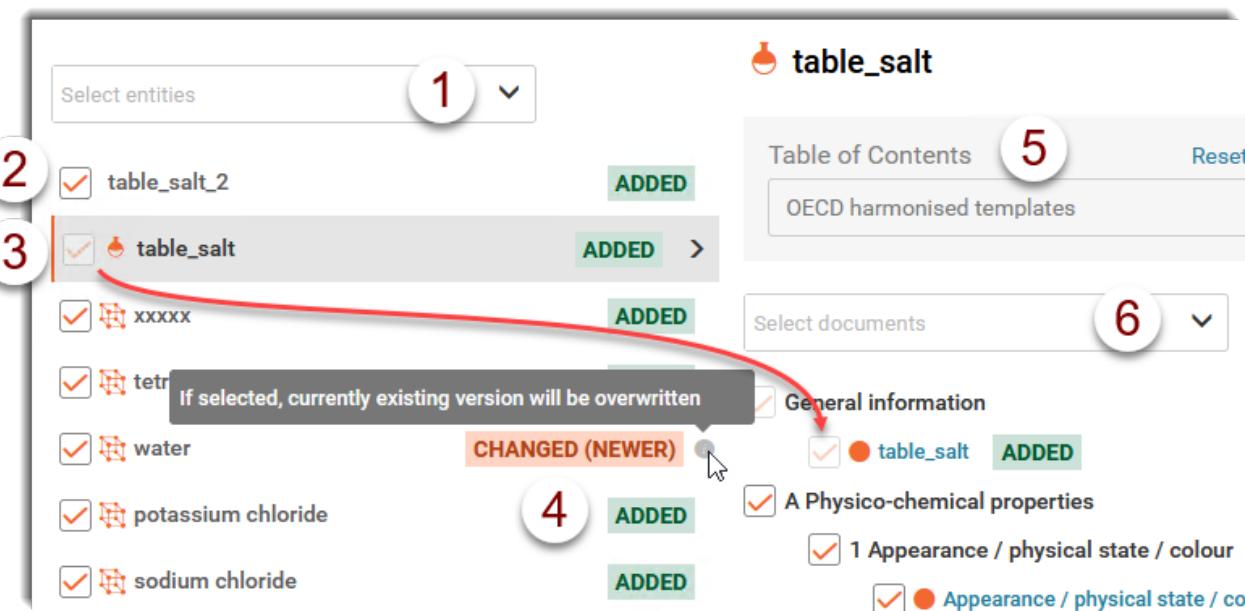
To extract data, start by viewing the record of the source *Dossier* and then select *Extract to dataset* from the upper menu labelled with three dots, as shown below.

**Figure 139: 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 is 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 140: Extract to dataset - Selection menu**



### Legend for Figure 140

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 <i>Last Modification Date</i> is older in the Dossier compared to the raw data in the database.	Entity or document will be overwritten in the raw data by the older version from the dossier.
CHANGE(NEWER)	The UUID is in the Dossier and the raw data. The data is different. The value of <i>Last Modification Date</i> 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 <i>Last Modification Date</i> 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 3.7.1.3 *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.

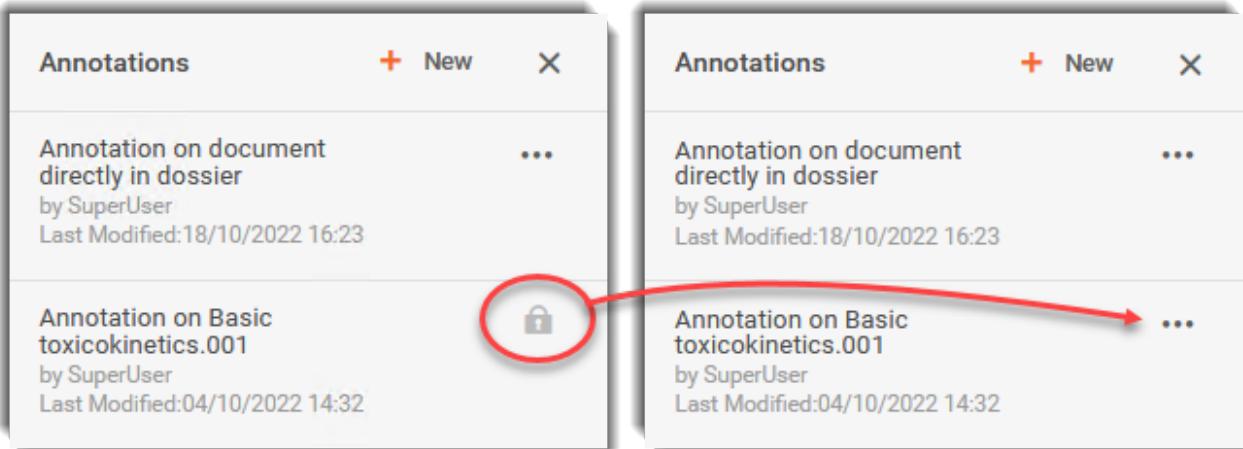
For example, if a *Template* in a Dossier is not selected, the link within the raw dataset to the *Template* is removed. Raw data in the database for the *Template* is not touched.

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 25.3.5.1 *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.

#### 8.4.1. 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.

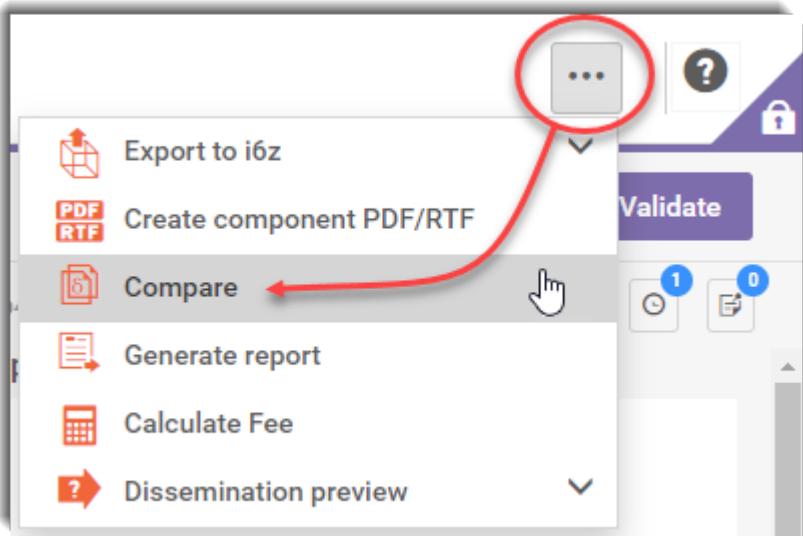
**Figure 141: Extraction of Annotations that were added after dossier creation (upper) and before (lower)**

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

## 8.5. Compare Dossiers

*Compare* produces a comparison of every value in any two *Dossiers*. Note that it is also possible to compare only two documents, as described in section 3.7.13 *Compare two documents*.

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

**Figure 142: Start the comparison of two Dossiers**

This opens a page from where the other, or target, *Dossier* is selected, as described in the figure below.

**Figure 143: Select the second, also known as target, Dossier in a comparison**

Subject name	Submission type	REACH Registration	Dossier UUID
1,2-dichloroethane / 203-458-1 / 107-06-2	REACH Registration 10 - 100 tonnes	0a479ce3-2e08-44fa-a3f3-f63f183083a6	
1,2-dichloroethane / 203-458-1 / 107-06-2	REACH Registration 10 - 100 tonnes	570bb02b-c0c1-4b95-a9eb-3e672248427	
1,2-dichloroethane / 203-458-1 / 107-06-2	REACH Registration 10 - 100 tonnes	4b1911c0-dc1f-4d16-b4e2-841ae49377	

**Legend for Figure 143**

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 Dossier>\_<name of target Dossier>\_comparison.html

Example: DossierA\_DossierB\_comparison.html

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**

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.

### 8.5.1. 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 144: Comparison report – First section: Dossiers**

<b>Dossiers</b>	
 <b>Source</b>	<b>Submission type:</b> REACH Registration 100 - 1000 tonnes <b>Subject:</b>  table_salt sodium chloride sodium chloride 7647-14-5 <b>EC Number:</b> <b>IUPAC Name:</b> sodium chloride <b>Chemical Name:</b> table_salt <b>Cas Number:</b> 7647-14-5 <b>Creation date:</b> Mar 15, 2019 18:29:07 (+0200)
 <b>Target</b>	<b>Submission type:</b> REACH Registration above 1000 tonnes <b>Subject:</b>  table_salt sodium chloride sodium chloride 7647-14-5 <b>EC Number:</b> <b>IUPAC Name:</b> sodium chloride <b>Chemical Name:</b> table_salt <b>Cas Number:</b> 7647-14-5 <b>Creation date:</b> Mar 20, 2019 17:32:41 (+0200)

### 8.5.2. 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 145: Comparison report – Second section: Dossier contents**

<b>Dossier contents</b>		
Source	Comparison	Target
 <b>Dossier headers</b>		
 R_10-100 / subject:  table_salt sodium chloride sodium chloride 7647-14-5	 <a href="#">Different</a>	 R_10-100 / subject:  table_salt sodium chloride sodium chloride 7647-14-5
 <b>Substances</b>		
 table_salt sodium chloride sodium chloride 7647-14-5	 <a href="#">Different</a>	 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.

### 8.5.3. 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

The screenshot shows the IUCLID web interface for a REACH registration dossier. The left pane displays a hierarchical tree structure of dossier sections. A red arrow points from the 'table\_salt' entry in the '1 General information\*' section to its detailed view on the right. The detailed view shows the following fields:

- Substance name\*: table\_salt
- Public name: Table Salt X
- Legal entity\*: [?](#)
- Third party: None

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

**Figure 146: 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	<a href="#">Identical</a>	table_salt sodium chloride sodium chloride 7647-14-5
1.2 - Composition		
• SubstanceComposition: Composition X	<a href="#">Identical</a>	• SubstanceComposition: Composition X

*Section Document comparison* is arranged and numbered as per the table of contents (TOC) for the *Dossier type* 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 147: Compare dossiers that have the same subject**

4.8 - Water solubility		
WaterSolubility: ws_record_1	Different	WaterSolubility: ws_record_1
WaterSolubility: ws_summary_1	Identical	WaterSolubility: ws_summary_1
WaterSolubility: ws_record_2	Identical	WaterSolubility: ws_record_2
WaterSolubility: ws_record_3	Identical	WaterSolubility: ws_record_3

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 148: Compare dossiers that have different subjects**

The screenshot shows two side-by-side dossier comparison windows and a detailed comparison table below them.

**Dossier Comparison Windows:**

- Left Window:** Shows section 4.8 Water solubility\*. It contains one summary document (ws\_summary\_1) and three record documents (ws\_record\_1, ws\_record\_2, ws\_record\_3). A red arrow points from ws\_record\_1 to the right window.
- Right Window:** Shows the same section 4.8 Water solubility\*. It contains the same summary document (ws\_summary\_1) and three record documents (ws\_record\_2, ws\_record\_1, ws\_record\_3). A red arrow points from ws\_record\_1 to ws\_record\_2.

**Detailed Comparison Table:**

4.8 - Water solubility		
● WaterSolubility: ws_record_1	<a href="#">Different</a>	● WaterSolubility: ws_record_2
● WaterSolubility: ws_summary_1	<a href="#">Identical</a>	● WaterSolubility: ws_summary_1
● WaterSolubility: ws_record_2	<a href="#">Different</a>	● WaterSolubility: ws_record_1
● WaterSolubility: ws_record_3	<a href="#">Identical</a>	● WaterSolubility: ws_record_3

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
	Identical	The descriptions below are for when the <i>Dossiers</i> have the same <i>Dossier</i> 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.
	Different	The entity or document has the same UUID in both <i>Dossiers</i> , but different content. For example, this could happen for an endpoint study record if the <i>Dossiers</i> being compared were created from the same <i>Substance</i> 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 <i>Different</i> is a hyperlink to the fourth level of the comparison

Icon	Label in interface	Description
		report, where the differing field(s) and their values are shown.
	Only in source	The entity or document is in the source <i>Dossier</i> , but not the target <i>Dossier</i> . This is based on UUID.
	Only in target	The entity or document is in the target <i>Dossier</i> , but not the source <i>Dossier</i> . This is based on UUID.
	Only in source, same content	The entity or document is in the source <i>Dossier</i> , but not the target <i>Dossier</i> . This is based on UUID. There is another document in the source <i>Dossier</i> with the same content.
	Only in target, same content	The entity or document is in the target <i>Dossier</i> , but not the source <i>Dossier</i> . This is based on UUID. There is another document in the target <i>Dossier</i> 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.

#### 8.5.3.1. 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 149: Links to duplicate content in the comparison report**

6.1.1 - Short-term toxicity to fish		
ShortTermToxicityToFish: EP1 (content reference: <Ref2>)	Identical	ShortTermToxicityToFish: EP1 (same content as <Ref2>)
ShortTermToxicityToFish: EP1-copy (same content as <Ref2>)	Only in source, same content	
ShortTermToxicityToFish: EP2 (content reference: <Ref4>)	Identical	ShortTermToxicityToFish: EP2 (same content as <Ref4>)
ShortTermToxicityToFish: EP3	Different	ShortTermToxicityToFish: EP3
ShortTermToxicityToFish: EP4	Only in source	
	Only in target, same content	ShortTermToxicityToFish: EP2-copy (same content as <Ref4>)
	Only in target	ShortTermToxicityToFish: EP5

#### Legend for Figure 149

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.

#### 8.5.4. 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 150: Comparison report – Fourth section: Field-level content differences**

**Field-level content differences**

R\_10-100 / subject: table\_salt sodium chloride sodium chloride 7647-14-5

Field	Source	Target
Document name	First dossier	Second dossier

1

2	• WaterSolubility ws_record_1
3	Type of information i Water solubility > Administrative data
4	Adequacy of study i Water solubility > Administrative data
5	Used for classification i Water solubility > Administrative data

3

4

5

Used for classification

ENDPOINT\_STUDY\_RECORD.WaterSolubility.AdministrativeData.UsedForClassification

#### Legend for Figure 150

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 151: Highlight the differences in a rich text field or render the HTML**

<p><b>Executive summary</b></p> <p><i>i</i> Acute toxicity: oral &gt; Applicant's summary and conclusion</p> <p> <a href="#">Highlight Differences</a></p>	<p><i>default</i></p> <p>Exec sum in dossier 1</p> <table border="1"><tr><td><b>Header 1</b></td></tr><tr><td>Value in first</td></tr></table>	<b>Header 1</b>	Value in first	<p><i>default</i></p> <p>Exec sum in dossier 2</p> <table border="1"><tr><td><b>Header 1</b></td></tr><tr><td>Value in second</td></tr></table>	<b>Header 1</b>	Value in second
<b>Header 1</b>						
Value in first						
<b>Header 1</b>						
Value in second						
<p><b>Executive summary</b></p> <p><i>i</i> Acute toxicity: oral &gt; Applicant's summary and conclusion</p> <p> <a href="#">Render HTML</a></p>	<p><i>default</i></p> <p>Exec sum in dossier 1</p> <p>Header 1</p> <p>Value in first</p>	<p><i>default</i></p> <p>Exec sum in dossier 2</p> <p>Header 1</p> <p>Value in second</p>				

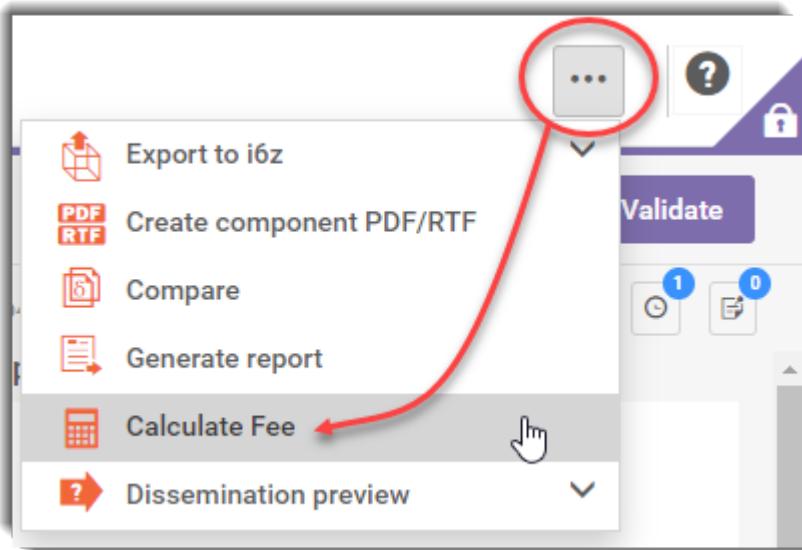
## 8.6. Calculate Fee

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.

### 8.6.1. Running the Fee calculator

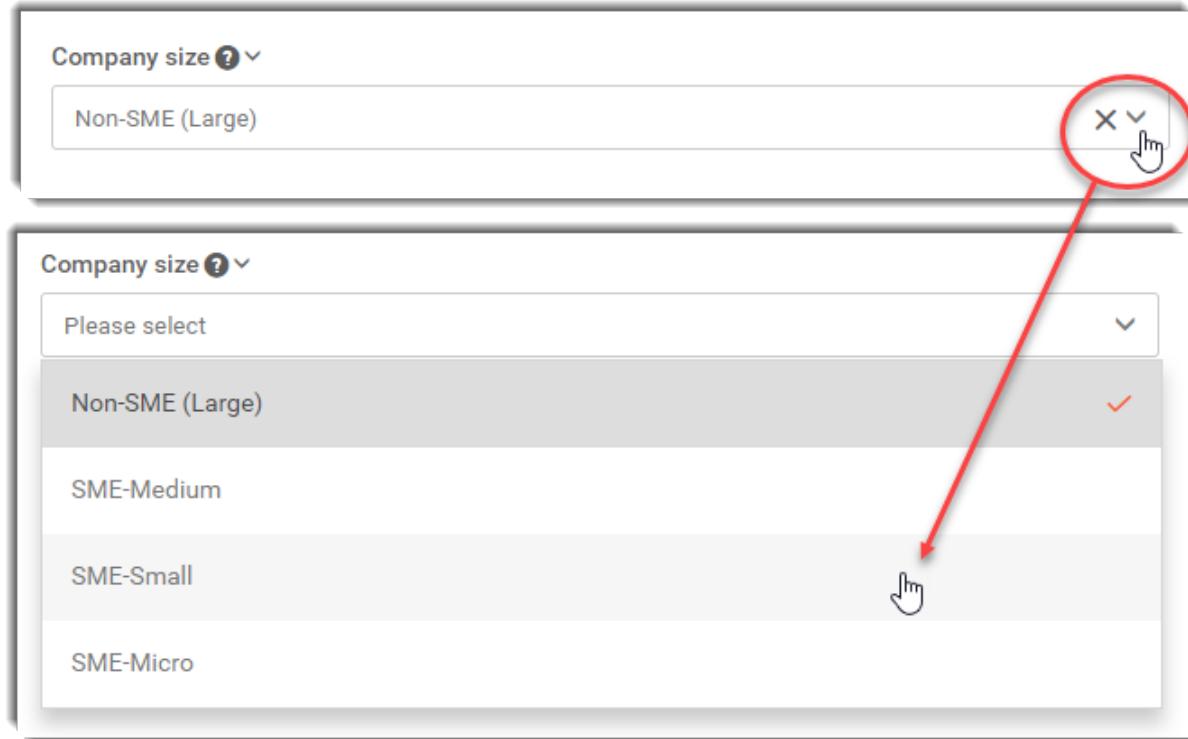
The *Fee calculator* is run from the top level of the record for a *Dossier*. Click on the button labelled with three dots, and then select *Fee calculator*, as shown ringed in red in the example below.

Figure 152: Run the Fee calculator



### 8.6.2. Selecting the company size

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

**Figure 153: Selecting the company size: example for SME-Small**

### 8.6.3. 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.

#### 8.6.3.1. 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 154: Hazardous substance indicator**

**Hazardous substance indicator**

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

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

#### 8.6.3.2. 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 155: Safety Data Sheet indicator**

**Safety Data Sheet indicator**

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

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

#### 8.6.3.3. 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 156: PBT/vPvB indicator**

**PBT / vPvB indicator**

This is a PBT/vPvB substance

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

#### 8.6.3.4. Annex III criteria indicator

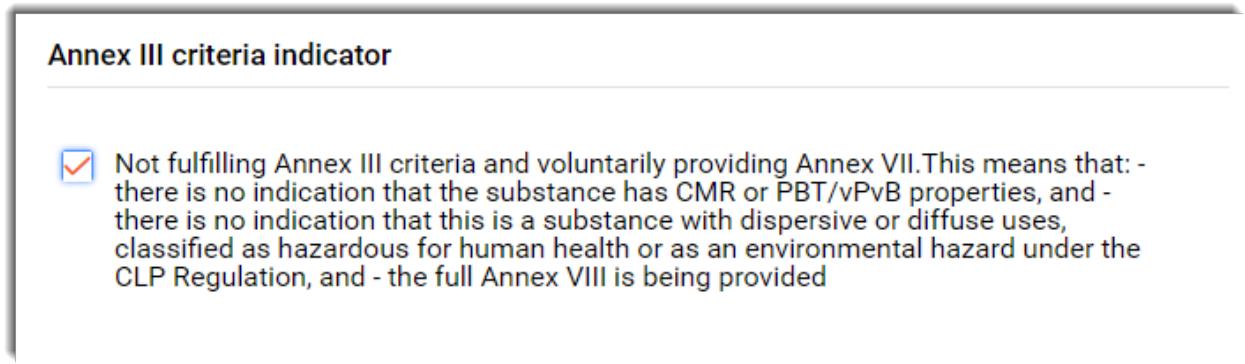
If the substance does not fulfil the Annex III criteria according to REACH Regulation, and the full Annex VII is voluntarily provided, tick the box next to the "Annex III criteria indicator".

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 157: Annex III criteria indicator**



#### 8.6.4. 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 158: Select the tonnage band of the previous submission, and information on intermediates

The screenshot shows two panels of the IUCLID web interface. The top panel is titled 'Tonnage band' and contains a dropdown menu with the placeholder 'Please select'. Below the dropdown is a list of tonnage bands: 'No standard registration fee paid before', 'between 1 to 10 tonnes/year, physicochemical requirements', 'between 1 to 10 tonnes/year, standard requirements', 'between 10 to 100 tonnes/year', 'between 100 to 1000 tonnes/year', and 'over 1000 tonnes/year'. A red arrow points from the 'between 10 to 100 tonnes/year' option to the bottom panel. Another red arrow points from the 'standard requirements' section of the dropdown to the same option in the bottom panel. A red circle with a hand cursor icon highlights the 'standard requirements' section. The bottom panel is also titled 'Tonnage band' and shows the selected option 'between 10 to 100 tonnes/year'. Below this panel is another section titled 'Isolated intermediates' containing two checkboxes: 'On-site isolated intermediates' (unchecked) and 'Transported isolated intermediates' (checked). A red arrow points from the checked checkbox to the bottom panel.

Tonnage band

Please select

No standard registration fee paid before

between 1 to 10 tonnes/year, physicochemical requirements

between 1 to 10 tonnes/year, standard requirements

between 10 to 100 tonnes/year

between 100 to 1000 tonnes/year

over 1000 tonnes/year

Tonnage band

between 10 to 100 tonnes/year

Isolated intermediates

On-site isolated intermediates

Transported isolated intermediates

### 8.6.5. 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 159: 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€
<b>Total Amount: 4,338€</b>	

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.

### 8.6.6. 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.

### 8.6.7. 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.

## 8.7. 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).

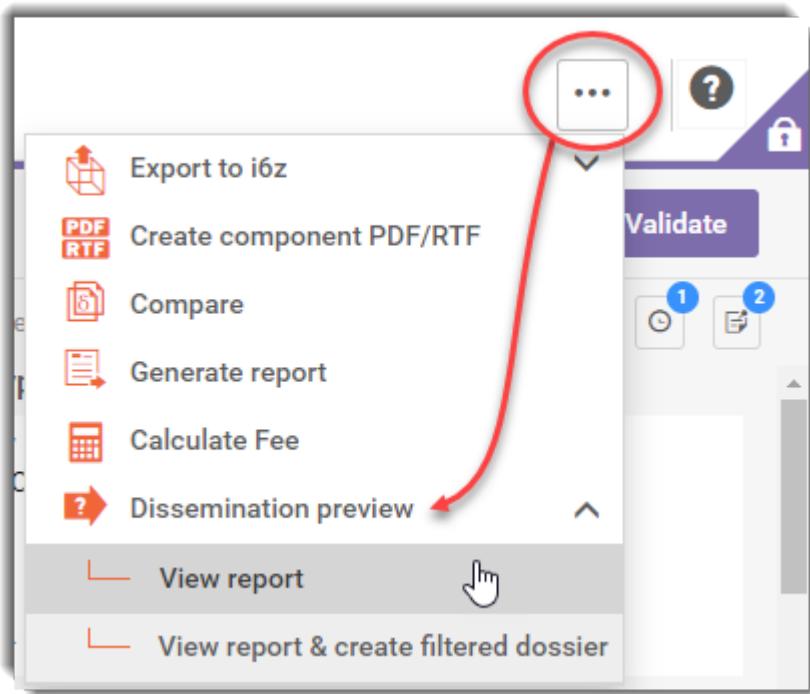
In addition, the information that will be disseminated for each *Substance* on the ECHA website will be aggregated from multiple registration *Dossiers* at different tonnage bands, and therefore may contain additional information to that indicated in the output of the *Dissemination preview*.

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.

### 8.7.1. 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 160: Run the Dissemination preview**

### 8.7.2. 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*.

#### 8.7.2.1. 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 161: The link between a referencing field and a referenced field in the Dissemination preview**

The screenshot shows a table with two columns. The first column is labeled 'sourceDocumentKey' and the second is 'referencedDocumentKey'. A red arrow points from the value 'a1c82b2f-4552-4670-90bc-01' in the 'referencedDocumentKey' column back up to the corresponding row in the 'sourceDocumentKey' column, which contains 'is|a1c82b2f-4552-4670-90bc-019bb'. This indicates a self-referencing relationship where a document links back to its own identifier.

sourceDocumentKey	referencedDocumentKey
is 4c51fd38-19b7-4382-8c10-7664c	c7-3c03bd98c480
d 4c51fd38-19b7-4382-8c10-7664c	c7-3c03bd98c480
d 4c51fd38-19b7-4382-8c10-7664c	c7-3c03bd98c480
d 4c51fd38-19b7-4382-8c10-7664c	d91223a6-15c0-4c09-9571-4a eac01c82b2f-4552-4670-90bc-01
d 4c51fd38-19b7-4382-8c10-7664c	c7-3c03bd98c480
d 4c51fd38-19b7-4382-8c10-7664c	c7-3c03bd98c480
d   d91223a6-15c0-4c09-9571-4aeac01	
is d91223a6-15c0-4c09-9571-4aeac01	c7-3c03bd98c480
d d91223a6-15c0-4c09-9571-4aeac01	c7-3c03bd98c480
is a1c82b2f-4552-4670-90bc-019bb	c7-3c03bd98c480

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 162: Example Dissemination report for a field in a Substance that links to a Reference substance**

A	B	C	D	E
entity	sectionName	documentField		outcome
Substance	1.1 Identification	SID_CONF_Substance / Substance name		Not published
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 163: The identifier of a Reference substance in *referencedDocumentKey* (Column G)**

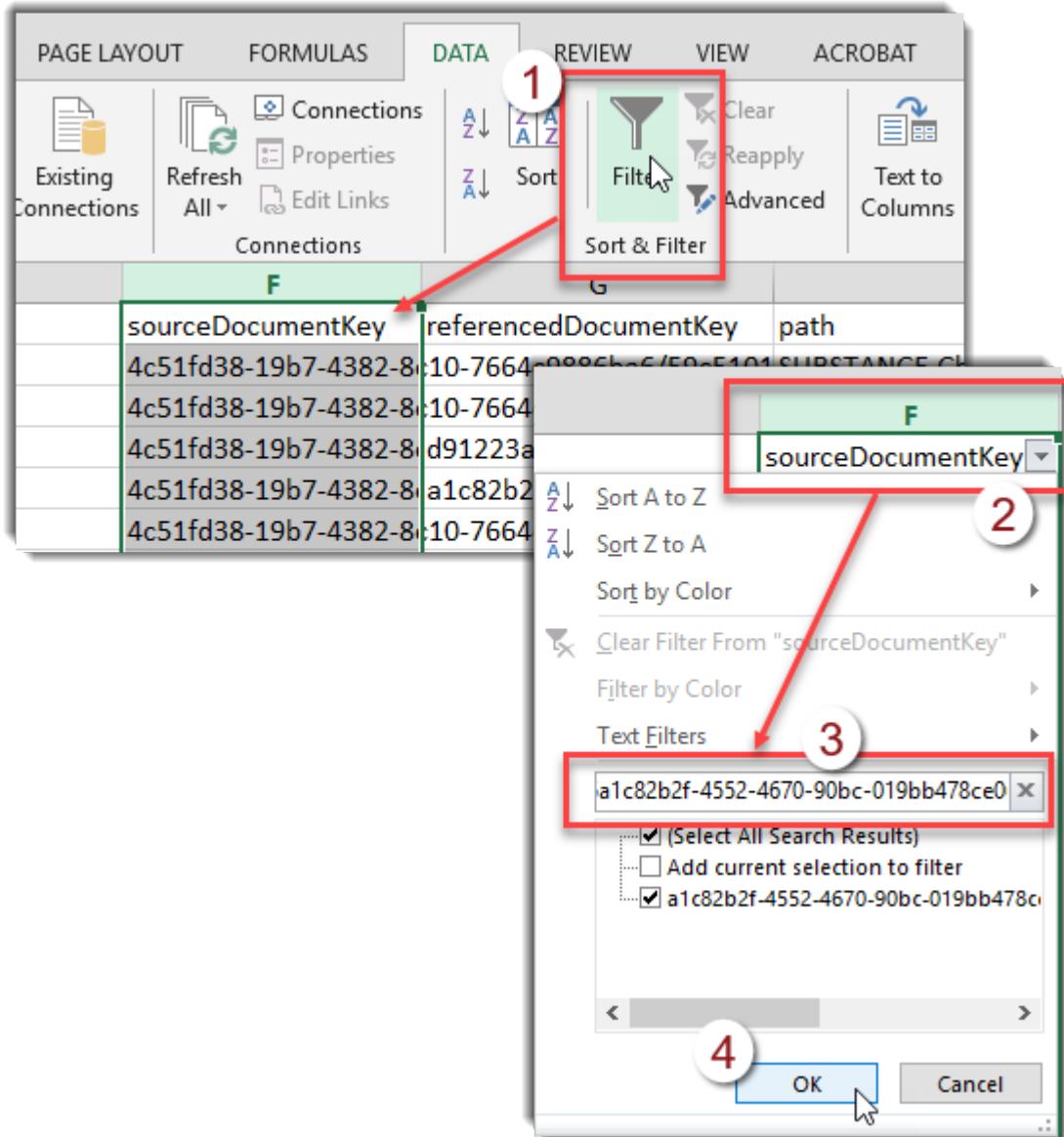
The screenshot shows a Microsoft Excel spreadsheet with a toolbar at the top containing buttons for DATA, REVIEW, VIEW, ACROBAT, and PPO Tool. Below the toolbar is a row of cells with headers F, G, H, I, J, K, L, M, and N. The cell in column G contains the value "a1c82b2f-4552-4670-90bc-019bb478ce06/59c5101c-87bc-4c3e-93c7-3c03bd98c480". A red arrow points from the text "The identifier of a Reference substance in *referencedDocumentKey* (Column G)" to this cell. The cell is highlighted with a green border. The rest of the spreadsheet rows show various substance properties like ChemicalName, PublicName, OwnerLegalEntity, and ReferenceSubstance.

F	G	H	I	J	K	L	M	N
urceDoc referenced path								
51fd38-19b7-4382-1SUBSTANCE.ChemicalName								
51fd38-19b7-4382-1SUBSTANCE.PublicName								
51fd38-1d91223a6-1SUBSTANCE.OwnerLegalEntity								
51fd38-1a1c82b2f-4SUBSTANCE.ReferenceSubstance								
51fd38-19b7-4382-1SUBSTANCE.TypeOfSubstance.Composition								

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 164: Apply a filter to *sourceDocumentKey* in MS Excel****Legend for Figure 164**

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 165: Output of the Dissemination preview filtered for a single reference to a Reference substance**

D	E	F	G
field	outcome	sourceDocumentKey <input checked="" type="checkbox"/>	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 dissemination)	a1c82b2f-4552-4670-90bc-019bb478ce0	
Reference substance / Reference substance information / Synonyms / 1 / Identity	Not published (ineligible for dissemination)	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 / category	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	

## 9. 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.

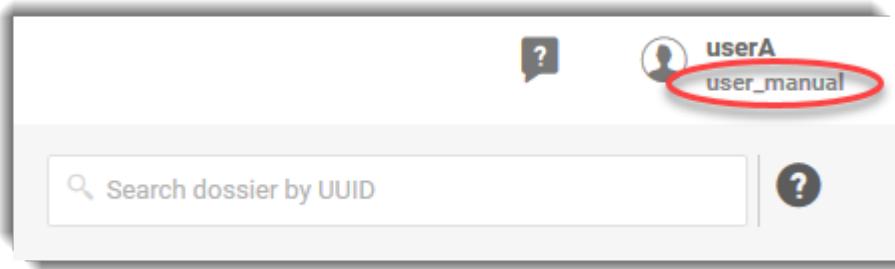
A *Legal entity* can be associated with various entities, such as *Substance*.

### 9.1. 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*.

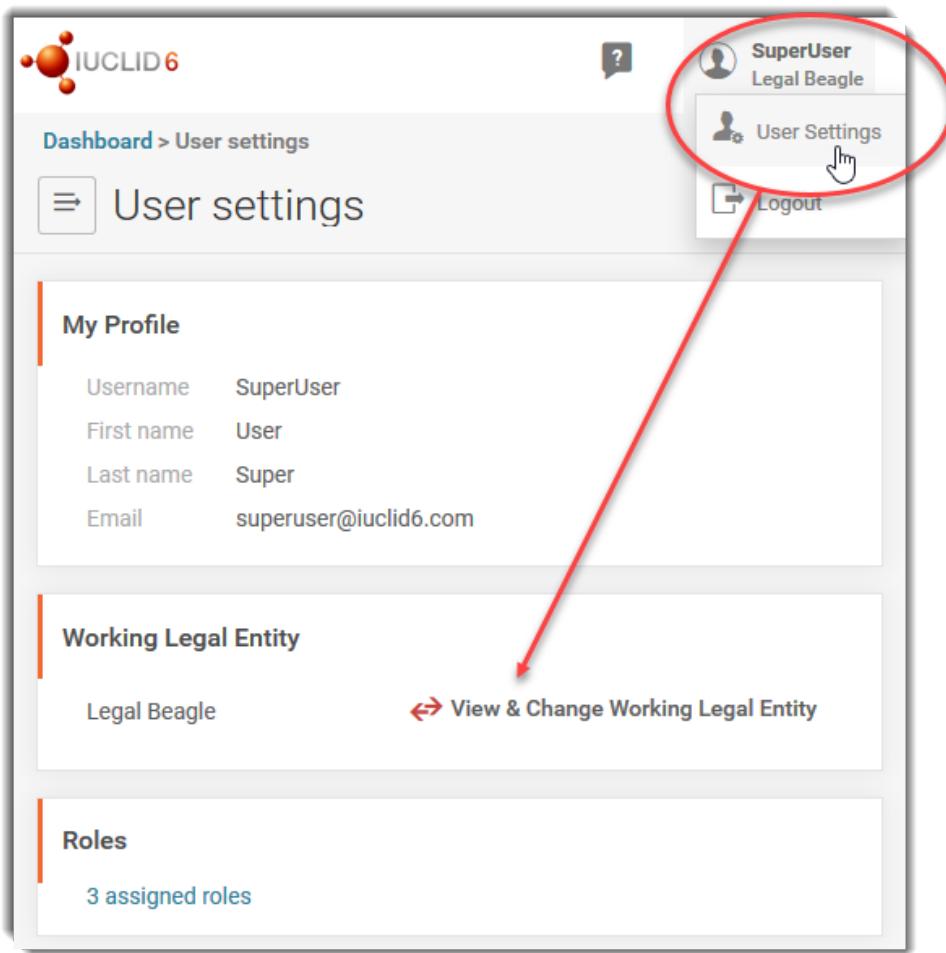
The *working Legal entity* is indicated at the top right of the interface, as shown below circled in red.

**Figure 166: 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 167: View and change the working Legal entity in IUCLID 6 Desktop**

## 9.2. 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.

## 9.3. 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.

## 9.4. 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*.

## 10. 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.

## 11. 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 web site under the section *Support / Get Reference Substances*. If the required *Reference substance* is not available on the web site, or if you otherwise prefer, it is possible to create a *Reference substance* within IUCLID. 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 168: The list page for Reference substances**

Reference substance	Date	Action
potassium chloride	12/10/2021 11:03	<input type="checkbox"/> <a href="#">Edit</a> <a href="#">More</a>
tetrasodium hexacyanoferrate	08/10/2021 19:24	<input type="checkbox"/> <a href="#">Edit</a> <a href="#">More</a>
water	08/10/2021 19:24	<input type="checkbox"/> <a href="#">Edit</a> <a href="#">More</a>

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 169: Enter a Reference substance into the field Impurities for a Substance**

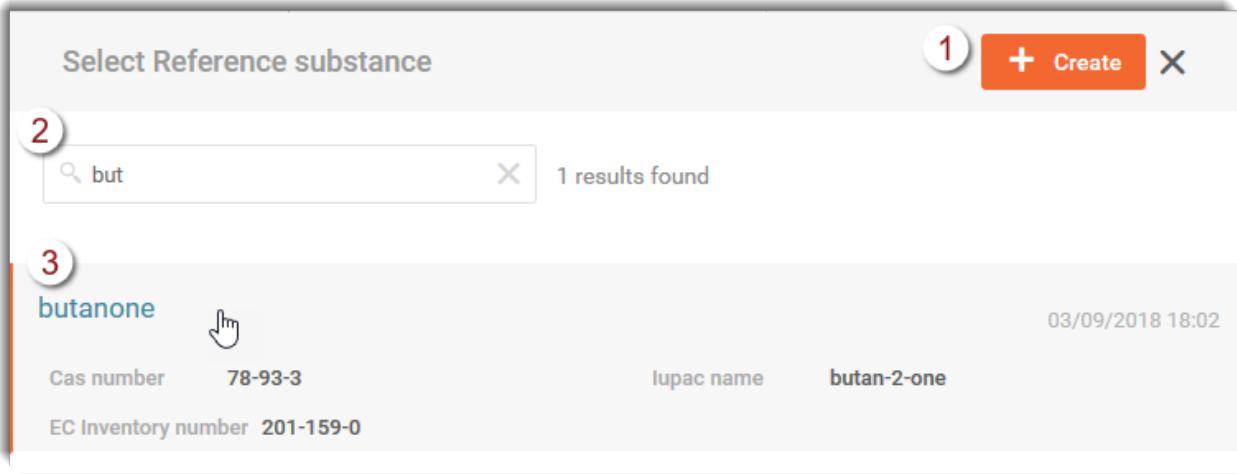
Impurities		
#	Reference substance	Typical concentration
1	(P) None (P) None potassium chloride   potassium chloride   7447-40-7	ca. 7 % (w/w)
2	(P) None (P) None water   water   7732-18-5	ca. 1 % (w/w)

Impurities		
#	Reference substance	
1	(P) None (P) None None	

Set values

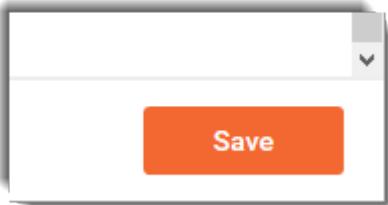
(P) None (P) None	Reference substance  
	
Typical concentration	
None	

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 170: 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.

After editing or creating a *Reference substance* or the entity or document that refers to it, click on the *Save* button at the bottom right of the interface:

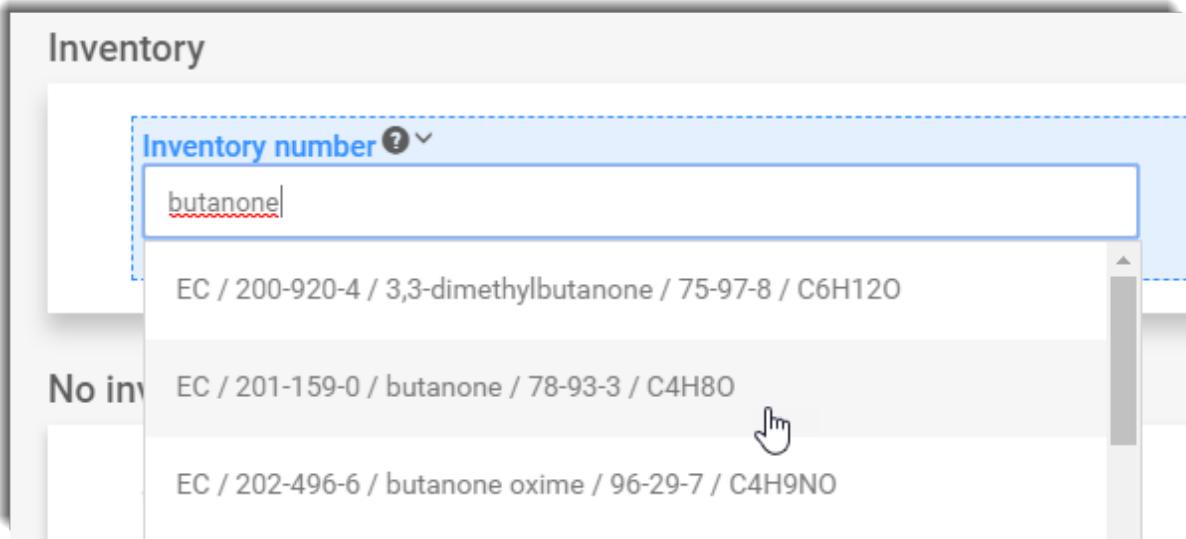
**Figure 171: Save**

## 11.1. General information

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.

## 11.2. Inventory

The field *Inventory* allows substance identity information to be retrieved from an *Inventory*. The EC Inventory is supplied with IUCLID. The field contains a dynamic search feature that tries to find a match between the value entered, and the values in the EC Inventory supplied with IUCLID. The matches are offered as selectable options, but they do not have to be selected. An example is shown below where the text "butanone" has been entered.

**Figure 172: Automatic searching of the EC Inventory in a Reference substance**

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

### 11.3. Reference substance information

*Reference substance information* is a collection of fields that contain identifiers for the *Reference substance* and related substances. In the field *Identifiers of related substances*, there is a field *Relation*, where the relationship can be described.

A single flag can be applied to all of *Reference substance information*, *CAS information* and *Related substances*.

### 11.4. Molecular and structural information

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

A single flag can be applied to all of *Molecular and structural information*.

See the example below.

**Figure 173: Molecular and structural information - example**

Molecular and structural information    None    None

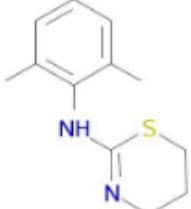
**Molecular formula**  
C12H16N2S

**Molecular weight**  
220.3338

**SMILES notation**  
Cc1cccc(C)c1NC2=NCSC2

**InChI**  
InChI=1/C12H16N2S/c1-9-5-3-6-10(2)11(9)14-12-13-7-4-8-15-12/h3,5-6H,4,7-8H2,1-2H3,(H,13,14)

**Structural formula**



## 12. 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 174: Contacts in the identification of a substance dataset**

Dashboard > Substances > table\_salt

## table\_salt

IUC5-2dd443b4-a92a-4f7b-9348-b7a896f4c38c

Working context

REACH Registration 10 - 100 tonnes

REACH Registration 10 - 100 tonnes

> table\_salt

Contact persons

UUID: IUC5-2dd443b4-a92a-4f7b-9348-b7a896f4c38c

+ New item

1 Person  
User, Manual; ECHA | User | Manual | ECHA

2 Person  
Tester, T; Not available | Tester | T | Not available

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 175: A newly created link to a Contact**

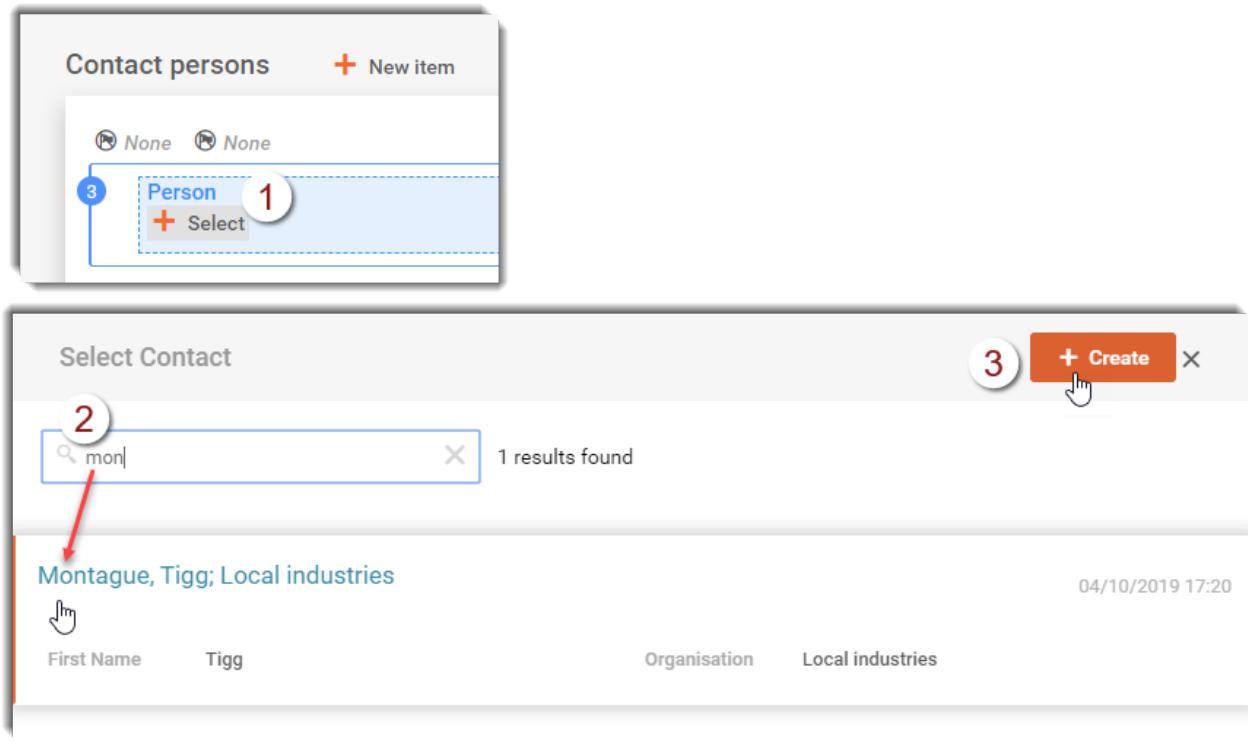
Contact persons

+ New item

None None

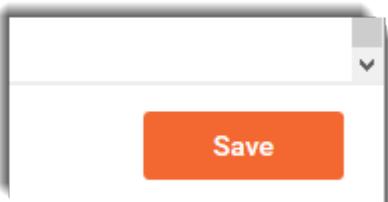
3 Person  
None

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 176: Place a Contact in an empty link****Legend for Figure 176**

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 177: Save**

## 13. 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*.

### 13.1. 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 178: Test material in a Mixture/Product – example where the Test material refers to the composition of the Mixture/product**

Edit Test material

**!** This IUCLID information is a re-usable data element. Note that any modification will impact all associated data.

test\_material\_butanone

Name  
test\_material\_butanone

Composition

1 + New item

2 Composition / purity: other information

3 other: Test material refers to the composition document named X in the Mixture/Product named Y.

#### Legend for Figure 178

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*.

## 14. Category

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

### 14.1. 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.

### 14.2. Category entity

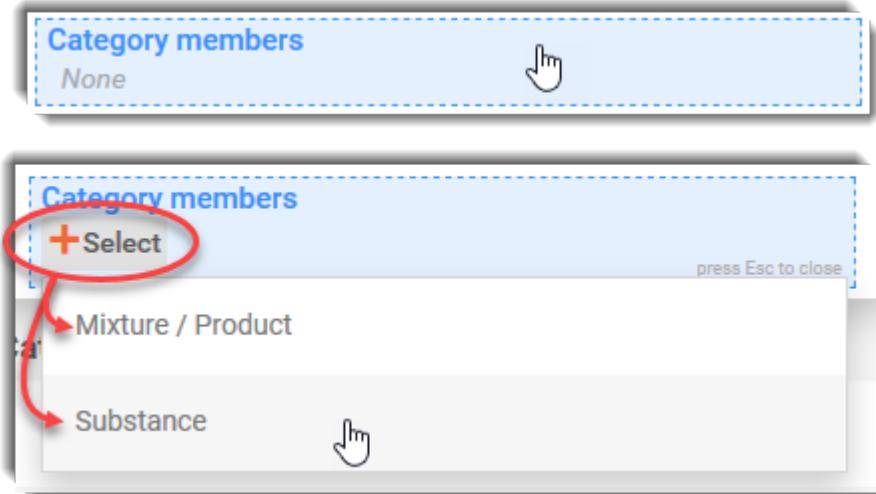
A *Category* entity contains a description of the rationale behind the chemical category, and a group of *Substance* entities that contain data about the members of the chemical category. A *Category* entity provides a functionality known as the category matrix. This displays links to all documents across 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 179: A newly created Category**

The screenshot shows the IUCLID web interface for creating a new category. The top navigation bar indicates the path: Dashboard > Categories > Alkali metal halides. The category name is displayed as "Alkali metal halides" with the UUID "df8e2ac9-cd59-4e9e-9a93-5a27e8bf4f74". The "Working context" dropdown is set to "Please select". The main content area includes fields for "Category name\*" (set to "Alkali metal halides"), "Public name" (set to "None"), "Legal entity\*" (with a note about predefined legal entities), "Regulatory purposes" (set to "None"), "Remarks" (set to "None"), and "Category members" (set to "None"). The "Category members" field is circled in red. Below this is a section for "Category documents" with a placeholder message: "Please add your category documents...".

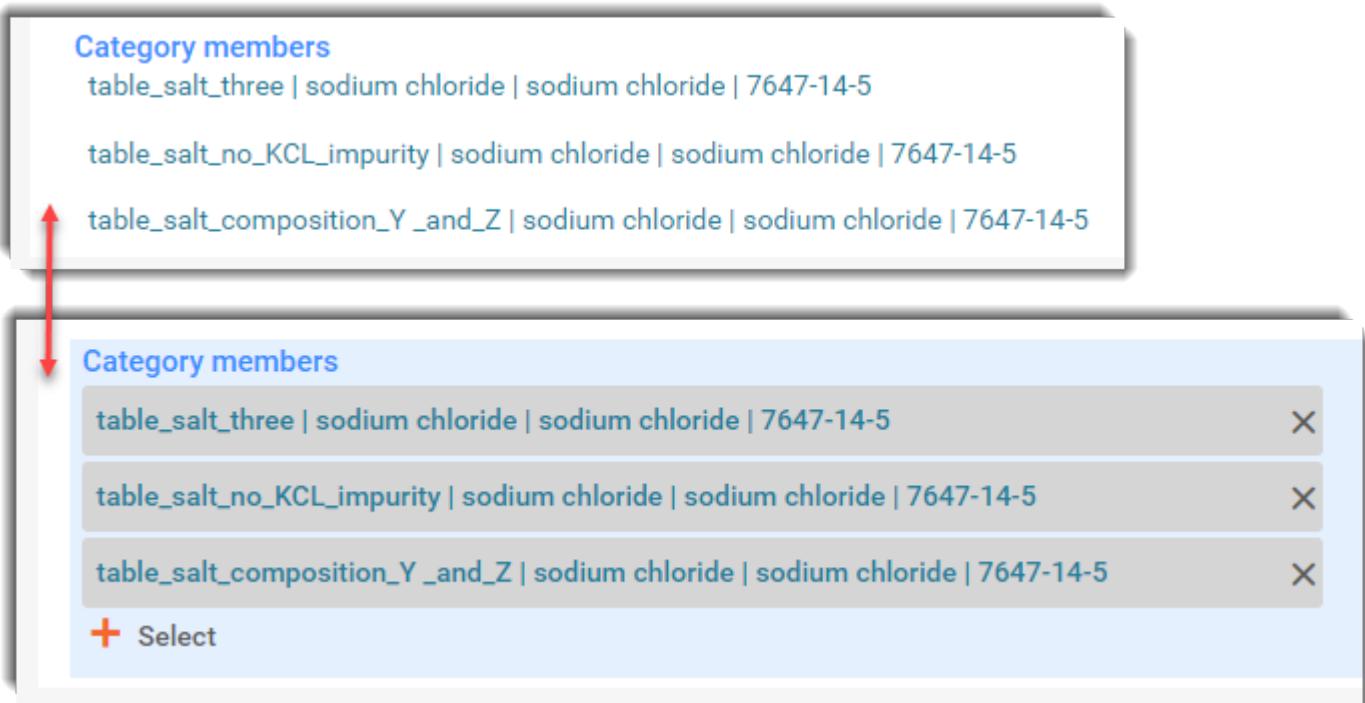
To add a member, first click within the field *Category members* to make it editable. An option *Select* appears. Clicking on *Select* gives an option of whether to add a *Substance*, or *Mixture/Product*, as shown below.

**Figure 180: Select whether the new member of a Category is to be a Substance or a Mixture/Product****Figure 181: Add a member to a Category**

The screenshot shows a search results page for substances. At the top, there is a search bar with the query '\*chloride' and a result count of '3 results found'. Below the search bar is a link to 'Advanced search'. The main area displays three substance entries in a table format:

Select Substance				+ Create	X
<input type="text" value="*chloride"/> <span>X</span> 3 results found					
<a href="#">► Advanced search</a>					
<b>Sodium chloride</b>				03/09/2021 18:50	
Inventory number	European Chemicals Agency	CAS number	UUID	IUPAC name	
Legal Entity	European Chemicals Agency	7647-14-5	c1bedae8-8cab-498a-aa9b-4f52e23a0ced	sodium chloride	
<b>table_salt</b>				03/09/2021 16:13	
Inventory number	231-598-3	CAS number	7647-14-5	IUPAC name	sodium chloride
Legal Entity	European Chemicals Agency	UUID	IUC5-2dd443b4-a92a-4f7b-9348-b7a896f4c38c		
<b>table_salt_no_KCL_impurity</b>				03/09/2021 15:32	
Inventory number	231-598-3	CAS number	7647-14-5	IUPAC name	sodium chloride
Legal Entity	Predefined Legal entity	UUID	ba28d2dd-2e5d-4dd3-885a-35a71076cb54		

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

**Figure 182: 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 183: Members of a Category in the table of contents**

The screenshot shows the 'Alkali metal bromides' category record. On the left, the 'Working context' dropdown is set to 'Please select'. The main panel displays the category details: UUID e98845be-deea-44f4-bd0a-0f9e33cba77, Category name\* Alkali metal bromides, Public name None, Legal entity\* Predefined Legal entity | Helsinki | No remarks | No remarks | No remarks, Regulatory purposes None, and Remarks None. A red box highlights the 'Category members' section, which lists 'Lithium bromide | Lithium bromide | Lithium bromide', 'Potassium bromide | Potassium bromide | Potassium bromide | 7758-02-3', and 'Sodium bromide | Sodium bromide | Sodium bromide | 7647-15-6'. A red bracket on the left points from the 'Alkali metal bromides' category name to the 'Category members' list, and another red arrow points from the 'Category members' list back to the 'Category members' section in the top modal of Figure 182.

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

### Justifications and discussions

**Category definition**  
Bromides of alkali metals.

**Category description**  
Describe

**Category rationale**  
For the manual.

**Reports** [+ New item](#)

#	Flags	Report	Actions
1	<input type="checkbox"/> None <input type="checkbox"/> None	<a href="#">csr_substance_x.pdf</a>	

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 184: Membership of a Category indicated in the Table of contents of a dataset**

The screenshot shows the IUCLID web interface. At the top, it displays the navigation path: Dashboard > Substances > Sodium bromide. Below this, the main title is "Sodium bromide" with the identifier "cf600a2c-964c-47e5-abd6-65191e30c22e". A "Working context" section contains a dropdown menu with the placeholder "Please select". Below this, a tree view shows the category structure: "Sodium bromide" is selected and highlighted in blue, while "CORE" is shown in grey. A dashed line separates this from another panel below.

**Linked Categories** 1

- ▼ Alkali metal bromides
- Predefined Legal entity
- Lithium bromide
- Potassium bromide

## 15. 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."*

## 16. 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 185: Literature references in the field Data source

The screenshot shows the IUCLID web interface for a substance named 'table\_salt'. On the left, a tree view shows sections like '6 Ecotoxicological information\*', '6.1 Aquatic toxicity\*', and '6.1.1 Short-term toxicity to fish\*'. The '6.1.1 Short-term toxicity to fish\*' section is expanded, showing items for 'Short-term toxicity to fish ESR1' and 'Short-term toxicity to fish ESR1'. The 'Short-term toxicity to fish ESR1' item is selected and highlighted in blue. On the right, a detailed view of this item is shown. The 'Data source' field is highlighted with a red circle and a red arrow points to it from the left. Below the 'Data source' field, a modal window titled 'Reference' is open, showing a list with one item: 'publication | A sample title for the user manual | Dr. Robin | 2022'. There are buttons for '+Select' and 'press Esc to close'.

## 17. 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.

### 17.1. 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 in 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.

### 17.2. 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.

#### 17.2.1. 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>

### 17.2.2. 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>

### 17.2.3. 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.

## 17.3. 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

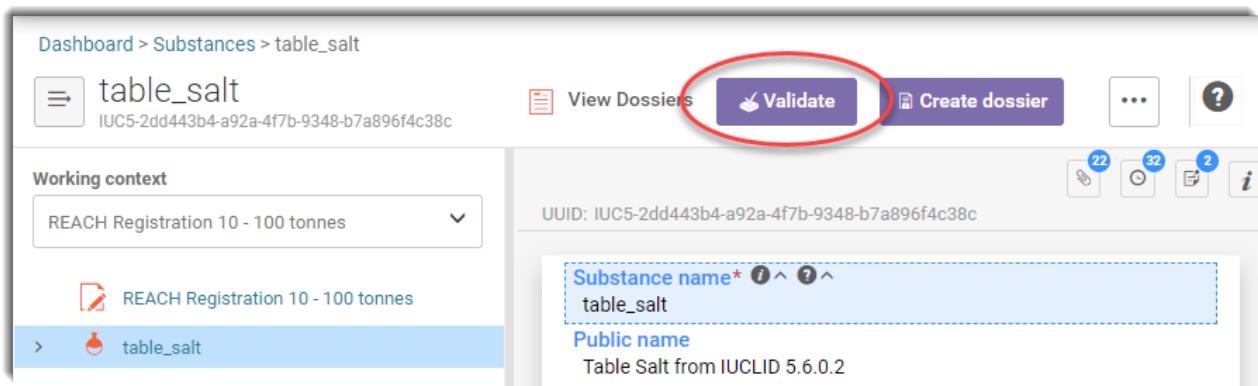
name of the entity in the breadcrumbs. The latter approach is useful if you have just edited a document, and you want to see the effect the edit has had on the validation.

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*.

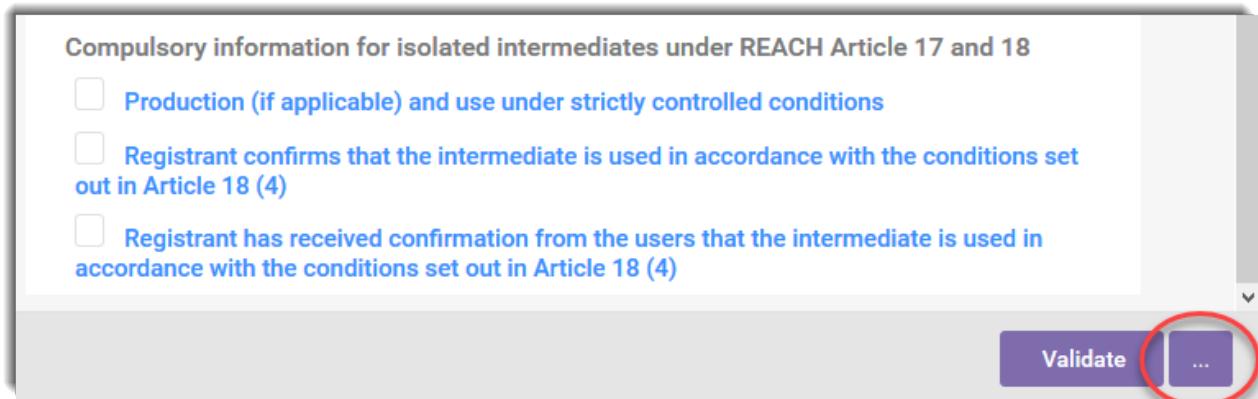
An example where to find the *Validate* button is shown for a *Substance* dataset.

**Figure 186: Run the Validation assistant on a Substance dataset**

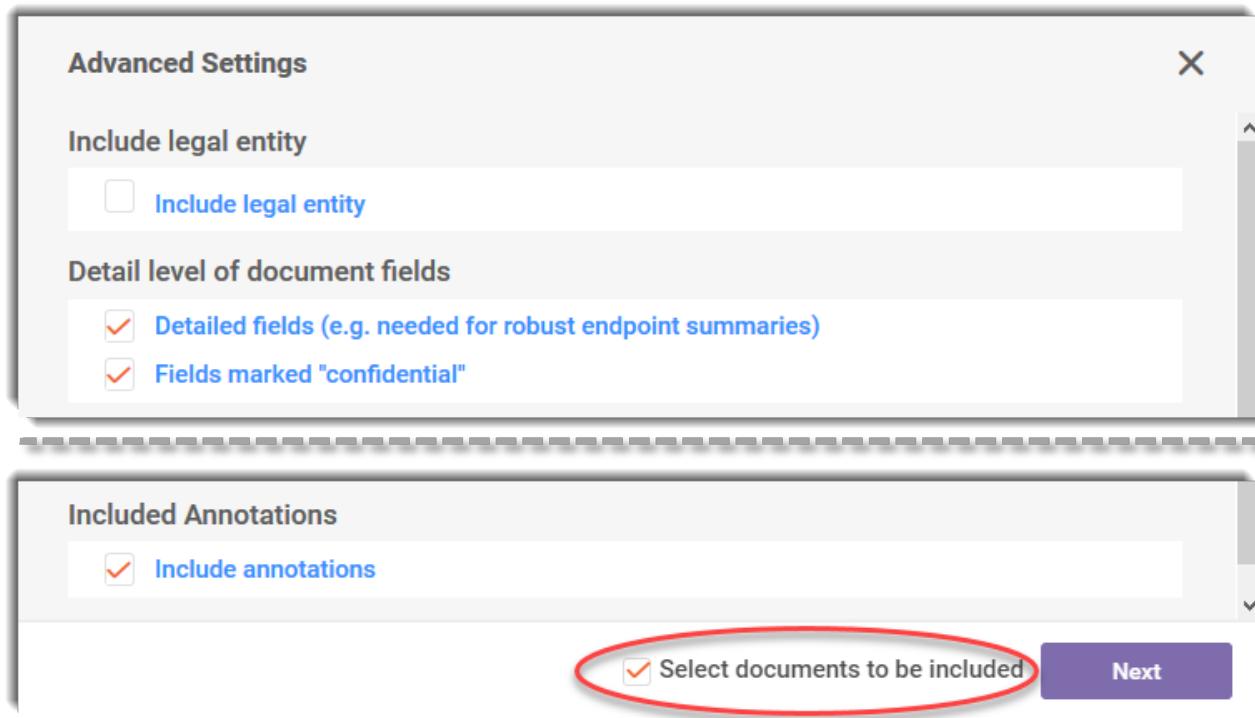


Fill out the *Dossier* header. To validate all of the dataset, click on the *Validate* button at the bottom right of the window. To exclude data from the validation, click on the button with three dots at the bottom right of the window, as indicated in the example below:

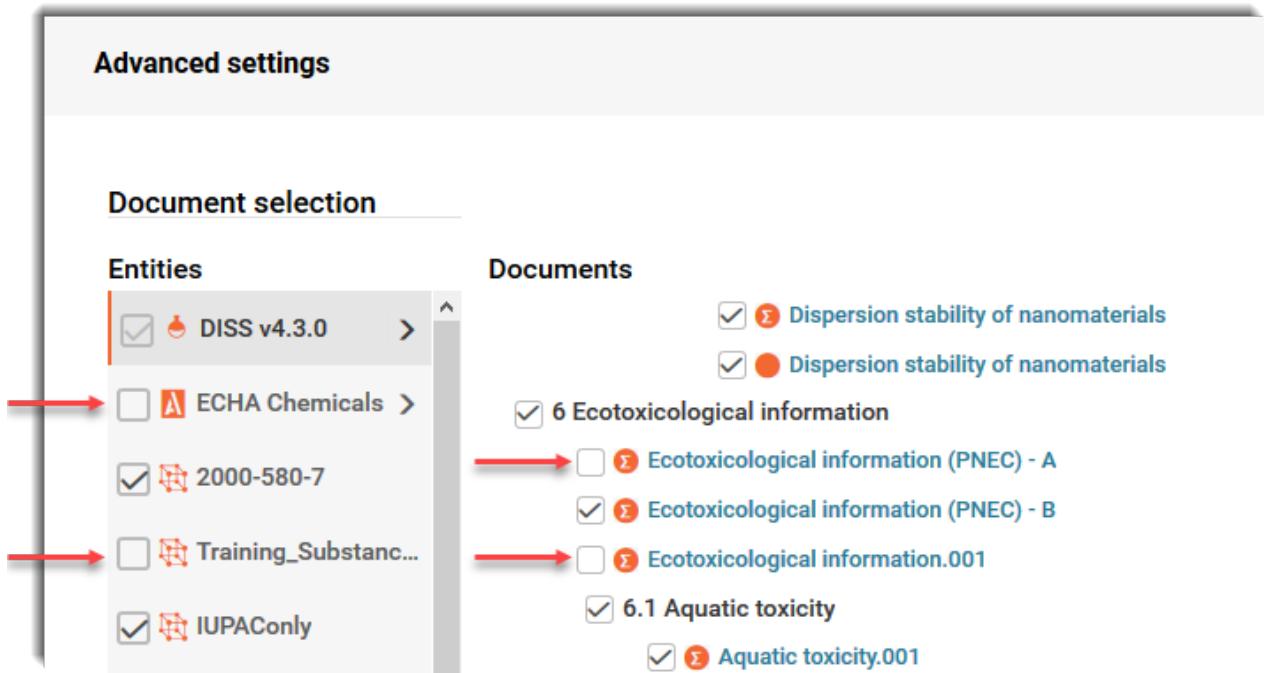
**Figure 187: Validate a subset of a dataset**



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

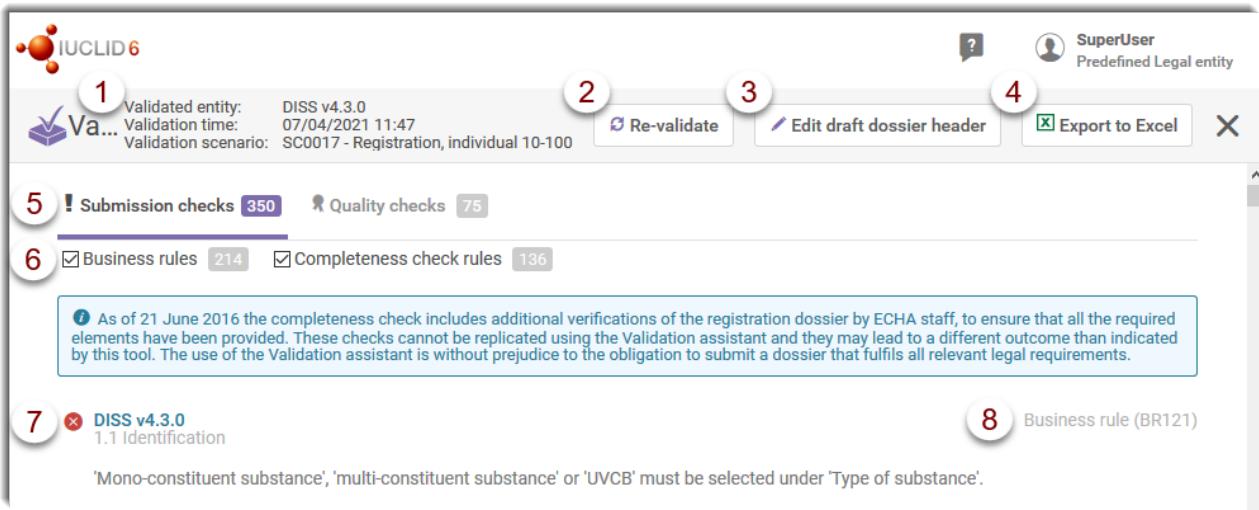
In the example shown below, some entities and specific documents have been excluded from the validation. To exclude a whole section in the table of contents, untick title of the section.

**Figure 189: 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.

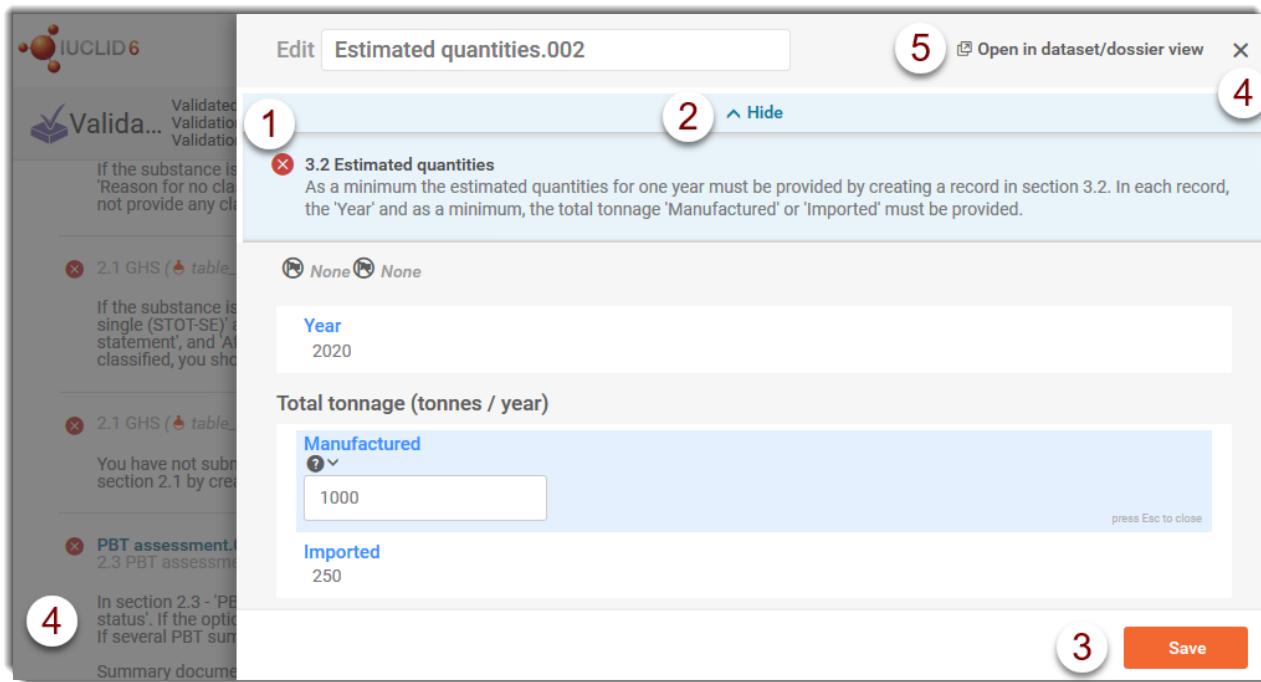
**Figure 190: The Validation assistant report: Submission checks**



#### Legend for Figure 190

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.

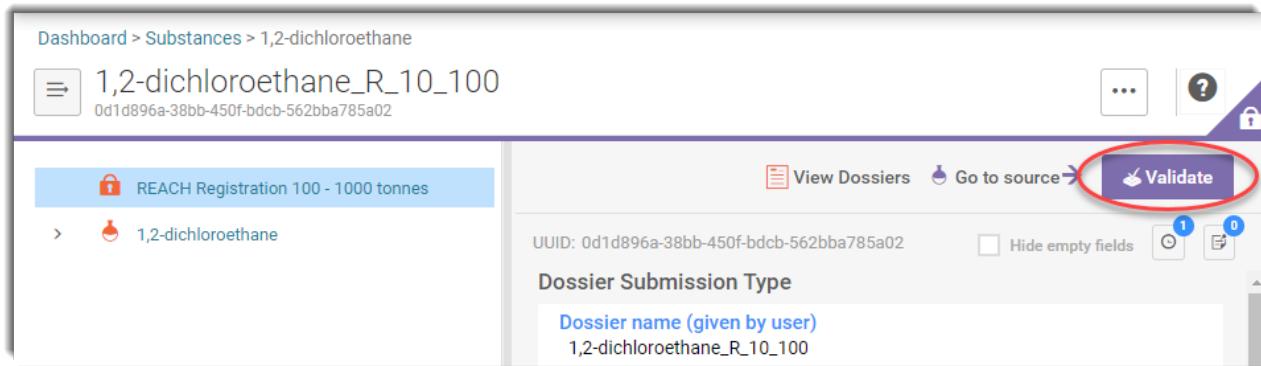
**Figure 191: Edit a document, and then go back to the validation assistant report**

### Legend for Figure 191

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.

## 17.4. 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 192: 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*.

## 17.5. 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.

## 17.6. 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.

## 18. 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.

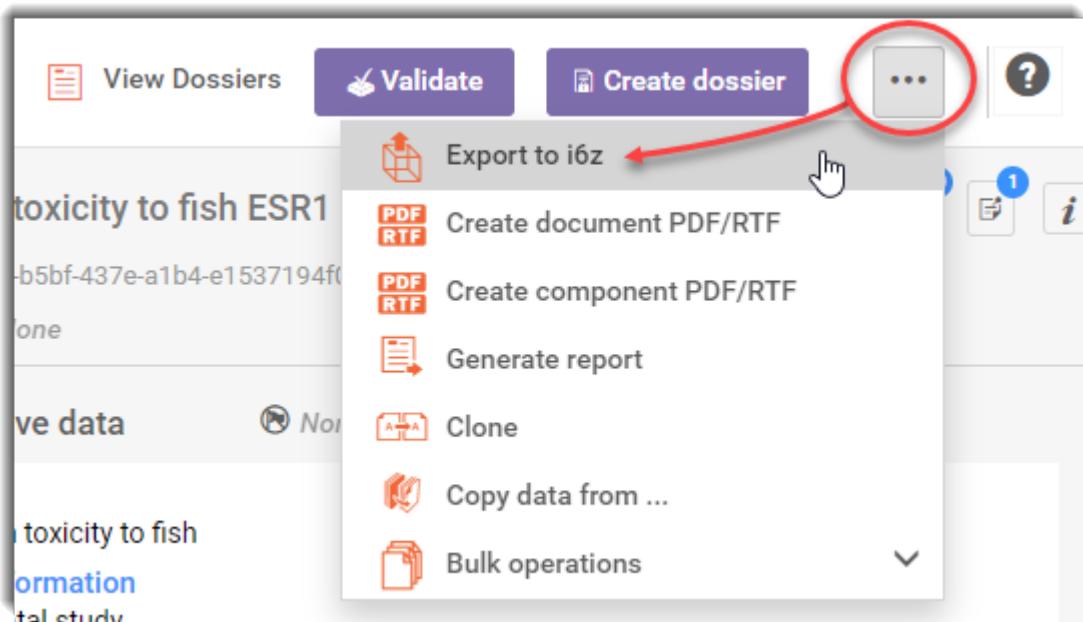
A document within an entity cannot be exported individually to an i6z file, but it can be exported in PDF or RTF format, as described in [20.2 Create document PDF/RTF - Create PDF/RTF](#). If *Export to i6z* is selected whilst a document is open in the data window, for example an endpoint study record, 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 is accessed from the menu under the three-dot button in the application window.

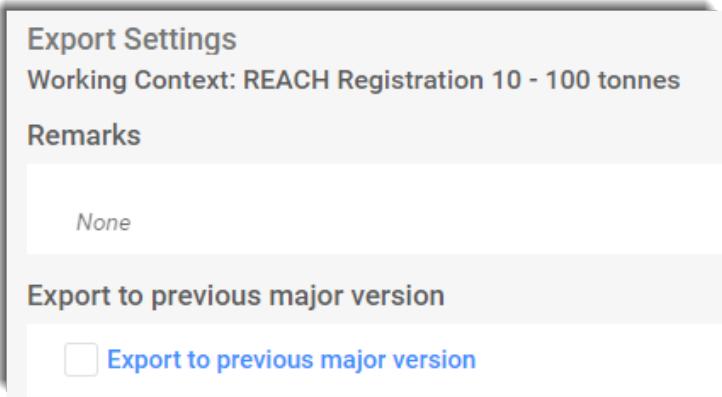
### 18.1. Export to i6z – raw dataset

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

Figure 193: Selecting Export to i6z for a Substance dataset



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

**Figure 194: 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.

### 18.1.1. Remarks

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

### 18.1.2. 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 ...
```

### 18.1.3. Detail level of document fields

See section 8.2.1.2 *Detail level of document fields*.

### 18.1.4. Flags for confidentiality

See section 8.2.1.3 *Flags for confidentiality*.

### 18.1.5. Flags for regulatory programmes

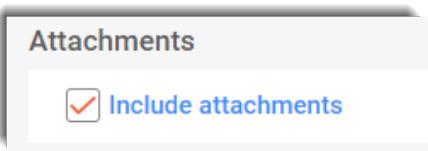
See section 8.2.1.4 *Flags for regulatory programme*.

### 18.1.6. Included annotations

See section 8.2.1.5 *Included Annotations*.

### 18.1.7. Included attachments

If the box is ticked, attachments will be exported.



### 18.1.8. Modification history

See section 3.7.16 *Modification History*.

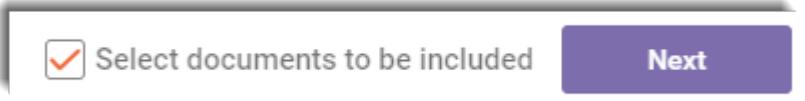
### 18.1.9. Reduced category content

See section 8.2.1.6 *Reduced category content*.

### 18.1.10. 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 195: 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 196: Exclude an entity from an Export to i6z file

Advanced settings

Document selection

Entities

- diethyl\_ether
- ref\_sub\_1
- Ethanol
- 2-methylpropan-2-ol

Documents

- diethyl\_ether
  - 1 General information
    - 1.2 Composition
      - Typical Composition 2013
      - Typical Composition 2013
      - Composition.003

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 substances* on the left that are referred to only in section 1.2.

**Figure 197: Exclude all the documents in a section from an Export to i6z file**

Advanced settings

Document selection

Entities

- diethyl\_ether >
- ref\_sub\_1
- Ethanol
- 2-methylpropan-2-ol
- butanone
- water
- diethyl ether

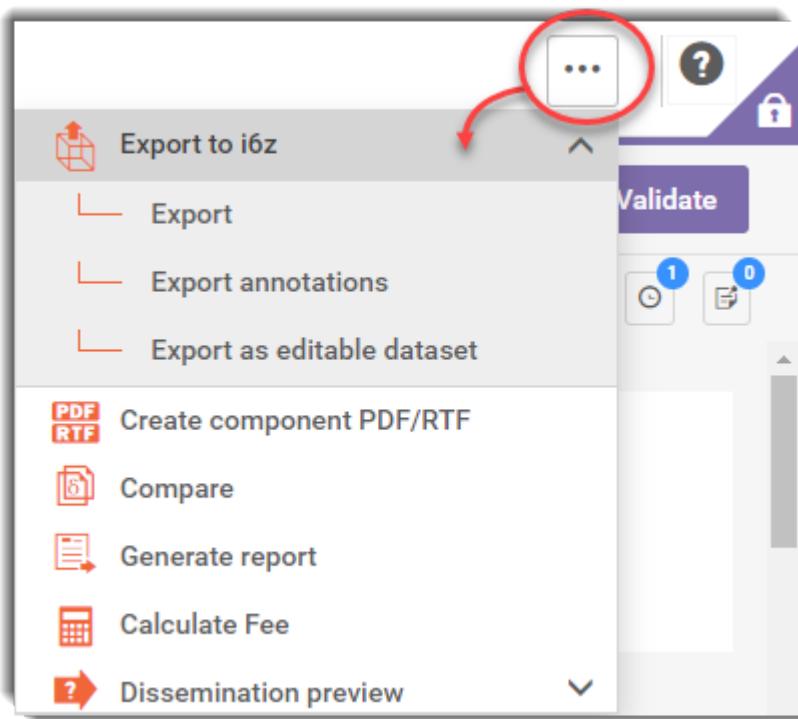
Documents

- diethyl\_ether
  - ✓ 1 General information
    - ✓ 1.2 Composition
    - Typical Composition 2013
    - Typical Composition 2013
    - Composition.003
  - ✓ 1.3 Identifiers
    - ✓ Identifiers
  - ✓ 1.4 Analytical Information
    - ✓ Analytical Information
  - ✓ 1.5 Joint submission

## 18.2. Export to i6z – Dossier

*Export to i6z* is run from the three dots button, as shown ringed in red in the example below. For a *Dossier*, there are three options.

Figure 198: Selecting Export to i6z for a Substance dataset



### 18.2.1. Export to i6z – Export of a Dossier

The *Dossier* is exported as an i6z file.

### 18.2.2. Export annotations

This exports to a zip archive, all the *Annotations* that are attached directly to the *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 it was created are not exported. These are shown in the *Annotations* window with a locked icon.

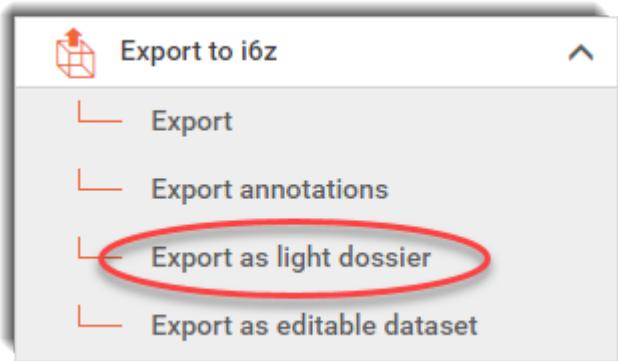
### 18.2.3. Export as editable dataset

This exports the subject of the *Dossier* as a raw dataset. For example, a *Substance dataset*. The raw dataset has the same UUID as the one used as the subject in the *Dossier*. The working context of the *Dossier* is not retained. This feature effectively acts as a tool to enable the re-use of the subject of a *Dossier* in a new *Dossier*. This is useful where the original dataset is no longer available.

#### 18.2.4. 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 199: 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 200: Selecting the base dossier for a light dossier**

A screenshot of a modal dialog titled 'Select the base dossier'. It shows a search bar and a button with a magnifying glass icon. Below it, it says '2 items found'. There are two entries: 'mix\_one\_3\_20\_0c' and 'mix\_one\_3\_20\_0 b'. Each entry includes columns for 'Subject name', 'Submission type', and 'Dossier UUID'. The first entry has a lock icon next to its Dossier UUID. Both entries have edit icons at the end of their rows.

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

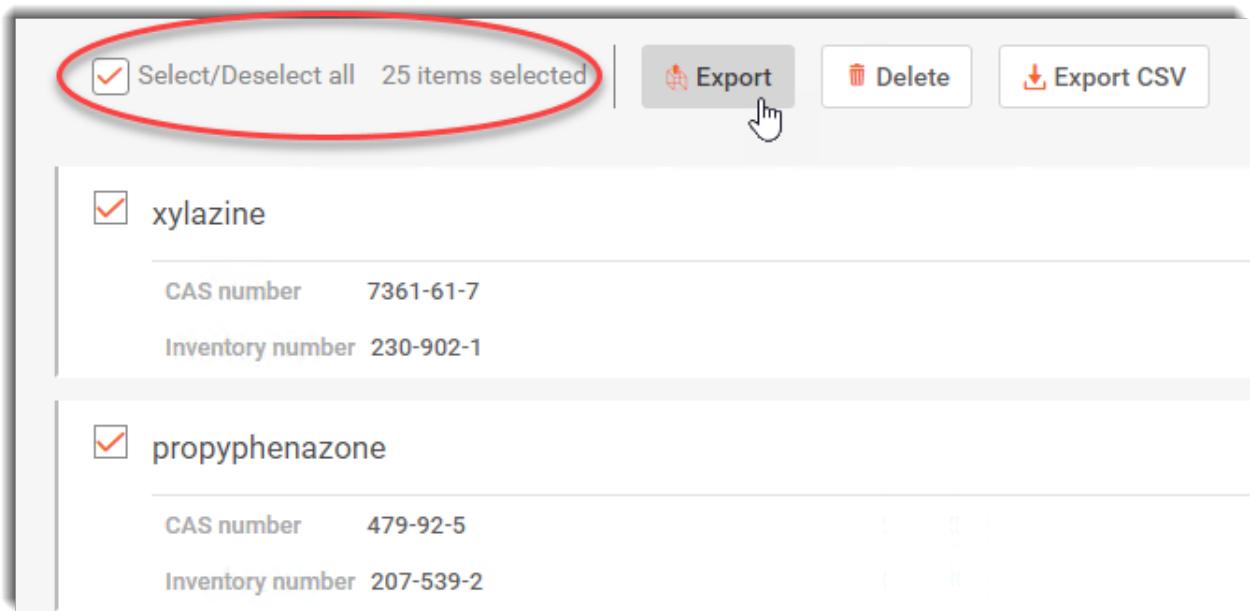
EU PPP Plant protection product authorisation

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.”.

## 19. 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 201: 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.

## 20. Output data to files of format PDF or RTF

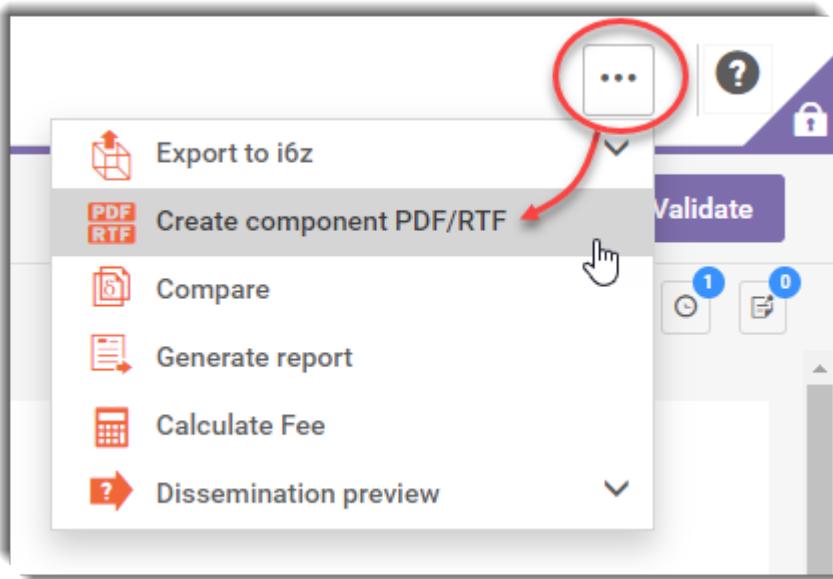
Documents and entities in raw datasets or Dossiers can be exported to files of standard formats that differ from the internal standard format of IUCLID (i6z). The options are PDF, and Rich Text

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.

## 20.1. Create component PDF/RTF

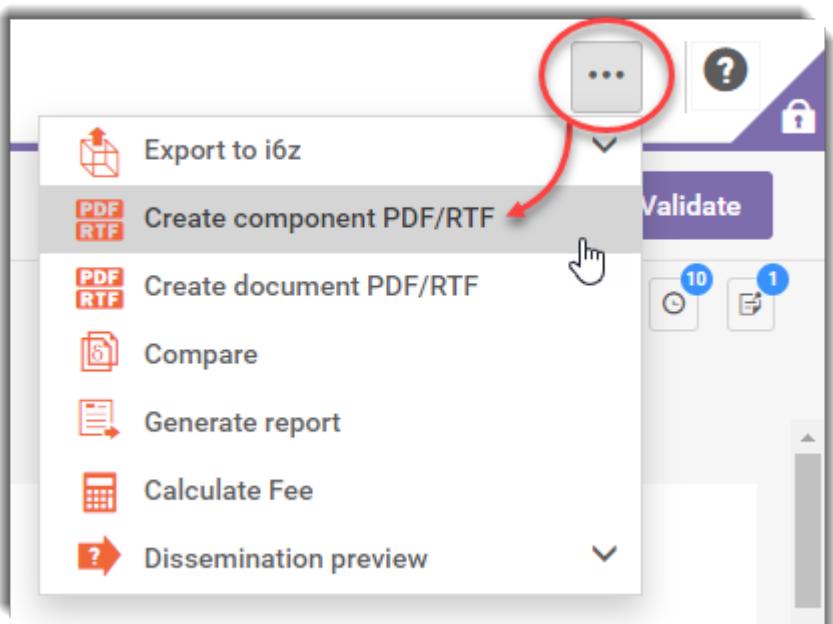
This option prints a whole raw dataset or Dossier. For example, where the Dossier header is selected it is the only option because the selection effectively means the whole Dossier.

**Figure 202: 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 203: Output all of a Dossier to a file whilst a document is selected**



## 20.2. 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 204: Output a single entity from a raw dataset

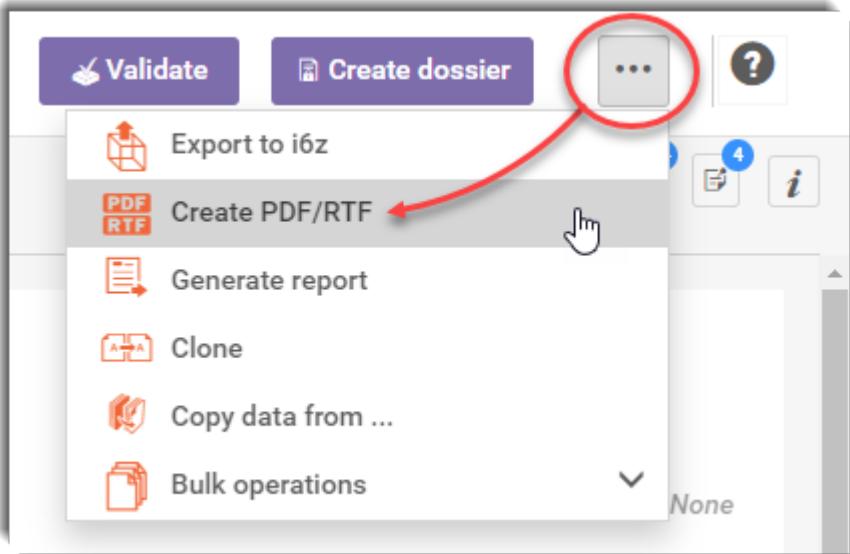
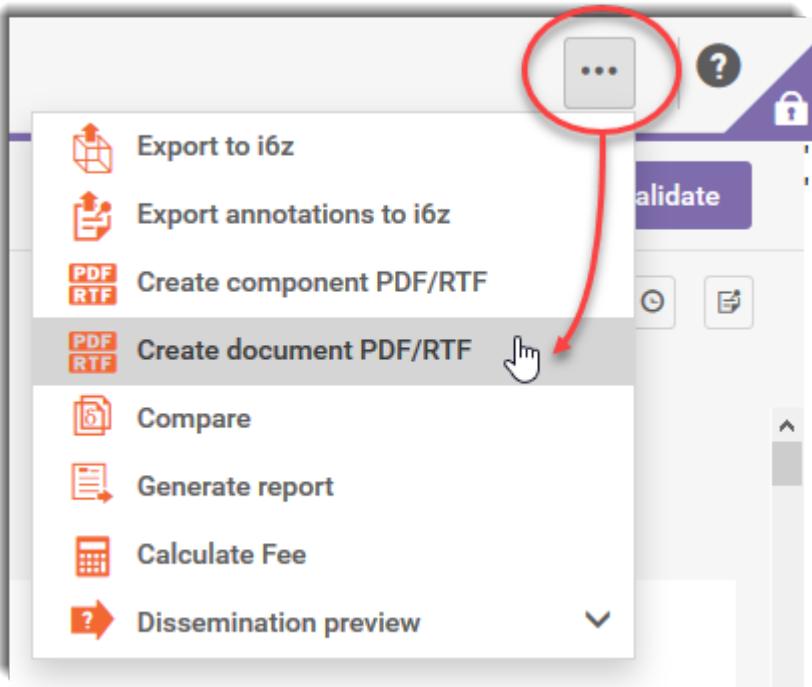


Figure 205: Export only the currently selected document from a Dossier to a file



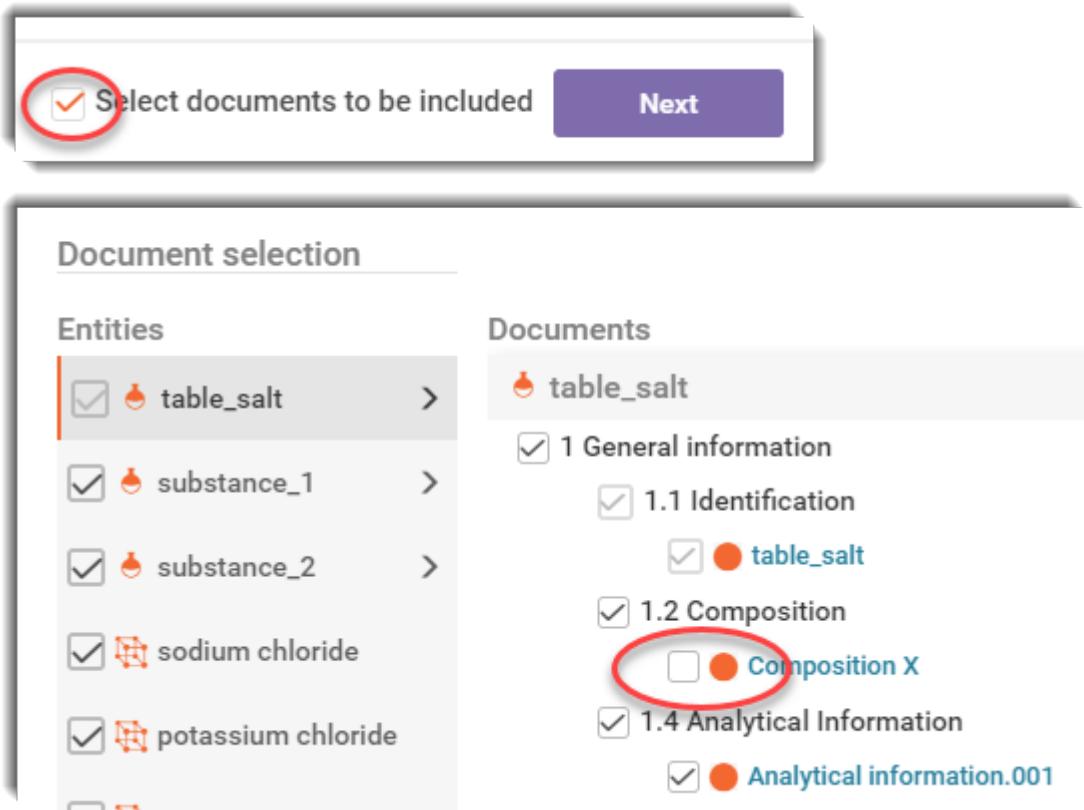
## 20.3. PDF/RTF Settings

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.

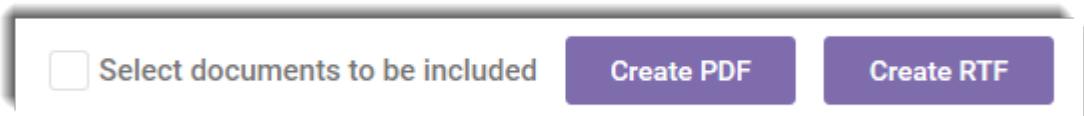
If the file is being created for a whole dossier, or a whole dataset, there is an option at the foot of the first page labelled *Select documents to be included*. This allows only certain individual documents to be excluded from the file. On the next page, documents can be excluded by unticking their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

**Figure 206: Exclusion of a document from the PDF file**



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

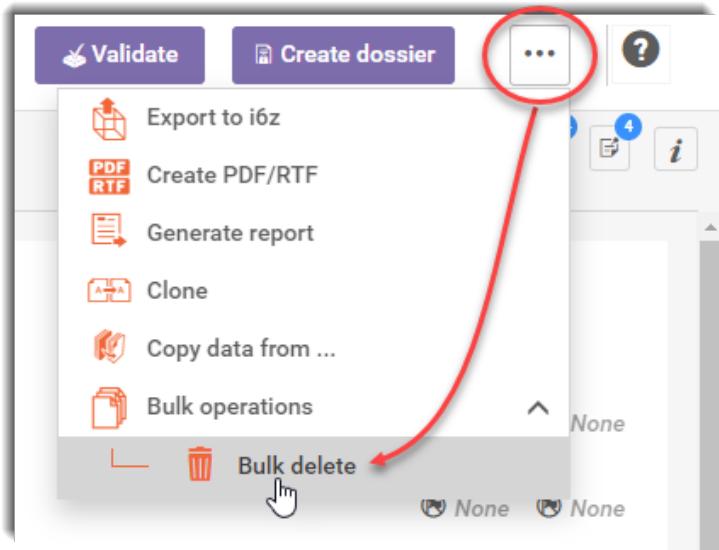
**Figure 207: Select the type of file to be exported**



## 21. 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 208: 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.

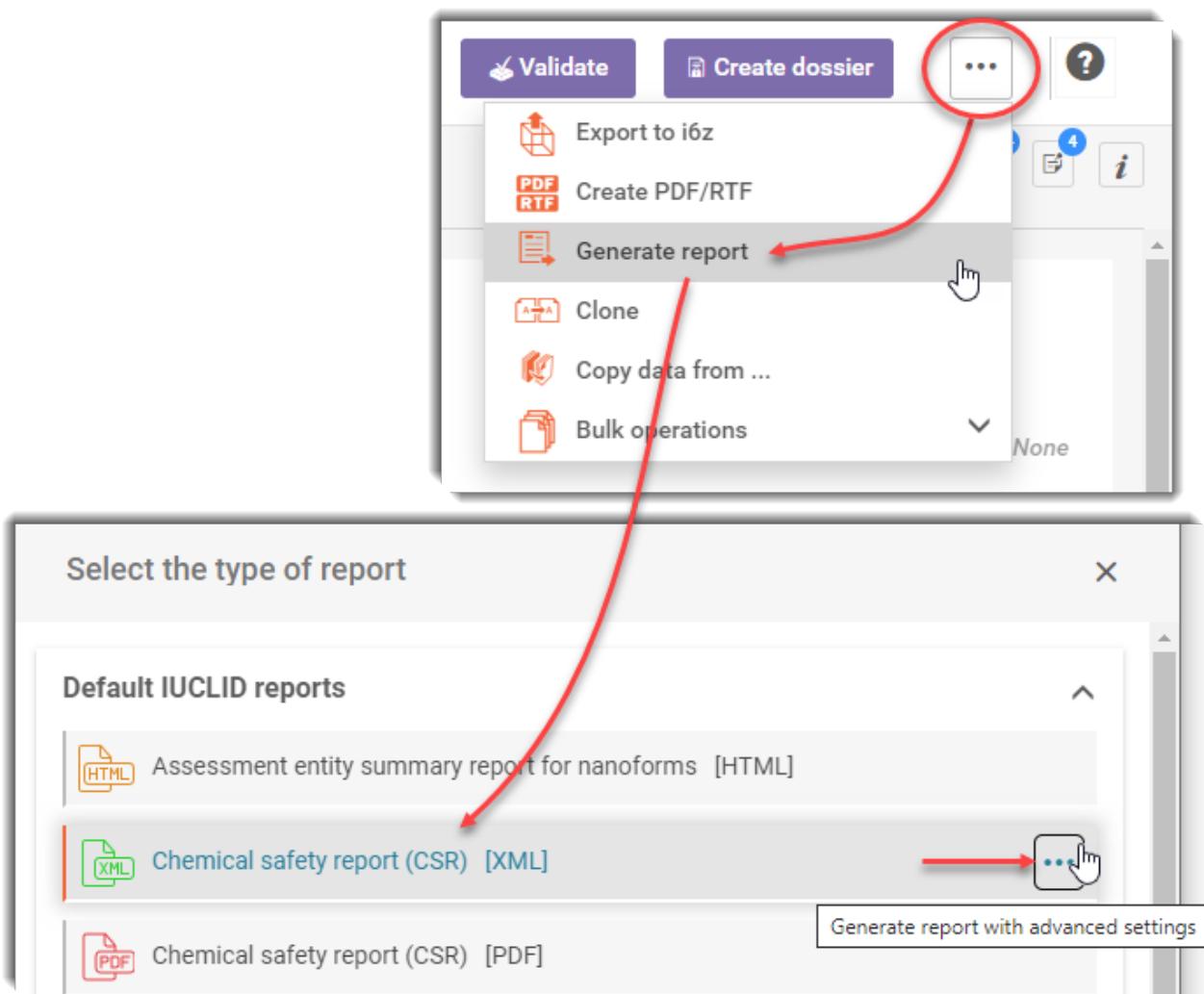
Figure 209: Bulk delete - Select documents to delete individually and by section

A screenshot of the 'Bulk delete' dialog. The title bar says 'Bulk delete'. Below it is a section titled 'Document selection'. On the left is a tree view of 'Entities': 'table\_salt', 'substance\_1' (which is expanded), 'substance\_2', 'newene', 'aquatic\_toxicity', 'Basic\_toxicokinetic...', and 'ECHA Chemicals'. To the right is a 'Documents' section. Under 'substance\_1', there are several sections: '1 General information', '1.1 Identification' (with a checkbox next to 'substance\_1'), '1.2 Composition' (with a checked checkbox next to 'Composition.001'), '1.4 Analytical Information' (with checkboxes next to 'Analytical information.001' and 'Analytical information.002'), '1.10 Assessment approach (assessment entities)' (with a checkbox next to 'Assessment approach'), and '2 Classification & Labelling and PBT assessment' (with an empty checkbox). The 'substance\_1' entity is highlighted with a red border.

## 22. 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 web 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 210: 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.

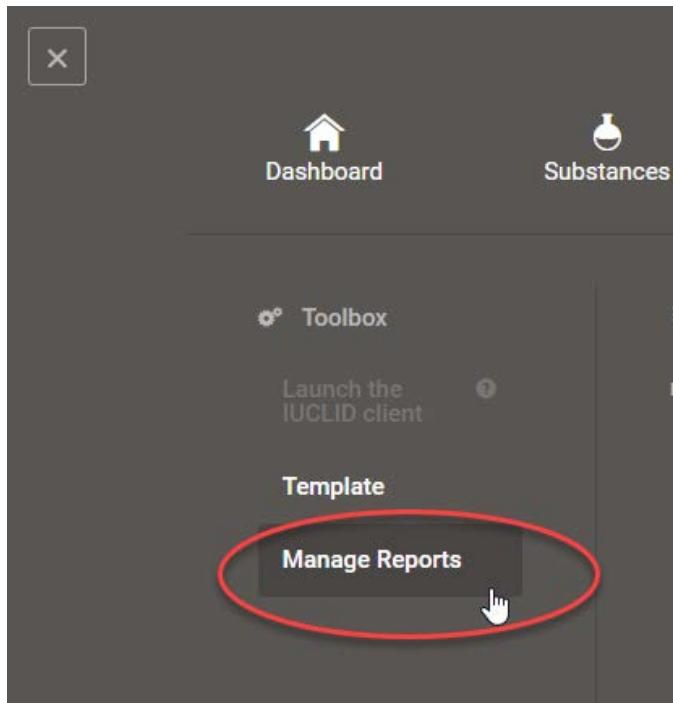
## 22.1. Manage reports

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 211: 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 212: The list page for reports**

The screenshot shows the 'Reports' section of the IUCLID web interface. At the top, there is a search bar and a 'New report' button. Below the search bar, it says '2 results found'. A sorting dropdown is set to 'Newest first'. Two reports are listed:

Name	Date	Actions
CSR_example_two	30/03/2021 16:33	...
CSR_example_one	30/03/2021 16:25	...

For each report, there is a column for 'Output format' (rtf) and 'Description'.

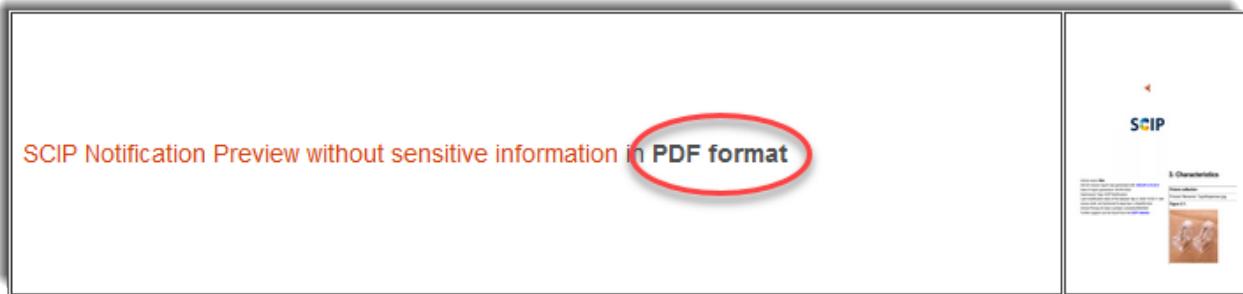
A report must have a name, and at least one type of file must be selected in the field *Output file*. In the example below, there is only one type of file that is appropriate, which is PDF.

**Figure 213: Selecting file types for a Report**

The screenshot shows the configuration page for a 'SCIP Notification Preview - custom' report. It includes fields for 'Name' (containing 'SCIP Notification Preview - custom'), 'Description' (empty), and 'Output file' (a dropdown menu). A red arrow points from the text 'Please select' in the dropdown to the word 'PDF' in the list below it.

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 214: An example of a report template on the IUCLID website**

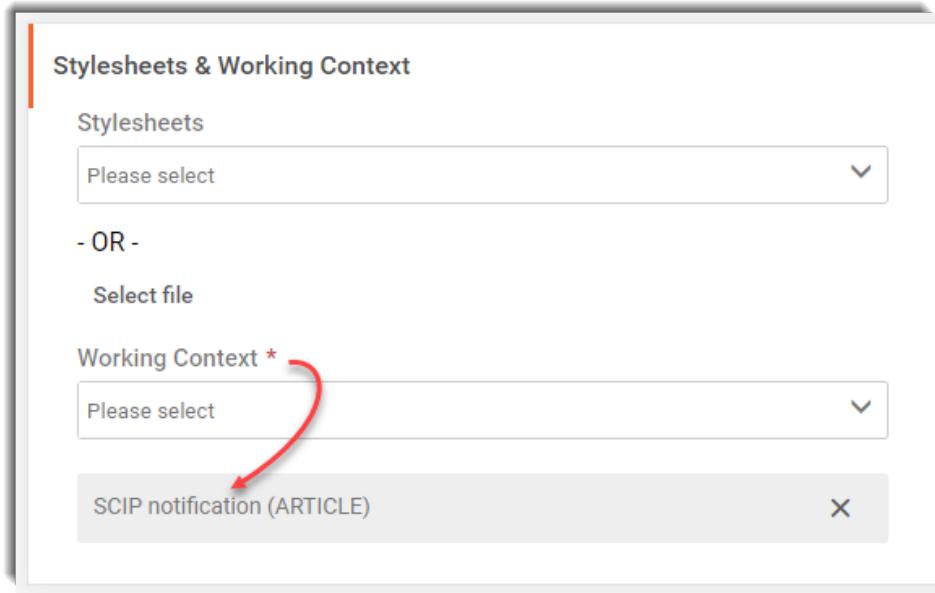


Upload a *main* template file and any additional template files required. The file extension is *ftl*. An example is shown below for a report definition available on the IUCLID website. *Main* templates have the word *main* in the filename.

**Figure 215: Upload report definition files**

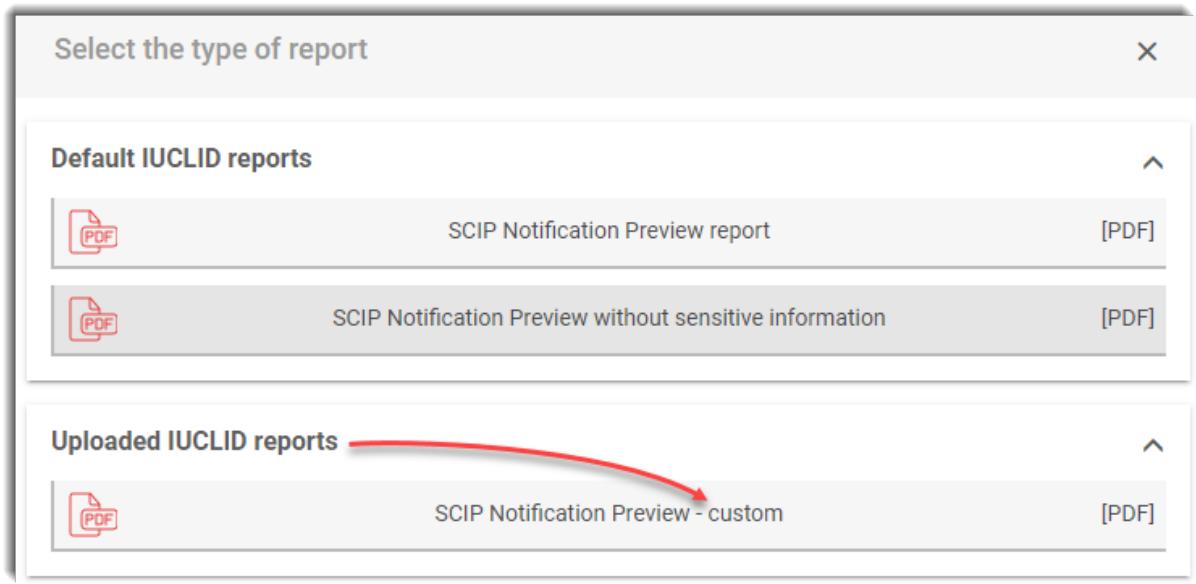


The next step is to define the format of the output of the report using either a style sheet, or by selecting a *working context*. If a *working context* is selected, the report will be available in the *Report generator* only where that *working context* is currently selected for the source of data.

**Figure 216: 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.

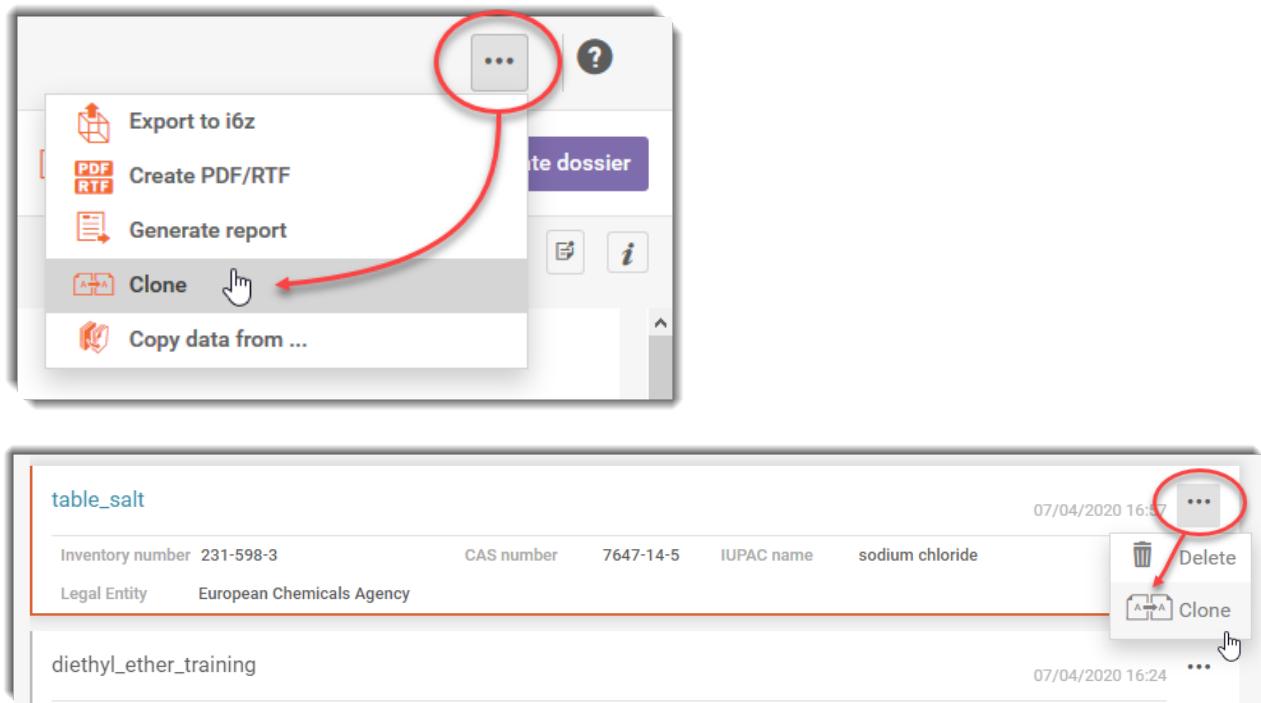
Uploaded reports are run from the *Report generator*, where they are shown under the default built-in reports, as shown in an example below.

**Figure 217: Selecting an uploaded definition of a report in the Report generator**

## 23. 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 218: 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 219: Cloning a substance dataset that has Assessment entities attached**

The screenshot shows two side-by-side substance datasets in the IUCLID web interface.

**Top Panel (Original Dataset):**

- UUID: IUC5-2dd443b4-a92a-4f7b-9348-b7a896f4c38c
- Substance name\*: table\_salt
- Public name: Table Salt X
- Icons in the top right: 2 (link), 16 (circles), 2 (envelope), and 1 (info).

**Bottom Panel (Clone Dataset):**

- UUID: 759523cd-fbae-48db-84d4-fc4c442ecd9d
- Substance name\*: table\_salt\_CLONE\_26.04.2022 n3
- Public name: Table Salt X
- Icons in the top right: 2 (link), 1 (circle), 0 (envelope), and 1 (info).

Red arrows point from the clone's assessment icons (2 link, 1 circle, 0 envelope) to the original dataset's assessment icons (2 link, 16 circles, 2 envelope).

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 220: Cloning a substance dataset that is in a Category**

The screenshot shows two side-by-side substance datasets in the IUCLID web interface, illustrating the cloning of a substance that is part of a category.

**Left Panel (Original Dataset):**

- REACH Registration 10 - 100 tonnes
- table\_salt
  - 1 General information\*
  - 2 Classification & Labelling and PBT assessment\*
  - 3 Manufacture, use and exposure\*
  - 4 Physical and chemical properties\*
  - 14 Information requirements
  - Inherited templates
  - Linked Categories

**Right Panel (Clone Dataset):**

- REACH Registration 10 - 100 tonnes
- table\_salt\_CLONE\_26.04.2022 n4
  - REACH Registration 10 - 100 tonnes
  - table\_salt\_CLONE\_26.04.2022 n4
    - 1 General information\*
    - 2 Classification & Labelling and PBT assessment\*
    - 3 Manufacture, use and exposure\*
    - 4 Physical and chemical properties\*
    - 14 Information requirements
    - Inherited templates

Red arrows point from the clone's category structure (14 Information requirements, Inherited templates) to the original dataset's category structure (14 Information requirements, Inherited templates).

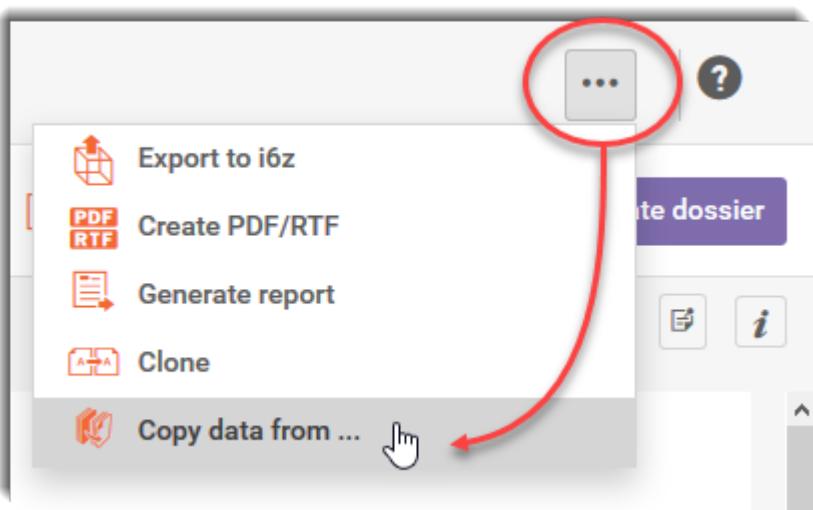
To add a link of the type shown on the left to the cloned Substance on the right, go to the Category, and create a reference to the cloned Substance. It is also possible to clone the Category, then create a reference to the cloned Substance.

*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*.

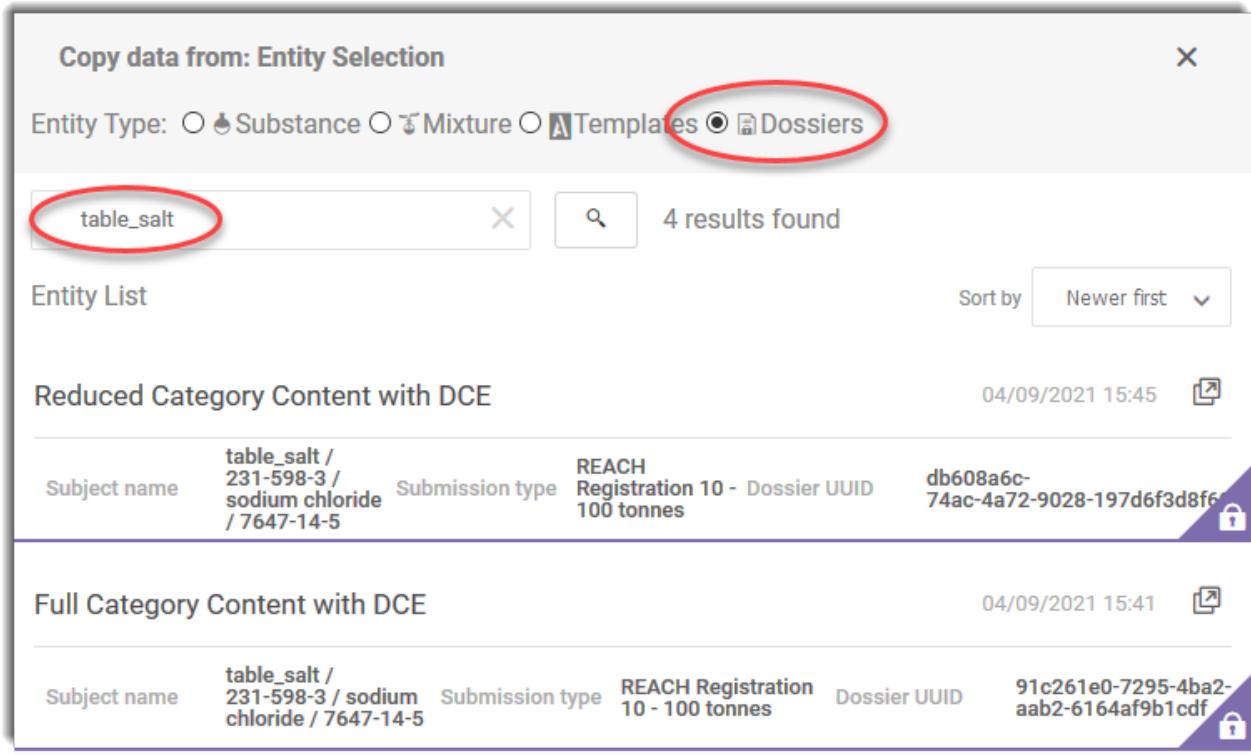
## 24. Copy data from ...

*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.

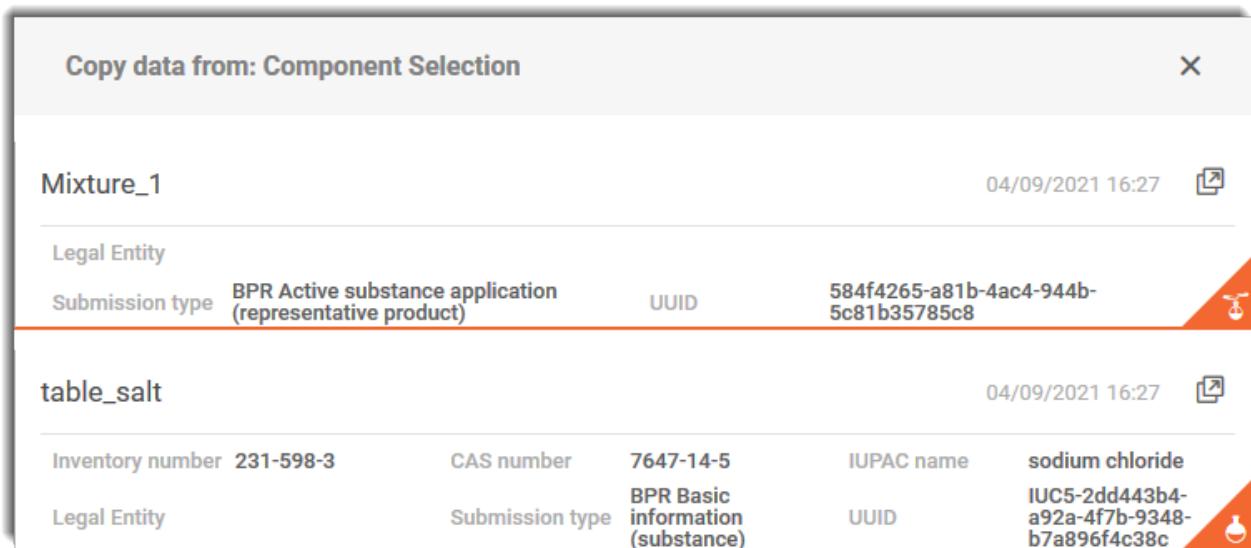
Figure 221: *Copy data from* ...



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 222: 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 223: 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 224: Select the document(s) to be copied**

The screenshot shows two expandable sections in the IUCLID web interface:

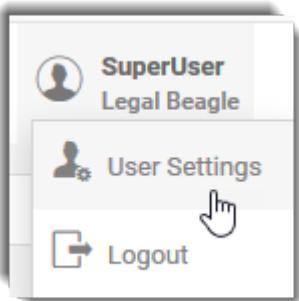
- Toxicological information**
  - Toxicokinetics, metabolism and distribution**
    - Basic toxicokinetics** (checked with a red arrow)
    - Basic toxicokinetics.001** (checked with a red arrow)
    - Dermal absorption** (unchecked)
    - Dermal absorption.001** (unchecked)
    - Toxicokinetics, metabolism and distribution.001** (unchecked)
- Dissociation constant**
  - pH** (unchecked)
  - pH.002** (unchecked)
  - pH.001** (unchecked)
  - Dissociation constant** (unchecked)
  - Dissociation constant.002** (checked with a red arrow)

A purple "Copy" button is located at the bottom right of the second section.

## 25. 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 log-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 9.1 *Working Legal entity*. The access is via a menu at the top right of the interface, as shown below.

Figure 225: 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 25.4 *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 226: User management with Instance Based Security (IBS) active

A screenshot of the IUCLID 6 web interface main menu. The menu items are: Dashboard, Substances, Mixture/Products, Articles, Categories, Toolbox, Inventory manager, User management (which is circled in red), Contact, User, About IUCLID, Template, Legal entity, Role, Help, Manage Reports, Sites, Group, About, Reference substance, Administration, Test material, and Literature reference.

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

## 25.1. 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 25.4.

## 25.2. 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 227: User management via the record page of a User

The screenshot shows a web-based application interface for managing users. At the top, a navigation bar indicates the path: Dashboard > Users > User One. Below this, the title "User One" is displayed next to a back arrow icon. The main content area is titled "User profile". It contains several input fields: "Username \*" with the value "User\_1"; "First name \*" with the value "User"; "Last name \*" with the value "One"; and an "E-mail" field which is empty. To the right of the "Last name" field, there is a link labeled "Change password" with a small circular icon. The entire interface has a clean, modern design with a light gray background and white text.

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.

## 25.2.1. 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.

### 25.2.1.1. 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 228: Password management

The screenshot shows a 'Change password' dialog box. At the top left is the title 'Change password' and at the top right is a close button ('X'). Inside the dialog, there is a section titled 'Password Rules' enclosed in a blue border. It contains the following text: 'Your new password must always satisfy the following rules :  
Password should be at least 4 characters in length  
Password should contain a capital letter  
Password should contain a number  
Password should be different from the last 3 passwords'. Below this section are two input fields: 'New password \*' and 'Confirm password \*'. Both fields have a placeholder 'None' and are currently empty.

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.

### 25.2.2. 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.

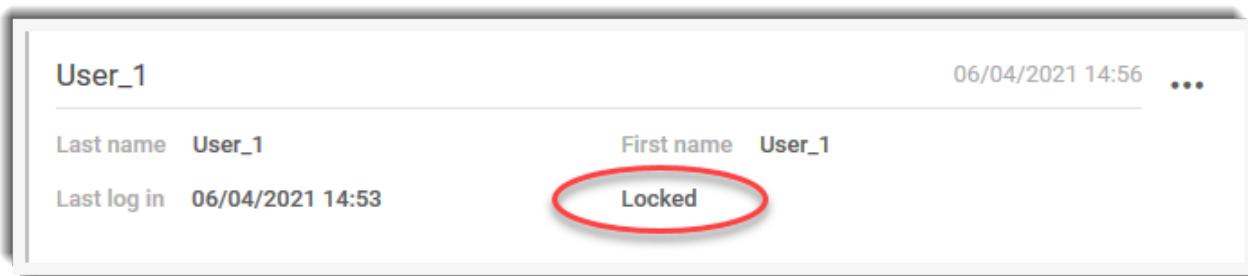
### 25.2.3. General

The option *Access All* is shown only when Instance Based Security (IBS) is active. For a description of IBS, see section 25.4 *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 229: 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*.

## 25.2.4. Roles

Figure 230: Adding a Role to a User under User management

#	Role	Action
1	User manager	
2	Full access	

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.

## 25.2.5. 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 231: Adding a Legal entity to a User under User management

#	Legal entity	Working legal entity	Action
1	Predefined Legal entity	<input checked="" type="checkbox"/>	
2	legal_entity_one	<input type="checkbox"/>	

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

## 25.2.6. Groups

This field is shown only when Instance Based Security (IBS) is on. For a description of IBS, see section 25.4 *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 232: Adding a User to a Group under User management**

#	Group	Action
1	Common	

### 25.2.7. 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 233: Default group access for a User**

Annotations	Common:	No access
	Group_A:	(R/W)
	Group_B:	(R/W/D)
Articles	Common:	No access
	Group_A:	(R/W)
	Group_B:	(R/W/D)

### 25.2.8. 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.

#### 25.2.8.1. 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.

#### 25.2.8.2. 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.

### 25.2.9. Import and Export of Users

If you need to import or export *Users*, use the classic interface. See the IUCLID website on how to open the classic interface.

## 25.3. 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.

#### 25.3.1. 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.

### 25.3.2. Permissions - access to operations

#### 25.3.2.1. Basic Operations

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

#### 25.3.2.2. 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.

### 25.3.3. Permissions - access to data

#### 25.3.3.1. Access to entities and inventories

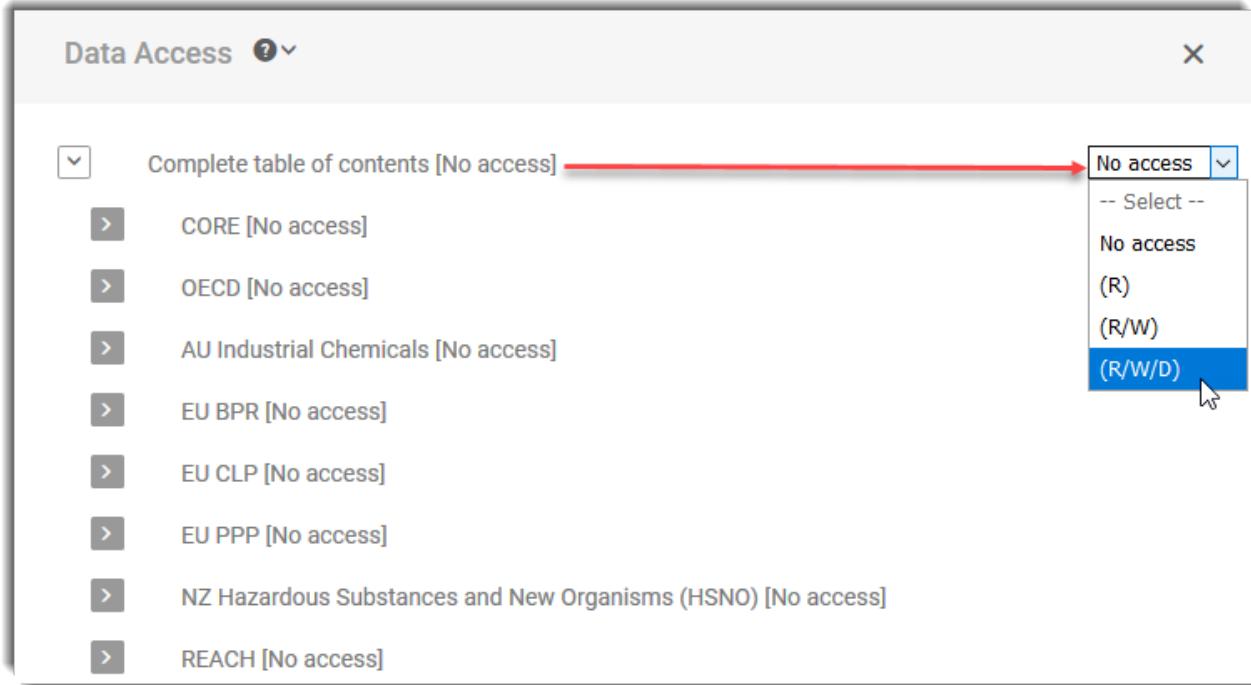
Here, access can be defined per type of entity, for example for all *Mixtures*. Clicking on a field opens a drop-down menu of the types of access available: no access, R (read), R/W (read and write), R/W/D (read and write and delete).

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

#### 25.3.3.2. Data access to section documents

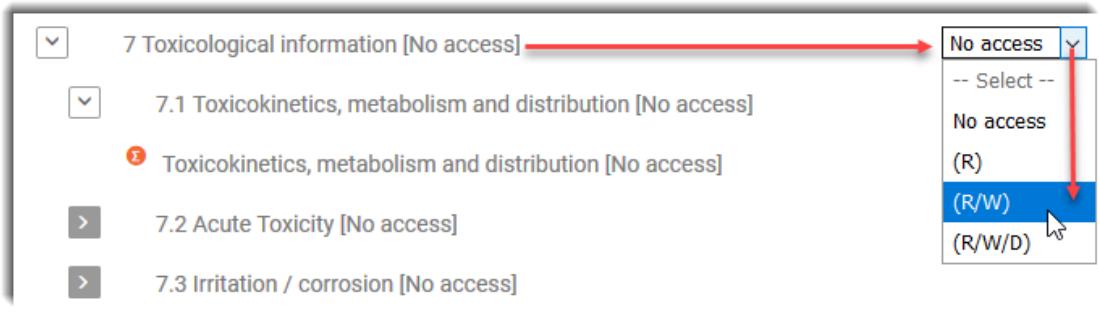
Here, access to data in datasets can be controlled at the level of section. The sections are shown in the default tree structure. To open the view, hover the cursor over the text “please view and select...”, then click on the grey box.

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 234: 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 235: 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*.

## 25.3.4. Application management

### 25.3.4.1. System configuration

*System configuration* is available only via the classic interface. See the IUCLID website on how to open the classic interface.

### 25.3.4.2. Security management

*Security management* is available only via the classic interface. See the IUCLID website on how to open the classic interface.

### 25.3.4.3. 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).

### 25.3.4.4. 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).

### 25.3.4.5. Assign Legal entities to users

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

### 25.3.4.6. Assign Roles to users

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

### 25.3.4.7. Remove Roles from users

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

## 25.3.5. 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.

### 25.3.5.1. IBS management

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

### 25.3.5.1.1. 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).

### 25.3.5.1.2. Assign users to groups

This right permits the changing of *Group* membership.

### 25.3.5.1.3. Manage private groups

This right permits the changing of ownership of a document. For more information see section 25.4.3 *Ownership*.

## 25.3.6. 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.

### 25.3.6.1. System administrator

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

### 25.3.6.2. Full access

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

### 25.3.6.3. Read-only

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

### 25.3.6.4. 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*.

### 25.3.6.5. 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*.

## 25.4. 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.

### 25.4.1. 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*.

#### 25.4.1.1. 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*.

#### 25.4.1.2. 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 236: Add a User to a Group from the record of the User**

#	Group	Action
1	Common	

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 237: Add a User to a Group from the record of the Group**

The screenshot shows the 'group\_1' group record in the IUCLID web interface. The 'Group information' section contains fields for 'Group name \*' (set to 'group\_1') and 'Group description'. The 'Assigned users' section lists two users: 'SuperUser' and 'User\_12345', both marked as managers. A red circle highlights the '+ New item' button in the 'Assigned users' section.

#	User	Manager	Action
1	SuperUser	<input checked="" type="checkbox"/>	
2	User_12345	<input checked="" type="checkbox"/>	

Select the *User* from those available. In the example below *User Reader\_12345* is selected.

**Figure 238: Select a User for membership of a Group**

The screenshot shows the 'Select User' dialog box. It displays two user records: 'FullAccess' and 'Reader\_12345'. The 'Reader\_12345' record is highlighted with a mouse cursor pointing at it. The 'FullAccess' record is also shown with its details: Last name 'Full Access', First name 'User', and Last log in 'Expired'. The 'Reader\_12345' record is also shown with its details: Last name 'Reader\_12345', First name 'Reader\_12345', and Last log in '13/04/2021 18:43'.

Last name	First name	Last log in
Full Access	User	Expired
Reader_12345	Reader_12345	13/04/2021 18:43

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*.

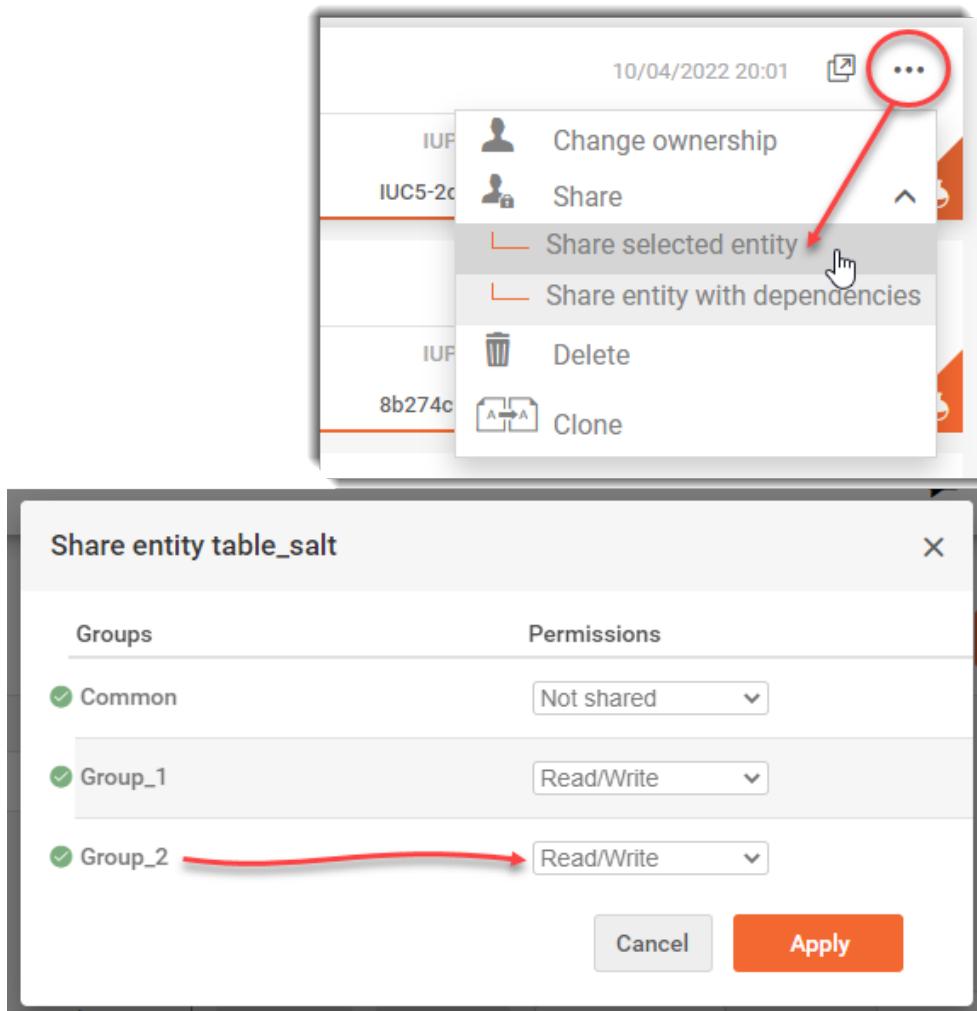
### 25.4.2. Share

*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 239: 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*.

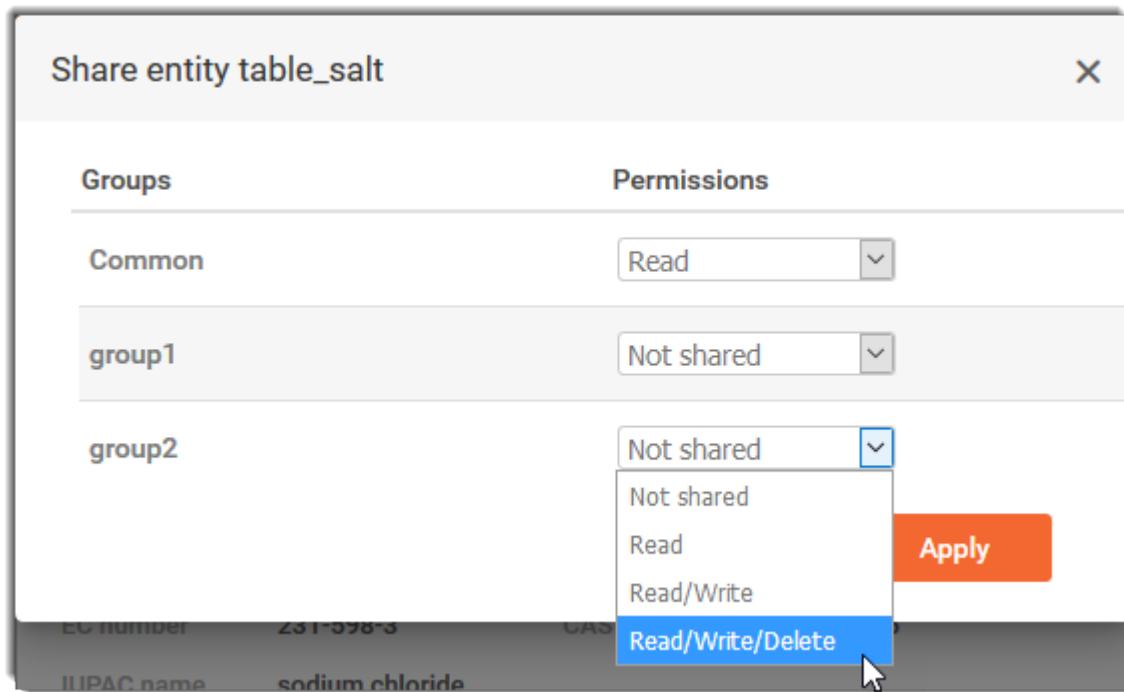
A *User* that has access to an entity only because of sharing, cannot edit the sharing of the entity.

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 240: Example of sharing a Substance dataset

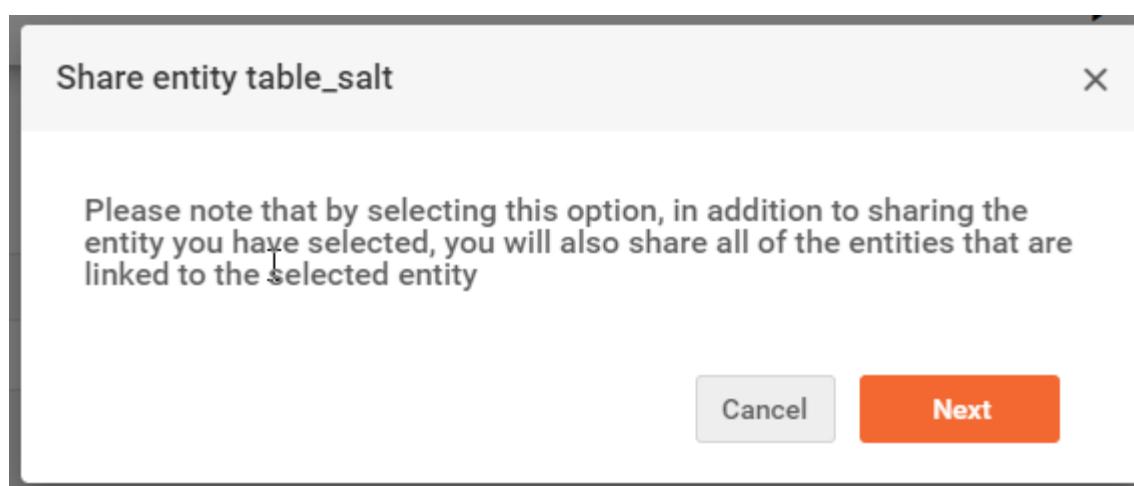


For *group2*, the permissions are being changed from *Not shared*, to *Read/Write/Delete*.

### 25.4.2.1. 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 241: Share entity with dependencies



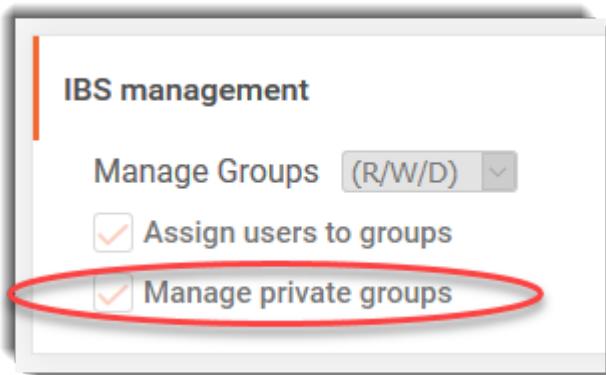
### 25.4.3. Ownership

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.

#### 25.4.3.1. Change ownership

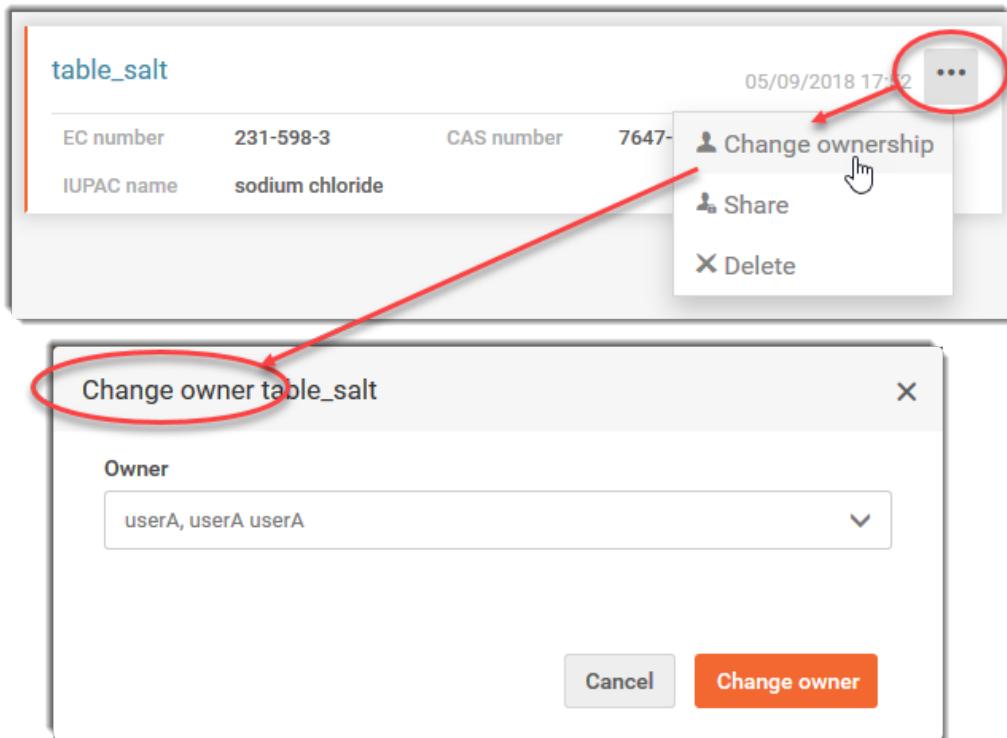
When an entity is created or imported, its ownership is set to that of the current *User*. An entity can have only one owner at a time. Ownership can be transferred only within the *Group* of the owner. Ownership can be transferred only by a *User* that is a manager of a *Group*, and has a *Role* in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

Figure 242: The right to change ownership



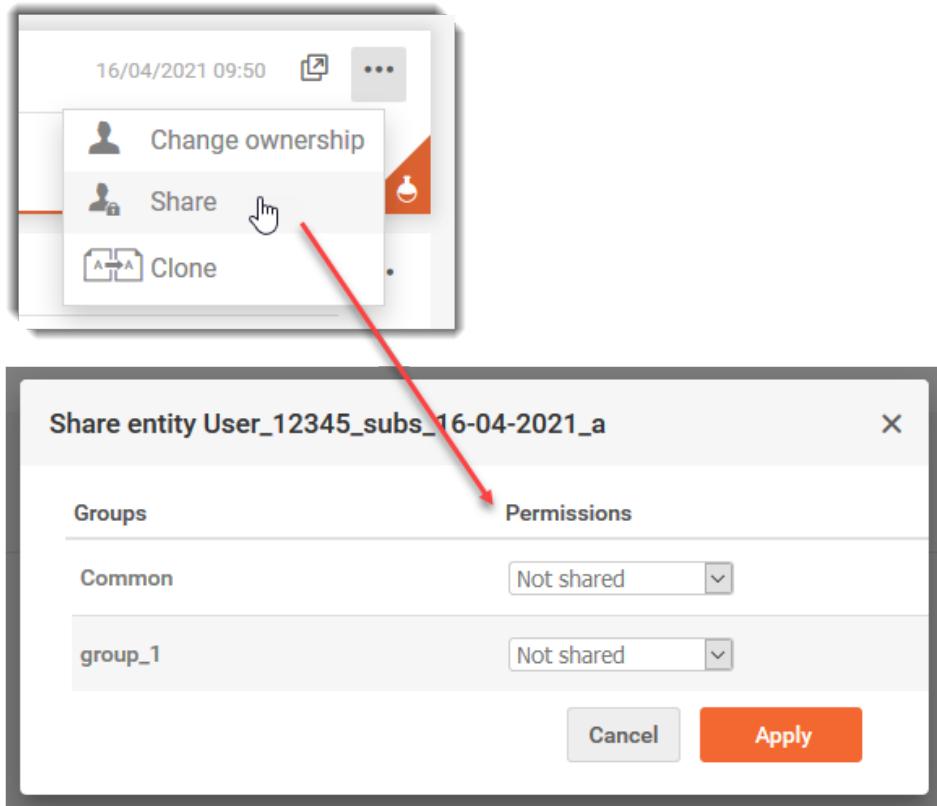
The predefined *Roles* that provide this right are *Administrator* and *Group manager*.

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

#### 25.4.3.2. 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 244: User manager access to an entity it does not own**

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

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

**result 2:** The following access has been granted.

**Table 12: IBS exercise - result 2**

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

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

**result 3:** The sharing allowed is shown below.

**Table 13: IBS exercise - result 3**

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

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

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

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

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

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

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

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

**Table 15: IBS exercise - result 7**

User	Access	Comment
userA	(rwd)	userA does not own Substance1 so it cannot share it, but it has rwd access because the User is in group1.
userB	(rwd), share	userB owns Substance1. Ownership gives full access, including sharing.
userC	(r)	Previously userC had no access rights, but now the userC can at least read the document because all <i>Users</i> have been granted that right as part of this

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

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

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

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

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

## 26. 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 26.1.5 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 26.1.6 Step 2: modification of relevant dose descriptors* and *section 26.1.8 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 26.3 *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.

## 26.1. 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.

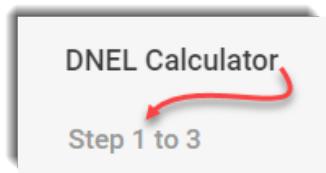
The data for reporting on the hazard assessment conclusions for human health (workers and general population) are in an endpoint summary at the top level of section 7 *Toxicological information* in a *Substance*. To launch the DNEL calculator, navigate to the endpoint summary, and then click on the button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

**Figure 245: Open the DNEL calculator**



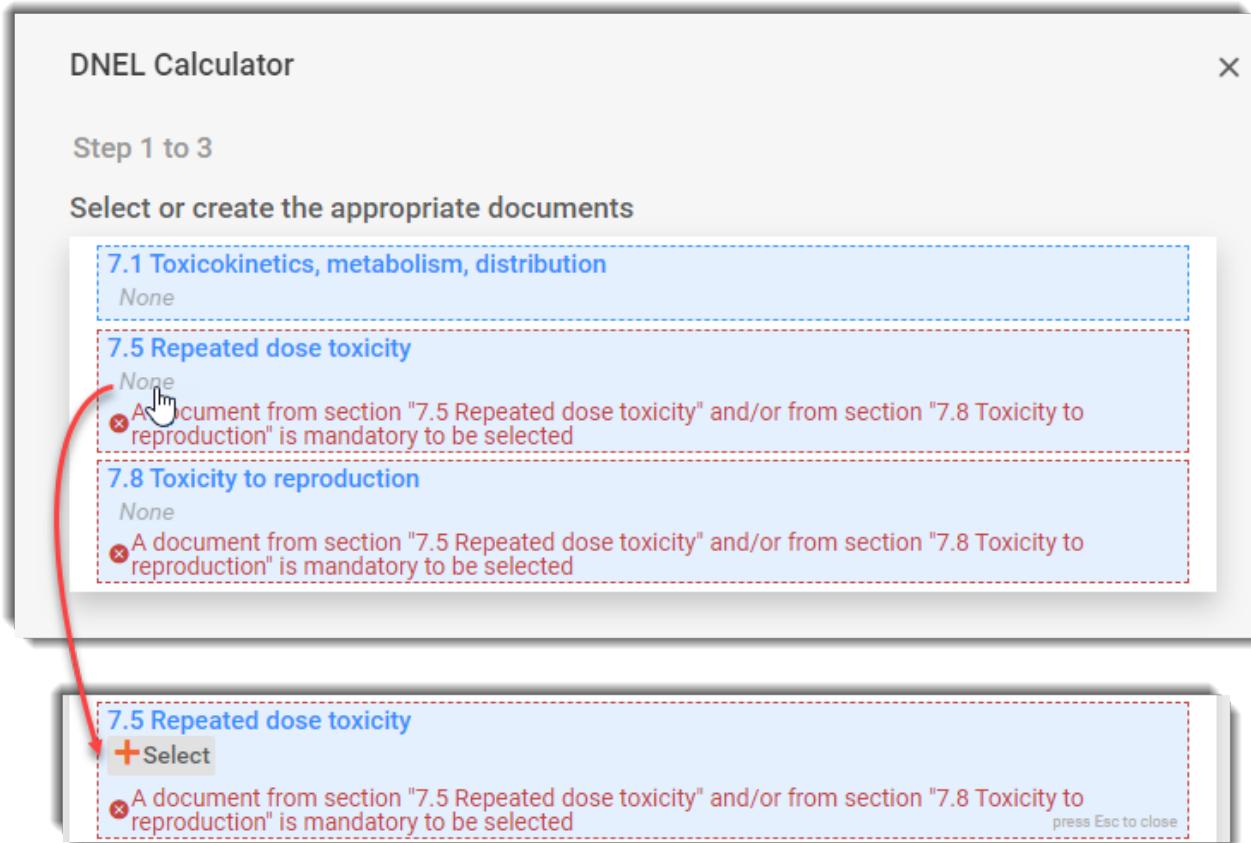
The DNEL calculator has three steps. The current step is indicated as shown below:

**Figure 246: Steps in the DNEL calculator wizard**

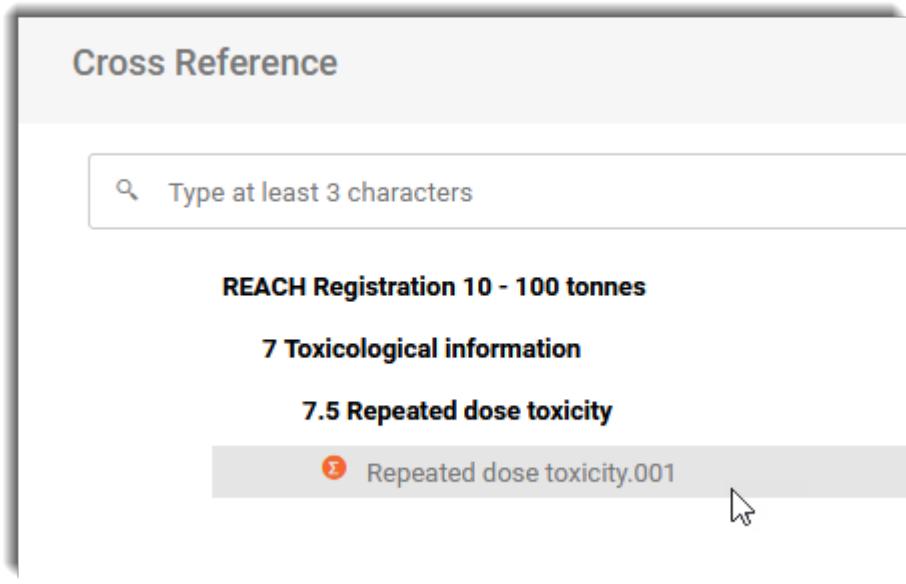


Guidance on entering data into the different steps of the calculator is provided in later sections.

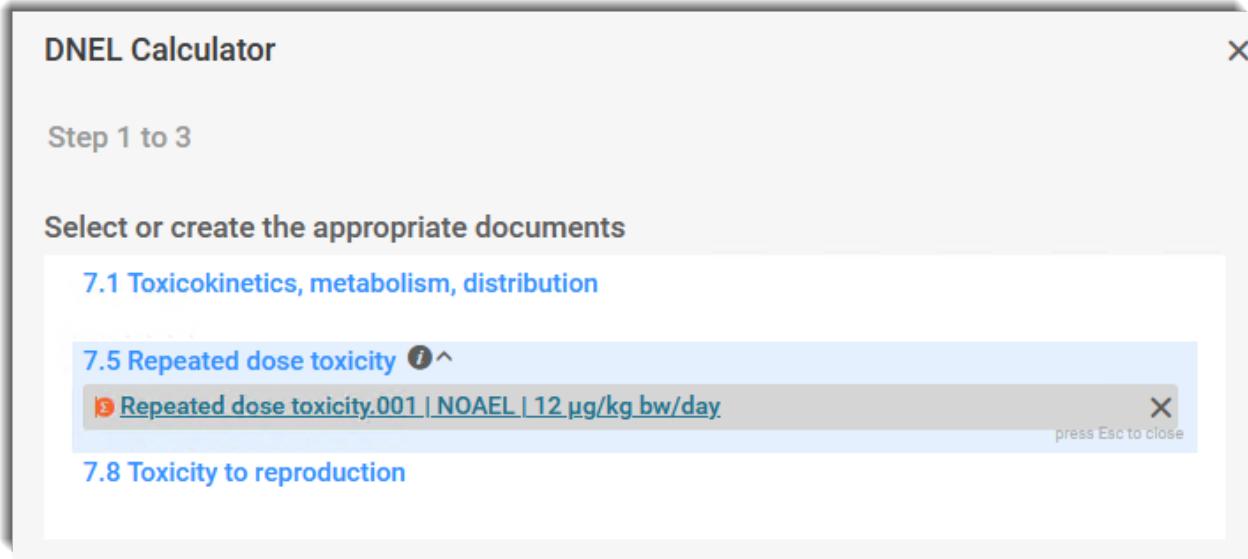
In the first step, the endpoint study summaries needed for the DNEL calculation are selected. Where nothing has been selected, there is a greyed-out comment *None*. To select a summary, click on the endpoint. Where a summary is mandatory and nothing is selected, a warning message is shown. An example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

**Figure 247: 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 248: 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.

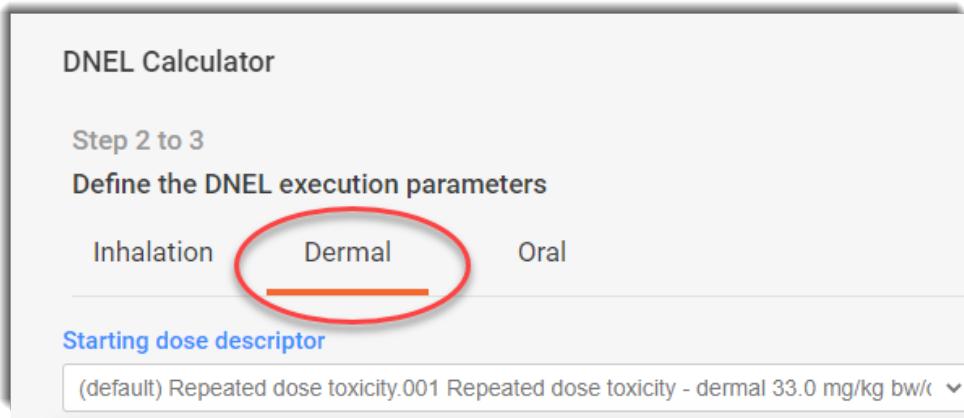
**Figure 249: An endpoint study summary selected in step 1 of the DNEL calculator**

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

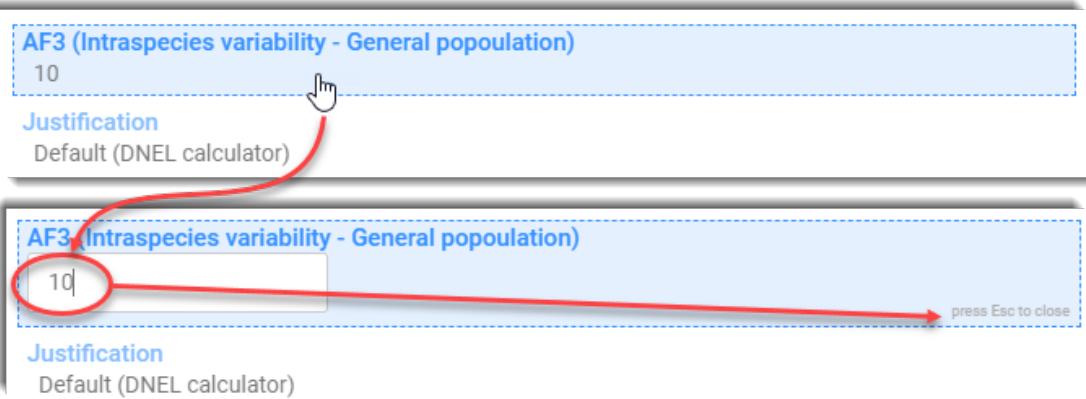
The *Next* button is available only if enough information has been provided to proceed with the calculation of DNELs.

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

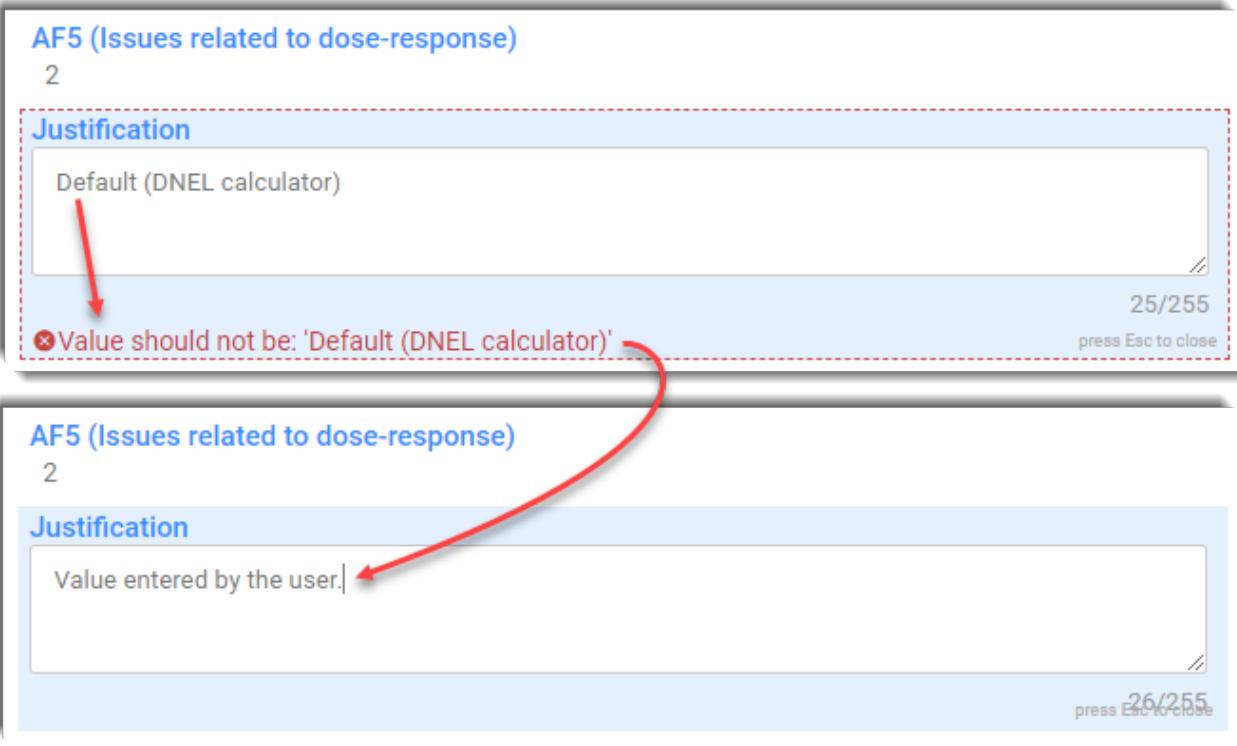
In steps 2 and 3, the data for different routes of exposure are grouped under tabs which are accessed by clicking on the tab. A selected tab is indicated by an orange bar under its title, as shown below in the example for *Dermal*. On moving between tabs, changes to data are remembered.

**Figure 250: 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 251: 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 26.3 *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 252: 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.

### 26.1.1. 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.

### 26.1.2. 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.

### 26.1.3. 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.

### 26.1.4. 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.

#### **26.1.5. 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 NOAEL(C), then the LOAEL(C) will be used for the derivation of the DNEL.

If more than one dose descriptor remains after applying the above selection criteria, the DNEL calculator derives all the corresponding DNELs following step 2 and 3 explained in sections 26.1.6 and 26.1.8, and selects the lowest DNEL.

#### **26.1.6. 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.

#### **26.1.7. 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

#### 26.1.7.1. 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:

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

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:

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

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

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

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

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

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

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

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

### 26.1.7.2. 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 m<sup>3</sup>/kg bw/8h) and humans performing a light activity (worker respiratory volume for light activity: 10 m<sup>3</sup>/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.

### 26.1.7.3. 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).**

<b>Route for dose descriptor</b>	<b>DNEL inhalation</b>		<b>DNEL dermal</b>		<b>DNEL oral</b>	
	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.

### 26.1.8. 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](#).

#### 26.1.8.1. 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

#### 26.1.8.2. 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.

#### 26.1.8.3. 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..

#### 26.1.8.4. 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.

#### 26.1.8.5. 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.

#### 26.1.8.6. 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](#).

### 26.1.9. 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 26.1.6 Step 2: *modification of relevant dose descriptors* and the assessment factors explained in section 26.1.8 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 26.1.5 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.

#### 26.1.9.1. 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)

#### 26.1.9.2. 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)

#### 26.1.9.3. 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)

#### 26.1.9.4. 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)

#### 26.1.9.5. 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)

## 26.2. Output information

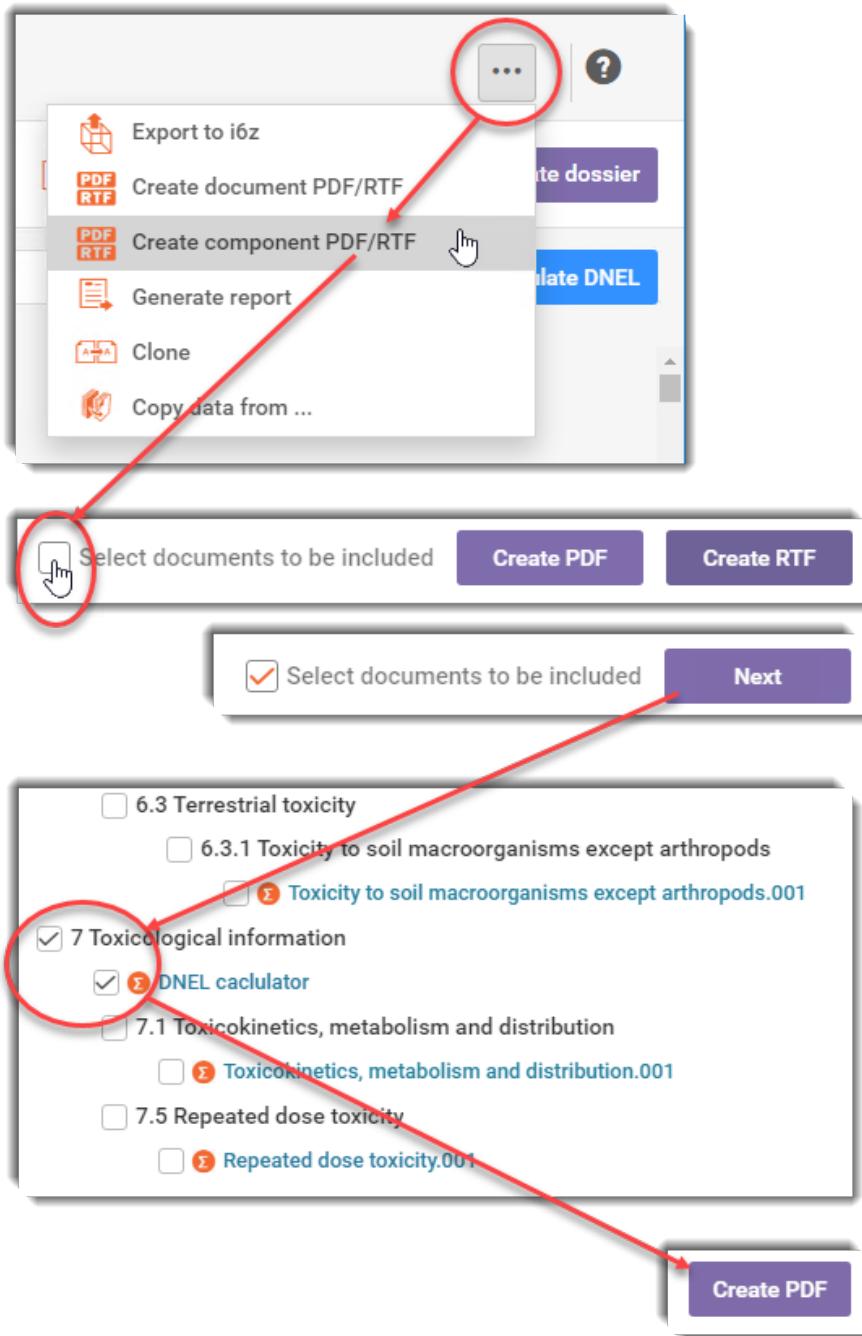
The output of the DNEL calculator is shown in step 3 of the DNEL calculator wizard.

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 253: Print the endpoint summary that contains the output of the DNEL calculator**

### 26.3. 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 26.1 *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 *26.1.5 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 *26.1.7.3 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.

## 26.4. 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.

## 27. 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:

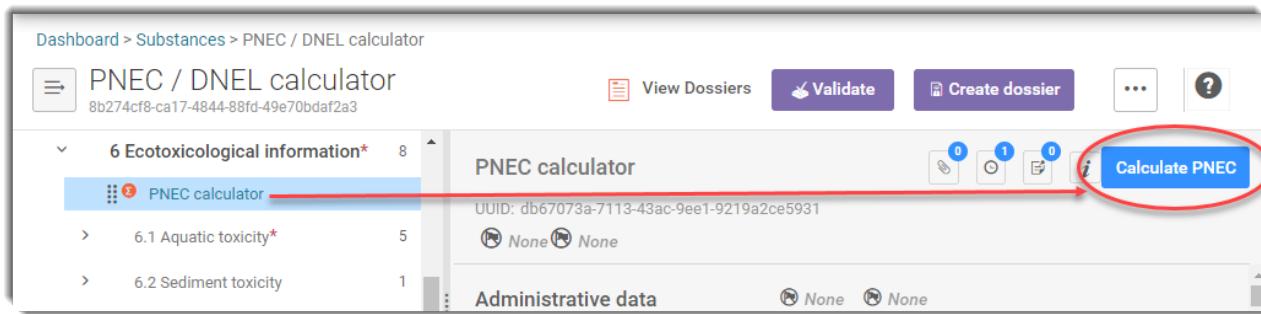
1. The assessor selects the relevant endpoint summaries in IUCLID section 6 - Ecotoxicological information in a substance dataset (or in a template) and launch the PNEC calculator in the menu that appears by right-clicking on it. The endpoint summaries of section 6 enable the reporting of the hazard assessment conclusions for the environmental protection targets.
2. The PNEC calculator performs the following for deriving PNECs
  - a. 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.
  - b. For aquatic and sediment protection target, data for freshwater are used as surrogate data in case the same type of data is not available for the marine and vice versa.
  - c. For sediment and soil protection target, the equilibrium partitioning method (EPM) may be used as an extrapolation method to calculate the PNEC and thus data for Koc is retrieved from the endpoint summary in IUCLID section 5.4.1.
  - d. Selects the relevant effect concentrations and the corresponding assessment factor (AF) to calculate the PNEC, or when relevant, using the EPM for the PNECs for sediments and /or soil, according to the rules in [ECHA Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.10](#).
3. The PNEC calculator reports all the results in a screen available to the assessor.
4. The assessor can *finish* the actions keeping the calculations as proposed by the tool or modify some assumptions by *editing* the calculations, as described in section *27.4 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.

## 27.1. Input data

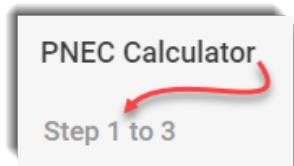
The input data for the PNEC calculator is the information available in the endpoint summaries in IUCLID sections 5.4.1 (Adsorption / desorption), 6.1.1 to 6.1.6 (Aquatic toxicity), 6.2 (Sediment toxicity) and 6.3.1 to 6.3.4 (Terrestrial toxicity).

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.

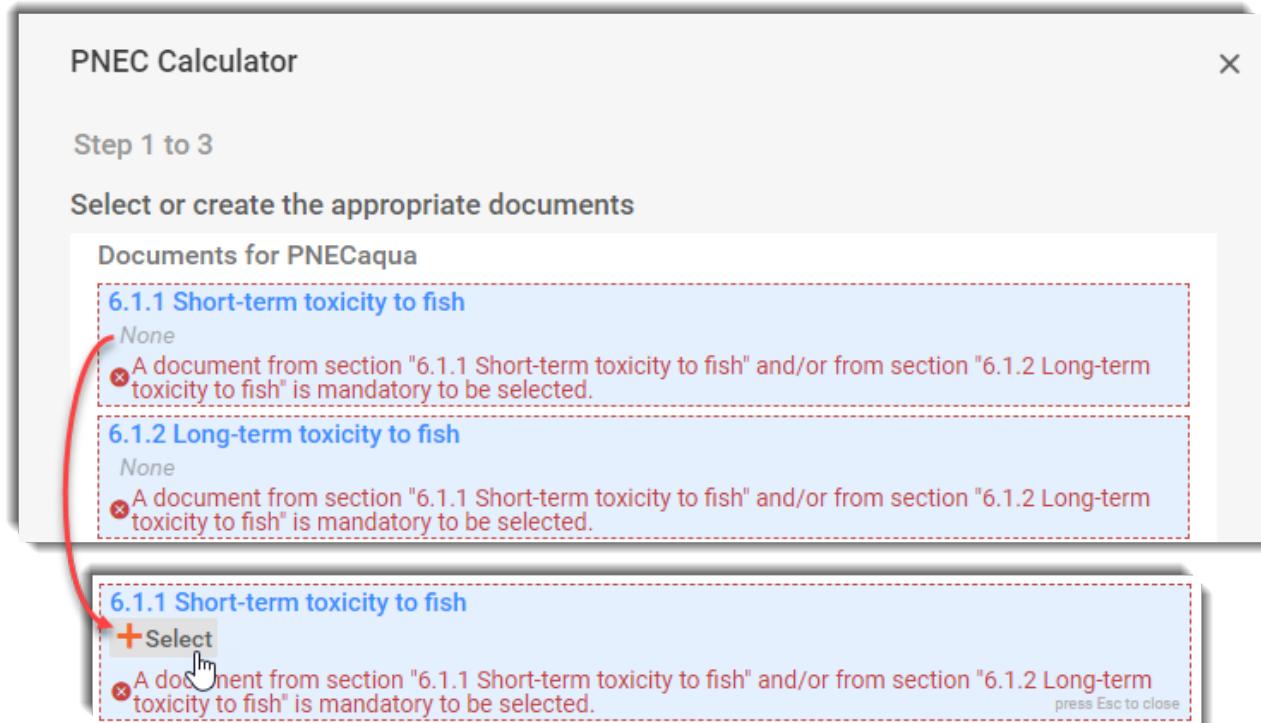
**Figure 254: Open the PNEC calculator**

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

**Figure 255: Steps in the PNEC calculator wizard**

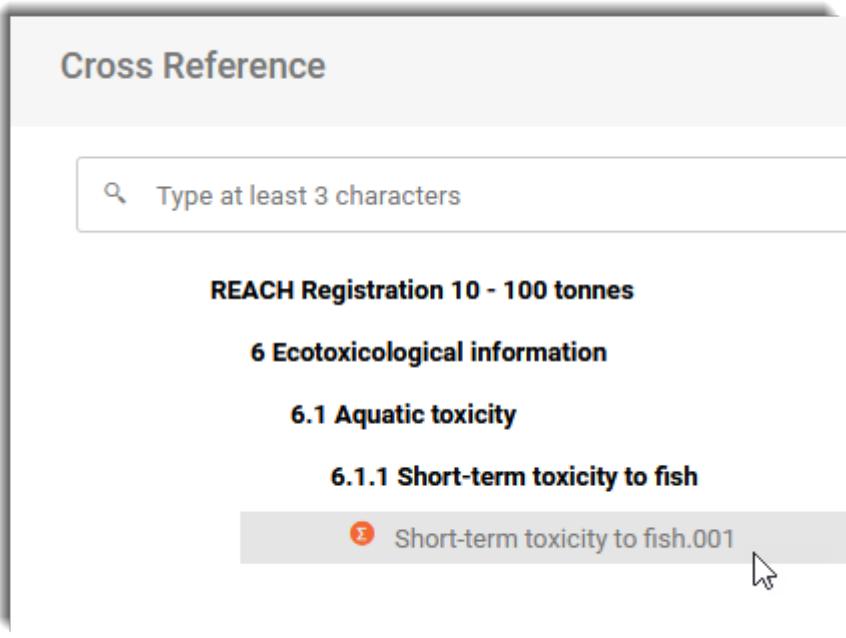
Guidance on entering data into the different steps of the calculator is provided in later sections.

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 256: Selecting summaries in step 1 of the PNEC calculator**

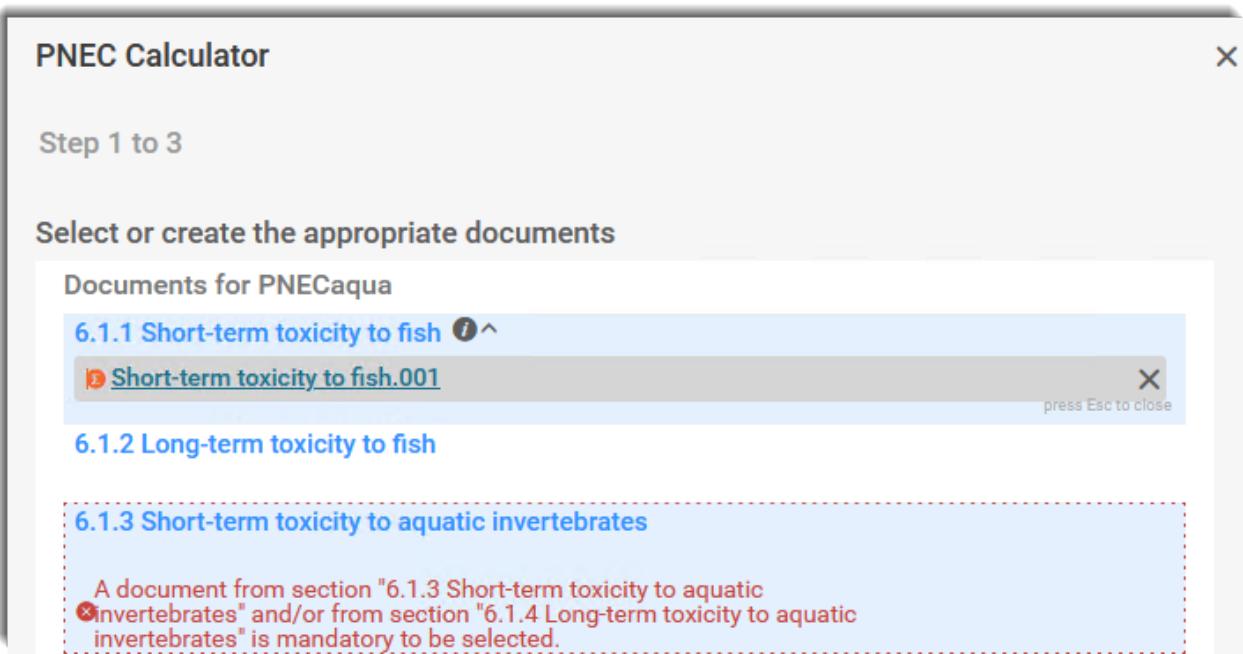
After clicking on the button labelled **+Select**, a window is shown in which you can select the relevant endpoint summary.

**Figure 257: 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 258: An endpoint study summary selected in step 1 of the PNEC calculator**



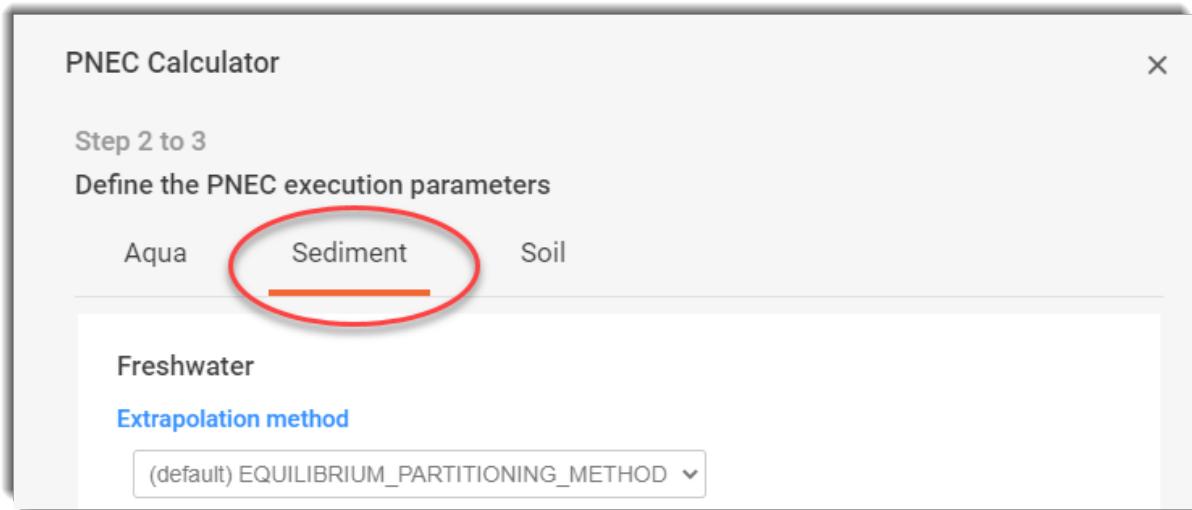
A selected endpoint summary can be deselected by clicking on the cross icon to its right.

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 259: 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 260: 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 27.4 *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 261: Entering a justification in to the PNEC calculator.**

Marine

Starting dose descriptor

(default) 6.1.1 Short-term toxicity to fish\_a - LC50 for marine water fish - 20.0 mg/L

Assessment Factor

12000

Justification

Value changed from the default of 10000 to 12000. Justification entered by user.

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

### 27.1.1. Endpoint summary 5.4.1 (adsorption/desorption- Koc)

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

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

### 27.1.2. 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.

### 27.1.3. 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.

#### 27.1.4. 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.

## 27.2. How the calculations are made

### 27.2.1. 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 27.4 *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:

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

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](#).

### 27.2.2. 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.

### 27.2.3. 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 *27.4 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 *27.4 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:

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

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

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

#### 27.2.4. 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 PNEC<sub>aqua,freshwater</sub> 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 *27.4 Modifying defaults from the PNEC calculator*.

If there is no experimental data, the PNEC<sub>soil</sub> is calculated with EPM:

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

If there is only one effect concentration available the PNEC<sub>soil</sub> 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, PNEC<sub>soil</sub> 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", PNEC<sub>soil</sub> 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", PNEC<sub>soil</sub> 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](#).

## 27.3. Output information

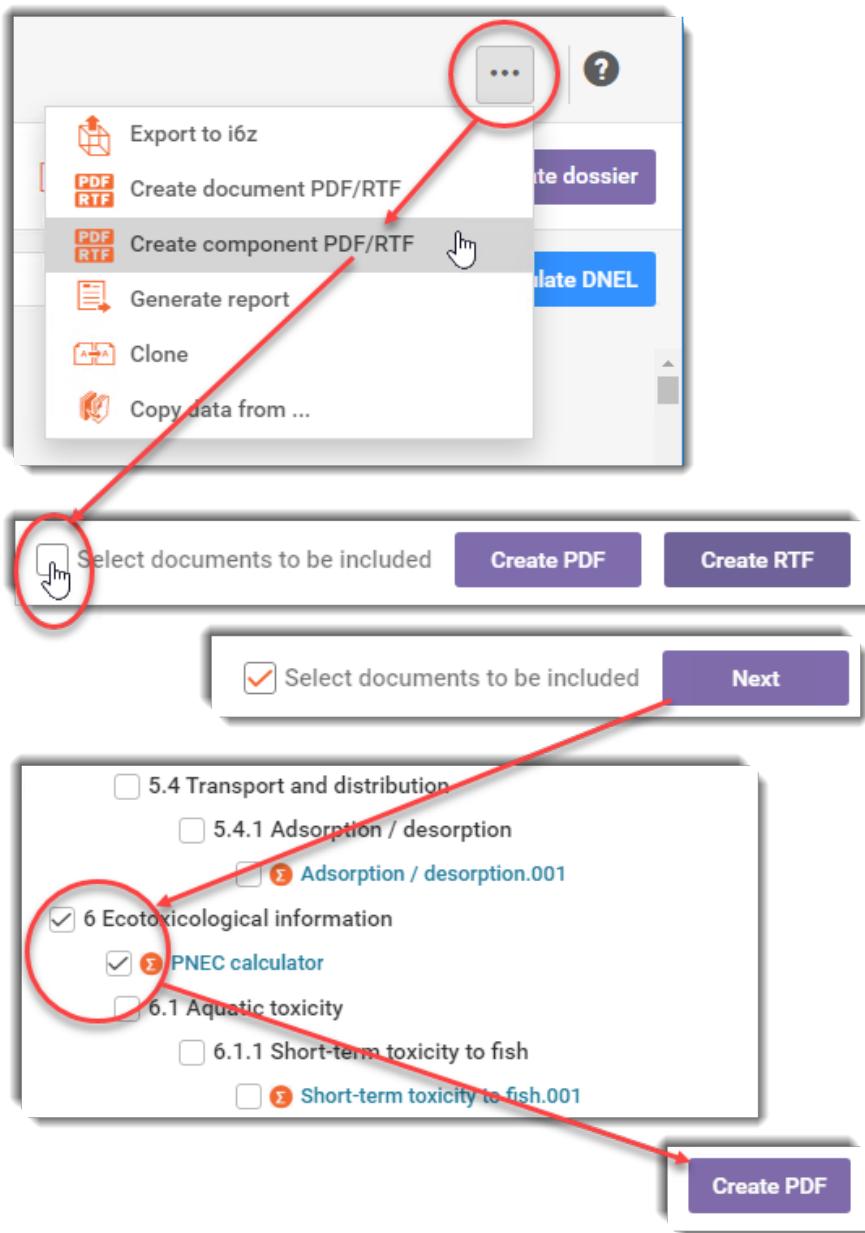
The output of the PNEC calculator is shown in step 3.

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 262: Print the endpoint summary that contains the output of the PNEC calculator**

## 27.4. 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 *27.4 Modifying defaults from the PNEC calculator*:

- 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.

## 27.5. Disclaimer

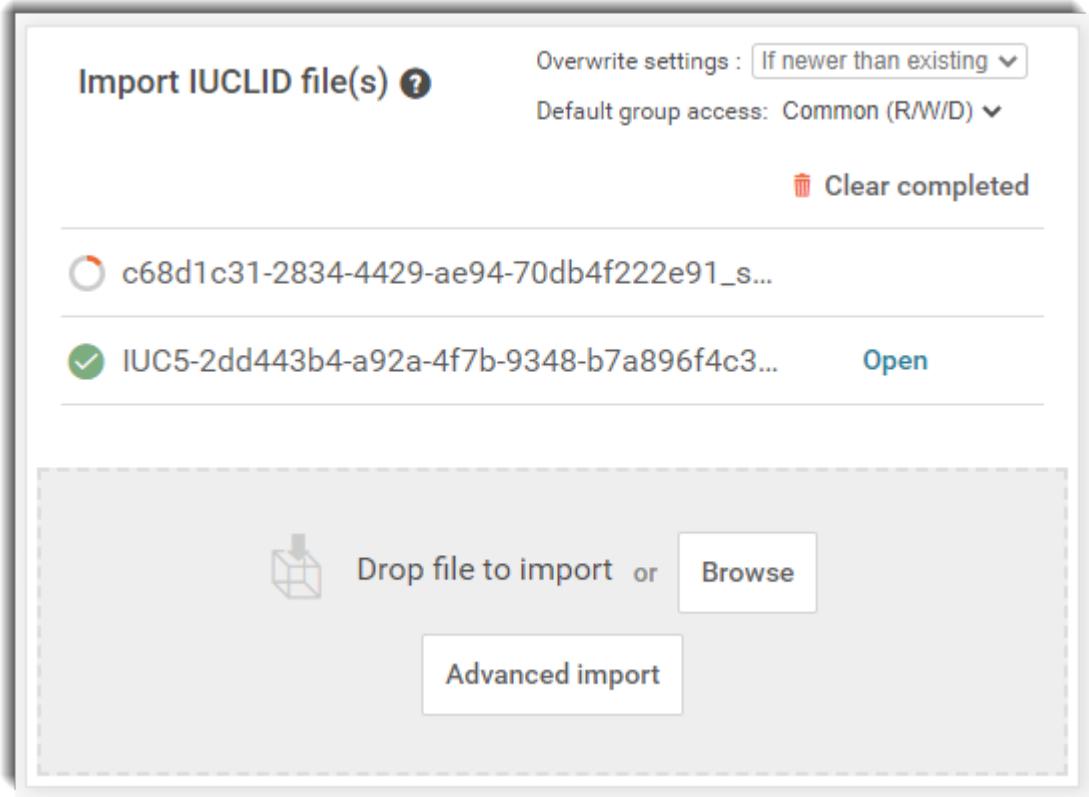
ECHA recommends the use of the optional PNEC calculator in IUCLID. Note that the registrants should link to the calculator all relevant endpoint summary(-ies) and that they remain responsible for the calculated PNECs.

## 28. 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.

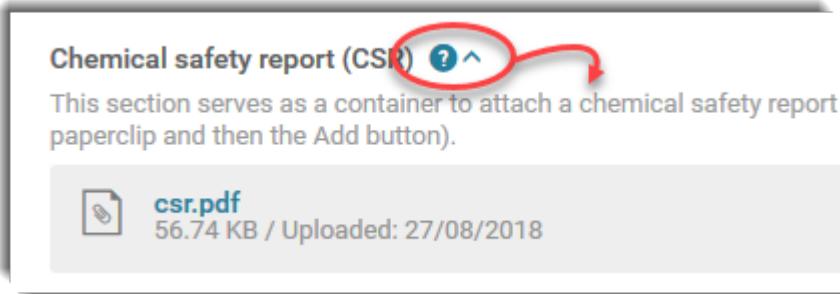
**Figure 263: Data is being imported**



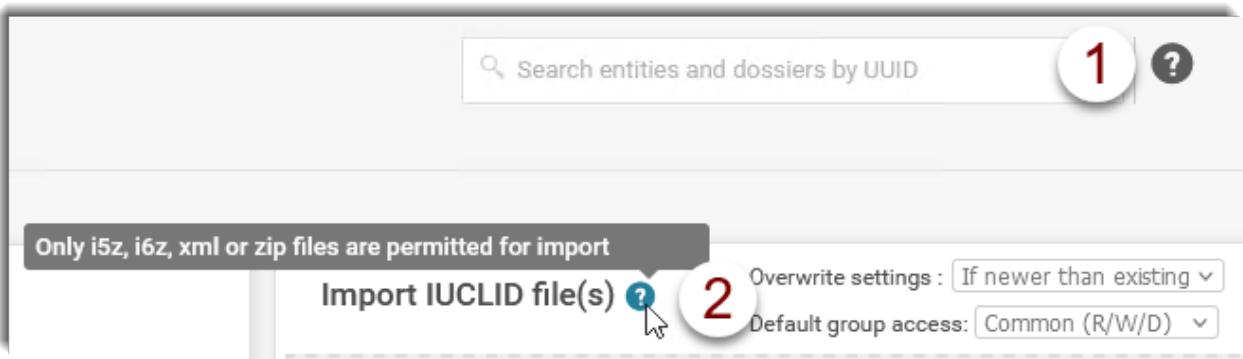
To shut down the IUCLID 6 Desktop application, close the window that opened when the application started.

## 29. 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:

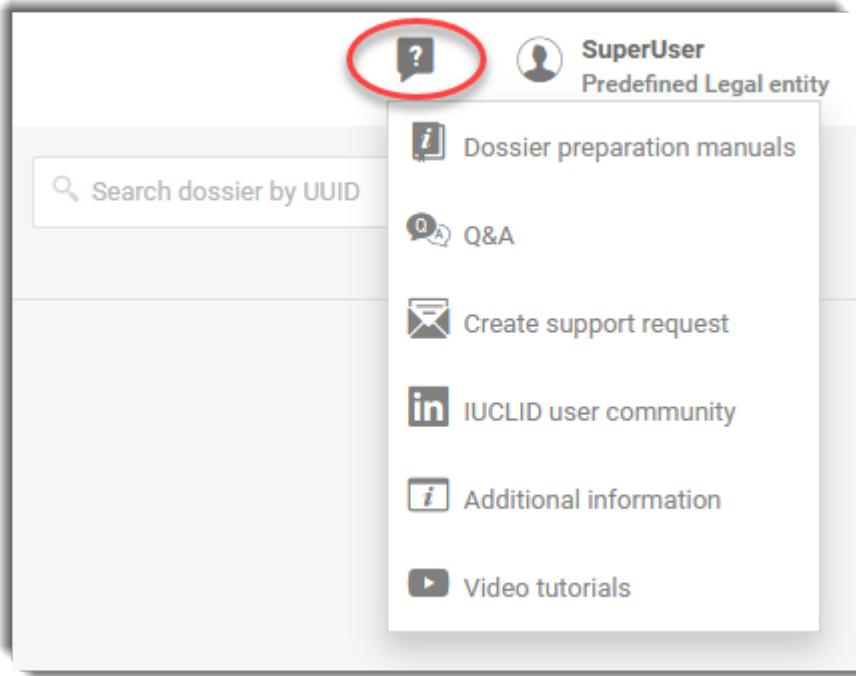
**Figure 264: Field specific help**

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 265: Function specific help**

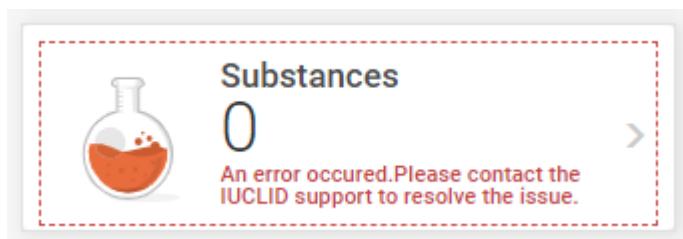
The dialogue icon with the question mark in the top bar of the interface contains links to external sources of help. An example of the links is shown below.

[Create support request](#) is a link to the European Chemicals Agency.

**Figure 266: External sources of help**

## 29.1. Error message on the dashboard

If the web 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 267: 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.

## 30. 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