

Biocides IT training
Helsinki – 25th of October 2018

IUCLID 6.3

Creation and update of a IUCLID dossier using a Web User Interface (IUCLID WebUI)

Background information

According to Article 6 (a) of the BPR, an application for approval of an active substance shall contain the information for the active substance, satisfying the requirements of Annex II. This is done by including the active substance dataset in the IUCLID dossier submitted for the application.

Article 6 (b) states that the information requirements of Annex III shall be provided for at least one representative biocidal product that contains the active substance.

IUCLID dossier type relevant for an active substance application is *BPR Active substance application (representative product)*.

In the context of Article 20 of the BPR Regulation, the application for authorisation for biocidal products other than biocidal products eligible for the simplified authorisation procedure, shall contain:

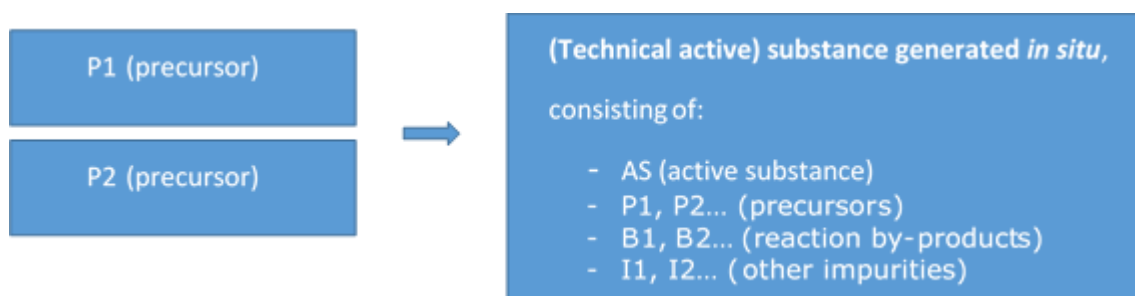
- A dossier or letter of access for the biocidal product satisfying Annex II requirements for every single active substance
- A dossier or letter of access for the biocidal product satisfying Annex III requirements; and
- A summary of biocidal product characteristics (SPC).

IUCLID dossier type relevant for a biocidal product authorisation is *BPR Biocidal product authorisation*.

IN SITU GENERATED ACTIVE SUBSTANCES

An in-situ generated active substance is understood to be an active substance that is generated at the place of use from one or more precursors.

All substances and/or mixtures used as precursors, as well as all components of a (technical active) substance generated in-situ, listed on a schema¹ below, shall be reported in the IUCLID technical dossier (*BPR Active substance application (representative product)* or *BPR Biocidal product authorisation*).



¹ according to the WG recommendation - Risk assessment and implications on data requirements for active substances generated in situ and their precursors, see https://www.echa.europa.eu/documents/10162/13564/situ_as_precursors_wg_recommendation_+2017_en.pdf/0c6aee50-5c29-bccc-3836-bb033a015144

Scenario

You are an applicant who needs to fill in a IUCLID 6 application satisfying the requirements as specified in Article 6 and 20. The active substance to be included in the biocidal product is considered as approved for the relevant product type. **This is an active substance generated in situ.**

As an applicant, you will need to:

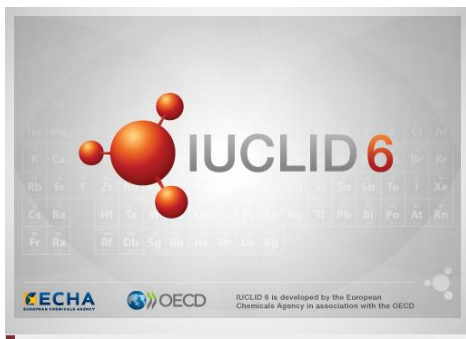
- **PART 1:** Launch IUCLID 6 and select the web user interface to be used
- **PART 2:** Create a biocidal product dataset
- **PART 3:** Create a BPR Active substance application (representative product) dossier and a BPR Biocidal product authorisation dossier, and export them
- **PART 4:** Correct an error in a product dataset in order to successfully create a BPR dossier (validation)

Please, complete the step-by-step instructions provided in the next pages.

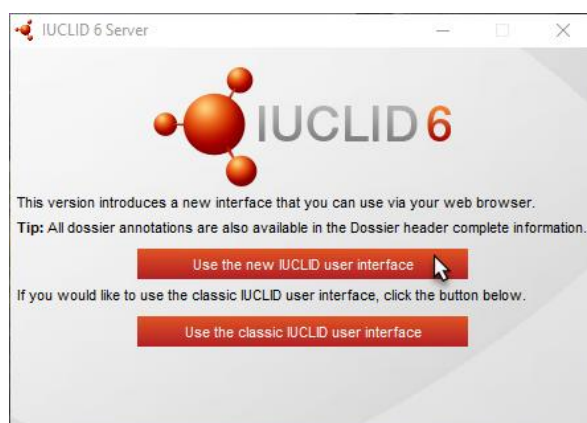
The scientific information provided in the following exercise is not necessarily accurate but will help you to carry out some necessary steps to complete your applications. Due to the time constraints we cannot go through all mandatory sections during the exercise.

PART 1: Launch IUCLID 6 and select the web user interface to be used

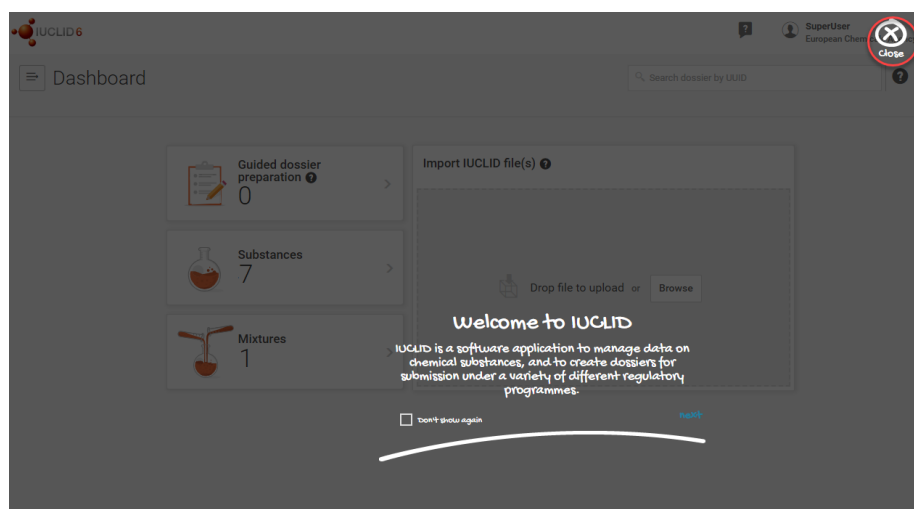
1. Click on the IUCLID icon available on your Desktop. IUCLID will start to open.



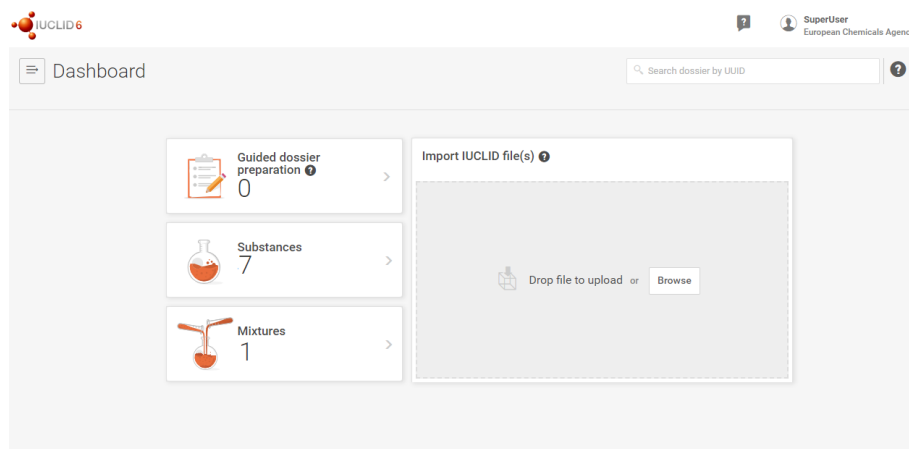
This window will disappear after 1-3 minutes, and after a while (no action visible on the screen) you will be asked to select between the new user interface and the classic interface. Select the new IUCLID user interface.



2. IUCLID will open in the browser. Firstly, the Dashboard User Journey will be displayed, you can close it by clicking on 'X'.




3. You can see now Substances widget with 7 substances, and Mixtures widget with 1 mixture. Those are the datasets that we will use during the exercise.

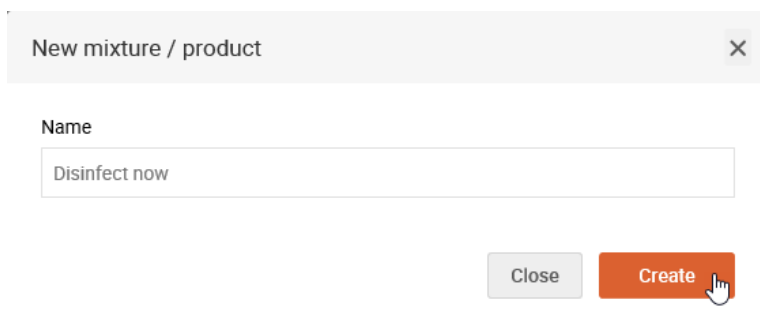


PART 2: Create a biocidal product dataset

The applicant needs to create a dataset for each precursor, active substance generated *in situ*, reaction by-product and other impurities in order to provide all required data. All these datasets shall be linked as components of a biocidal product, defined in the composition document of the biocidal product dataset. In this part of the exercise you will create a biocidal product dataset using five predefined substance datasets, mentioned in [part 1](#).

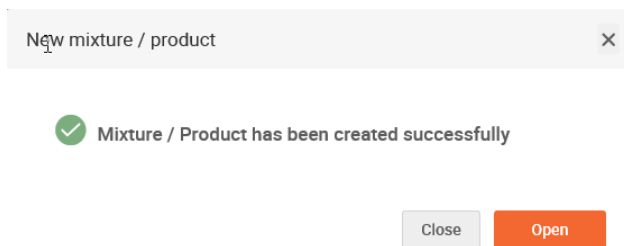
The biocidal product dataset needs to contain the initial composition which describes how much of each precursors will be used, and a composition of the (technical active) substance generated *in-situ* (see the schema in '[Background information](#)'). Therefore at least² two composition documents shall be created, and **the first composition should always contain an active substance dataset**.

1. Click on Mixtures widget and then on .
2. Insert a product name 'Disinfect now' and create a mixture / product dataset by clicking 'Create'.



² If any of the compositions varies depending on conditions, intended uses, or other factors, then more composition records should be provided; during the training we will create only two composition documents.

3. Mixture / Product has been created successfully, so you can open it by clicking 'Open'

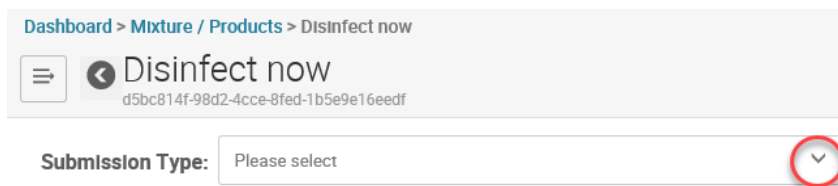


4. A new mixture / product opens by default with the *Complete table of contents*. Therefore, you need to define submission type(s) relevant to a biocidal product (instruction will follow). It is needed to ensure that the displayed table of contents will follow the requirements of the Biocidal Products Regulation, and that the created dossier(s) will have correct types. In this exercise we will create two dossiers:

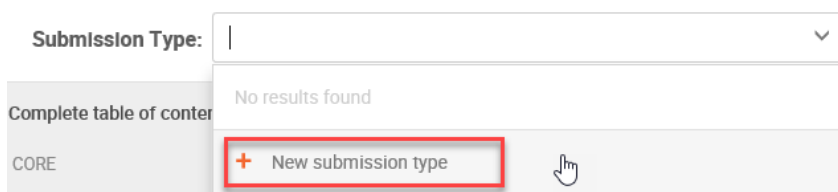
- BPR Active substance application (representative product) dossier, and
- BPR Biocidal product authorisation dossier.

Therefore, select both submission types in the field 'Submission type' as indicated in the following steps:

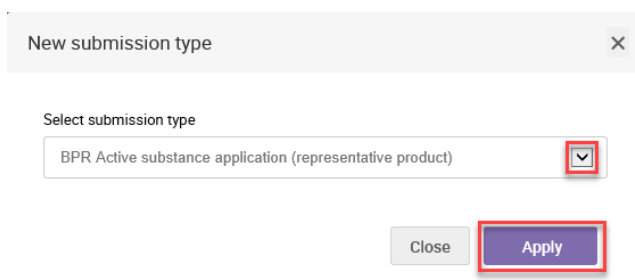
a) Click the arrow on the right



b) Click on '+New submission type'

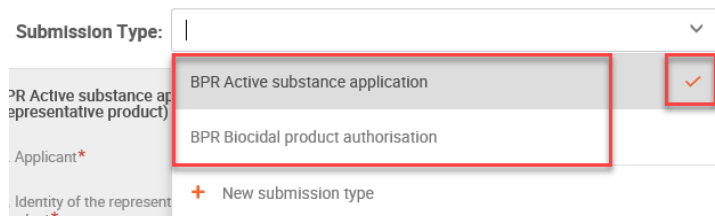


c) Select from the list 'BPR Active substance application (representative product)', and click 'Apply', and then 'Close'



d) Repeat this procedure for the 'BPR Biocidal product authorisation'.

5. You should see two submission types. By clicking on one of them you decide which table of contents will be displayed. Both these submission types follow as strictly as possible the requirements indicated in the Annex III of the Biocidal Products Regulation, both have the same sections set as mandatory and optional. However, some section names are different, and validation rules assigned to each submission type are different. Select 'BPR Active substance application'.



6. Indicate the composition of the biocidal product 'Disinfect now' (instruction will follow the data overview).

Data overview:

Composition of the technical active substance generated *in situ* (the right side of the schema in [Background information](#)):

- chlorine dioxide (active substance, ca. 60% w/w)
- reaction by product ABC (impurity, ca. 40% w/w)

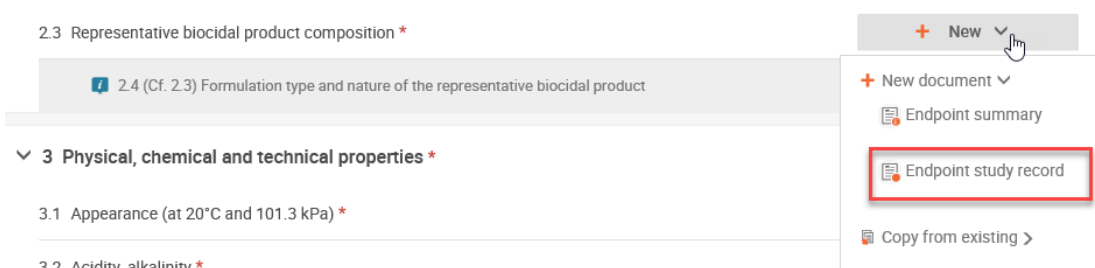
Formulation type: GA


Initial composition before precursors start to react (the left side of the schema in [Background information](#)):

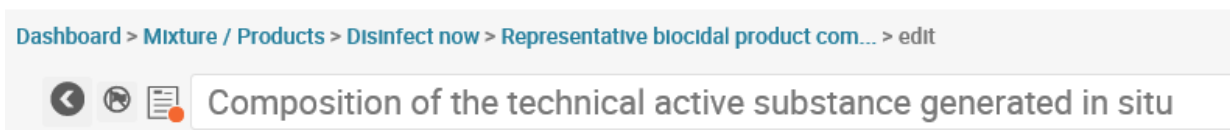
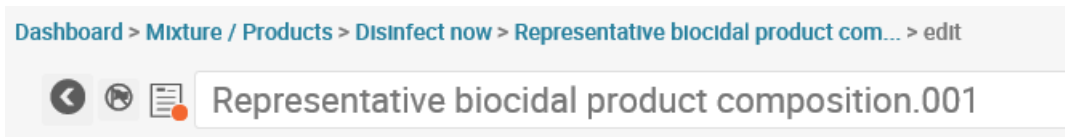
- sodium chlorite (precursor, ca. 45% w/w)
- sodium bisulfate (precursor, ca. 45% w/w)
- hydrochloric acid (precursor, ca. 10% w/w)

Instruction of creating the first composition record (Composition of the technical active substance generated *in situ*):

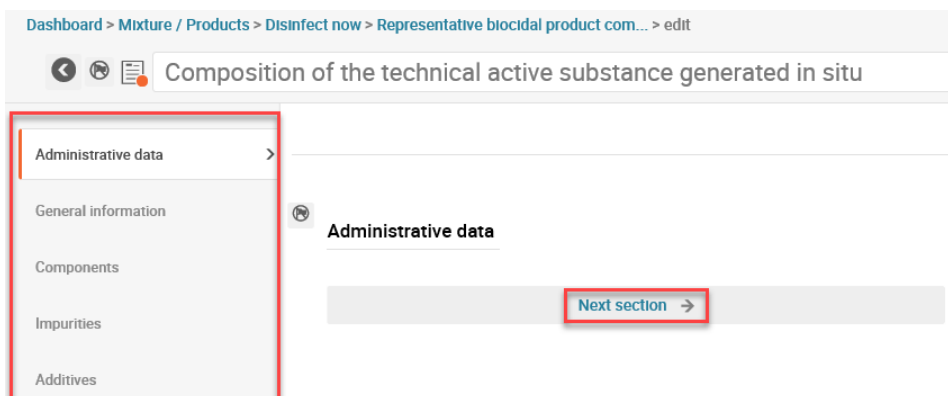
- a) Go to section 2.3 Representative biocidal product composition, click '+New', and add a new document by selecting 'Endpoint study record'




- b) Change document's name to 'Composition of the technical active substance generated in situ' and click  in the right bottom corner.



Note: You can navigate through different subsections using the menu on the left side or clicking a sign 'Next section'.

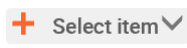


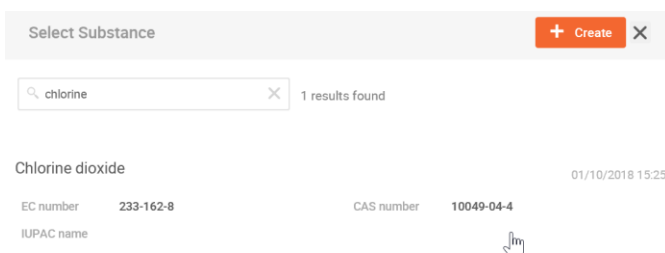
- c) Under 'General information' insert 'Mixture/product name' which is 'Disinfect now', and 'Formulation type' which is 'GA Gas (you might need to scroll down). You can also add an invented trade name, and a brief description. Click .

- d) Under 'Components' add an active substance, following the instruction below:

- chlorine dioxide (active substance, 60% w/w)

Click . The sliding window will appear.

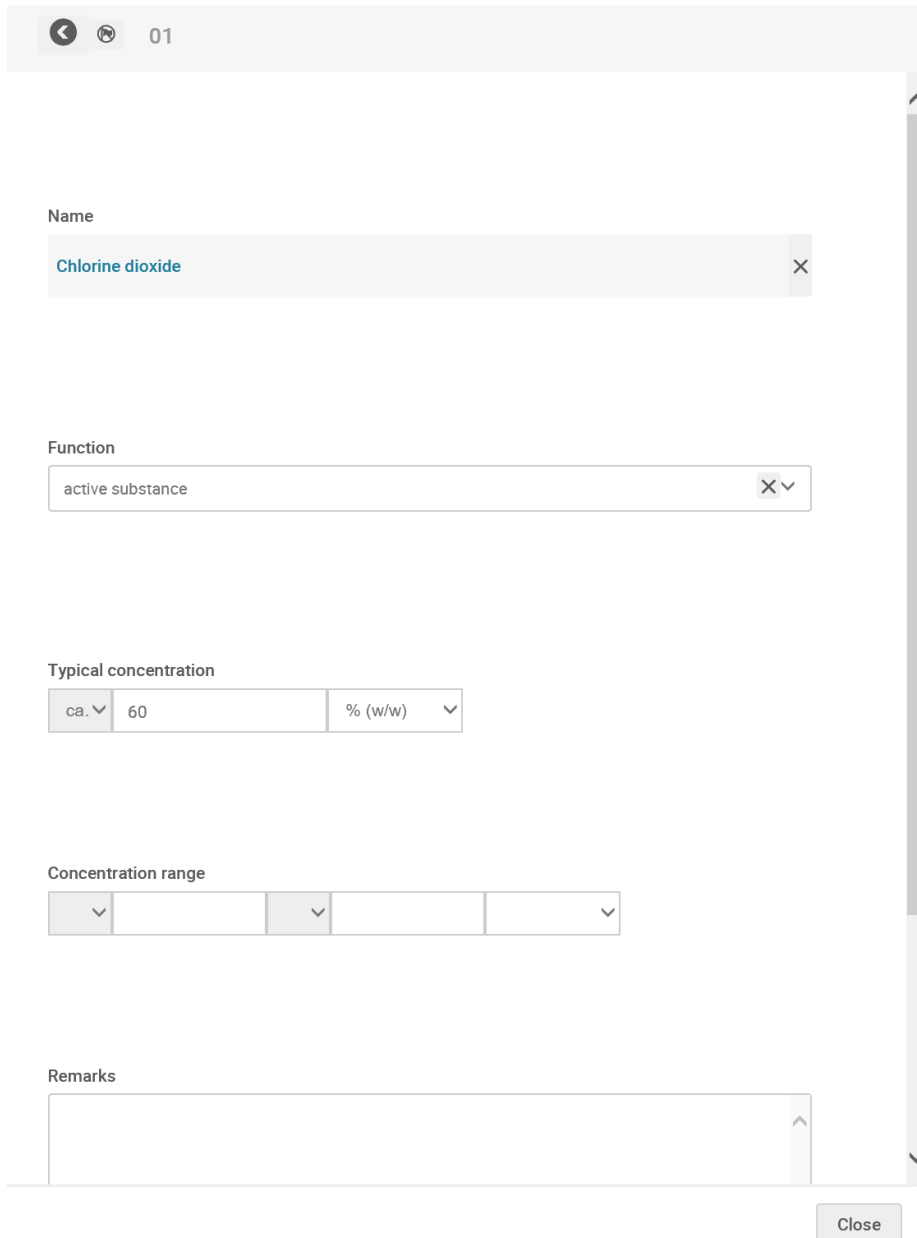
Click , and select 'Substance' from the drop down list. Select Chlorine dioxide and click on it.



Select the function 'active substance' from the drop down list.

Indicate the 'Typical concentration' of 60% w/w.

Note: You always leave the 'Concentration range' empty in a composition record of a biocidal product. If there is a need to indicate that a substance may remain at different concentrations in a (technical active) substance generated *in situ*, then the maximum expected value must be reported (as an exact value) and in the remarks field the range of possible concentration values needs to be specified.



01

Name
Chlorine dioxide

Function
active substance

Typical concentration
ca. 60 % (w/w)

Concentration range


Remarks


Close

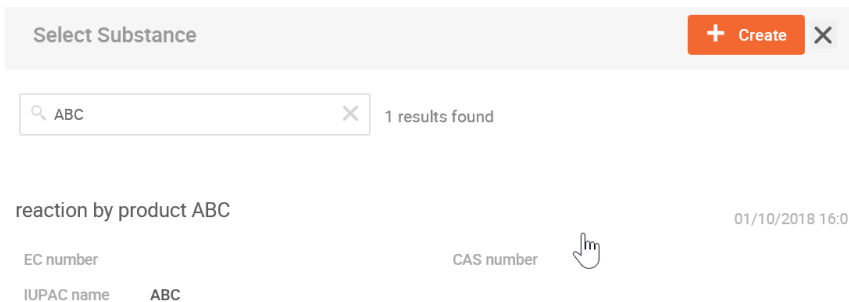
Click **Close** and **Save**.

e) Under 'Impurities' add a reaction by product, following the instruction below:

- reaction by product ABC (impurity, 40% w/w)

Click . The sliding window will appear.

Click , and select 'Substance' from the drop down list. Select 'reaction by product ABC' and click on it:



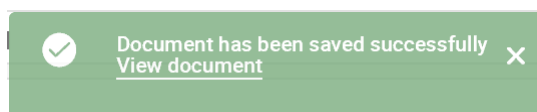
Indicate the 'Typical concentration' of 40% w/w.

Indicate that this substance is a substance of concern:

Substance of concern

Click  and .

Click on green message to view the composition document.



Note: the green message disappear after few seconds, if you did not manage to click on it, press 'Save' button again.

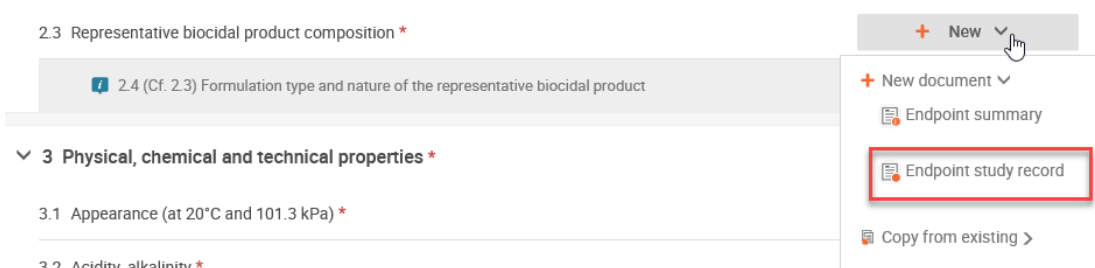
Instruction of creating the second composition record (Initial composition before precursors start to react):

a) Come back to the product 'Disinfect now'




[Dashboard](#) > [Mixture / Products](#) > [Disinfect now](#) > Composition of the technical active...

- b) Go to section 2.3 Representative biocidal product composition, click '+New', and add a new document by selecting 'Endpoint study record'

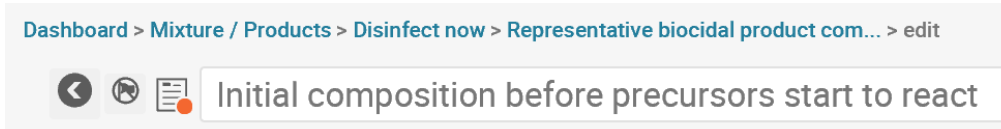


The screenshot shows a web interface for '2.3 Representative biocidal product composition'. A dropdown menu is open under a '+ New' button, listing options: '+ New document', 'Endpoint summary', 'Endpoint study record' (highlighted with a red box), and 'Copy from existing >'. The main content area shows sections for '2.4 (Cf. 2.3) Formulation type and nature of the representative biocidal product' and '3 Physical, chemical and technical properties'.


- c) Change document's name to 'Initial composition before precursors start to react' and click  in the right bottom corner.



The screenshot shows a breadcrumb trail: 'Dashboard > Mixture / Products > Disinfect now > Representative biocidal product com... > edit'. Below it, a title bar contains navigation icons and the text 'Representative biocidal product composition.001'.



The screenshot shows the same breadcrumb trail as above. The title bar now displays 'Initial composition before precursors start to react'.

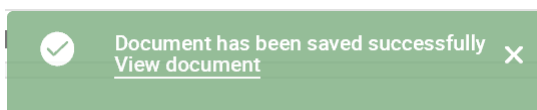
- d) Under 'General information' insert 'Mixture/product name' which is 'Disinfect now'. Click .

- e) Under 'Components' add three substances:

- sodium chlorite (precursor, 45% w/w)
- sodium bisulfate (precursor, 45% w/w)
- hydrochloric acid (precursor, 10% w/w)

For each of them, select the function: 'other: precursor', indicate the 'Typical concentration', and indicate that they are substances of concern.

After adding all three substances save your data, and click on green message to view the composition document.



The screenshot shows a green notification box with a checkmark icon, the text 'Document has been saved successfully', a link 'View document', and a close 'X' button.

Components



Component flag	
Name	Sodium chlorite sodium chlorite 7758-19-2
Function	other: precursor
Typical concentration	ca. 45 % (w/w)
Concentration range	
Remarks	
Substance of concern	✓

Component flag	
Name	Sodium bisulfate sodium hydrogensulphate 7681-38-1
Function	other: precursor
Typical concentration	ca. 45 % (w/w)
Concentration range	
Remarks	
Substance of concern	✓

Component flag	
Name	Hydrochloric acid hydrogen chloride 7647-01-0
Function	other: precursor
Typical concentration	ca. 10 % (w/w)
Concentration range	
Remarks	
Substance of concern	✓

f) Come back to the product 'Disinfect now' to see the whole composition.

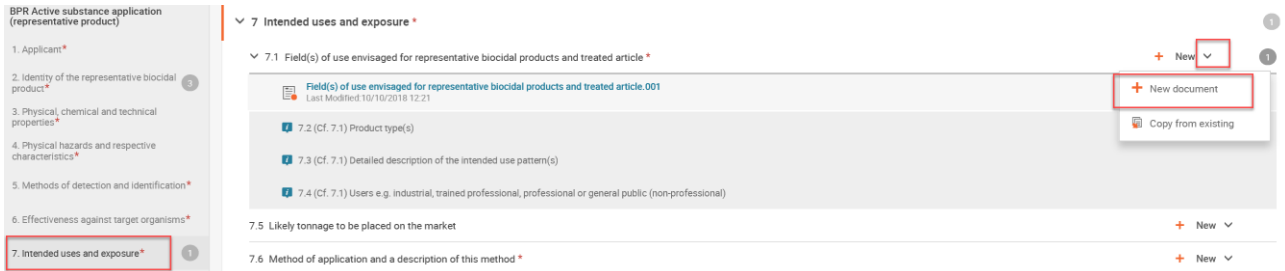
✓ 2.3 Representative biocidal product composition *

 Composition of the technical active substance generated in situ Last Modified:10/10/2018 10:34
 Initial composition before precursors start to react Last Modified:10/10/2018 11:11

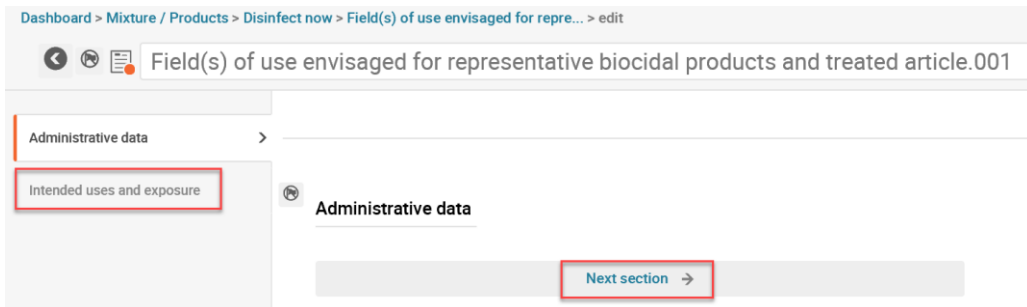
Note: In this exercise we do not insert data on disinfection by-products, due to the time constrains. Disinfection by-products may be generated when the technical active substance generated *in situ* (i.e. any of its components) reacts with microorganisms or other organic matter when exerting its biocidal effect. The disinfection by products should be reported as 'Impurities' in IUCLID.

7. Before a dossier can be created, all mandatory sections of the dataset have to be filled in, accordingly to the requirements set up in Annex III of the Biocidal Products Regulation. It is also very important to indicate all possible links between relevant sections and the composition records. Let us see one example:

- a) Select from the menu section 7 Intended uses and exposure, and create a new document in section 7.1

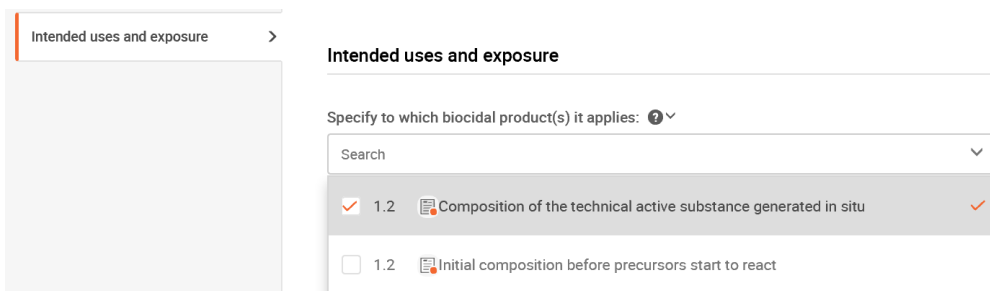


- b) Go to the 'Intended uses and exposure' by selecting this title from the menu or clicking 'Next section'

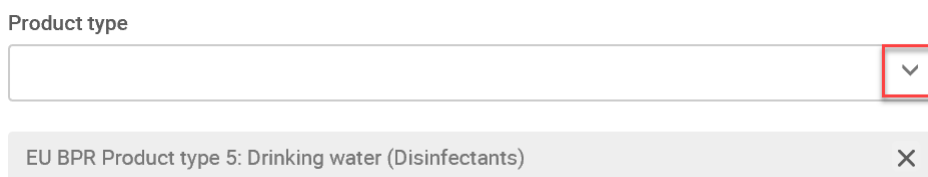


- c) In the first field 'Specify to which biocidal product(s) it applies:' specify to which composition the information inserted in this section, applies.


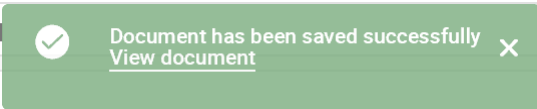
Select the 'Composition of the active substance generated in situ' as this is the composition containing the active substance.



- d) Indicate the 'Product type'

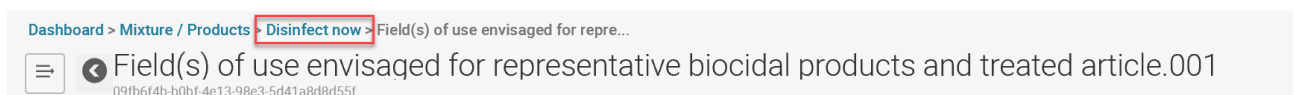


e) You might fill in other fields with the information of your choice.


Click  and  to see the document.

PART 3: Create two dossiers: BPR Active substance application (representative product) dossier and a BPR Biocidal product authorisation dossier, and export them

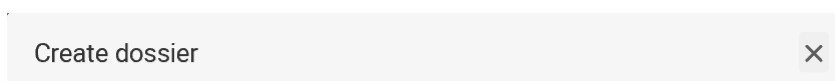
1. Come back to the product 'Disinfect now'




2. Click on the button .

3. Indicate dossier name 'Disinfect now – representative product' and click on .

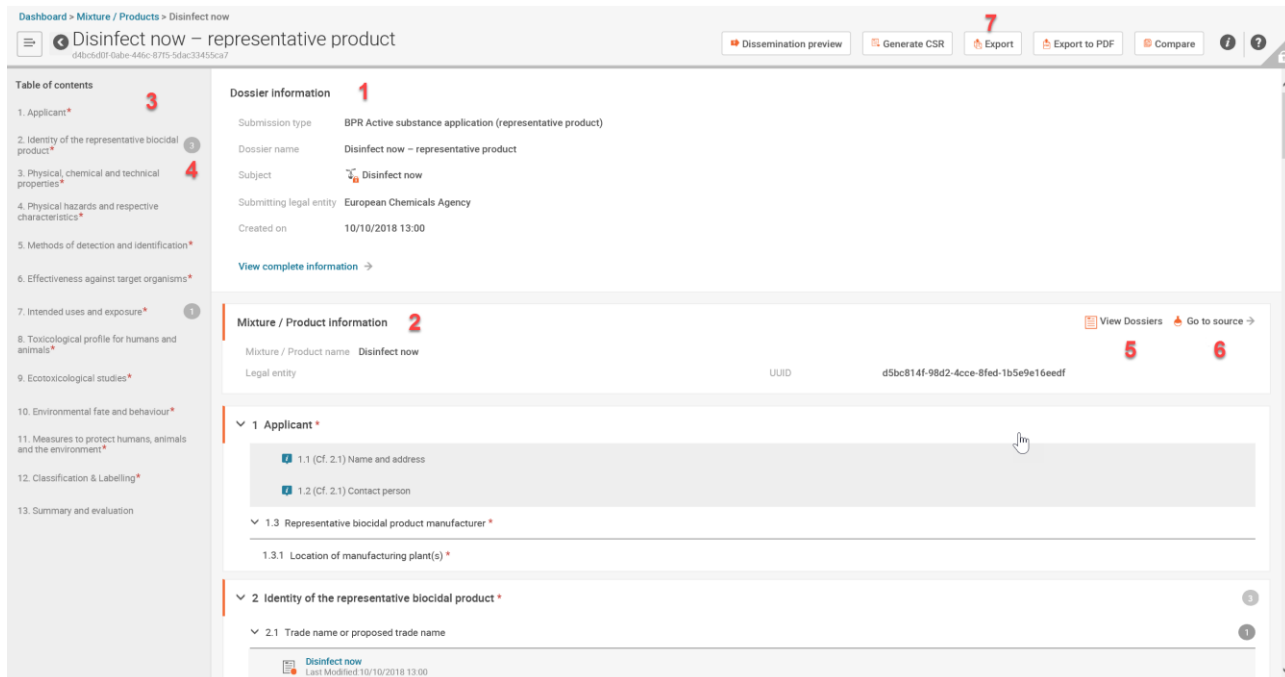
4. The dossier has been created and you can open it by clicking 'Open'.



 Dossier creation was completed successfully.
Do you want to open the created dossier?

You can see the dossier information (1), mixture/product information (2), and you can navigate through all the sections using the table of contents on the left side (3). Numbers on grey background displayed in the table of contents indicate how many documents have been created in each section (4). You can see all dossiers created based on this product (5), and you can access the source dataset (6). Among the functionalities available for a dossier, you can find 'Export' (7).

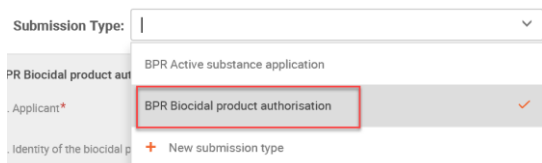


The screenshot shows the ECHA IT tool interface for a dossier titled "Disinfect now – representative product". The interface includes a top navigation bar with options like "Dissemination preview", "Generate CSR", "Export" (marked with a red 7), "Export to PDF", and "Compare". On the left, a "Table of contents" (marked with a red 3) lists 13 sections, with numbers on grey backgrounds indicating document counts (e.g., 3, 4, 1, 5, 6). The main content area shows "Dossier information" (marked with a red 1) and "Mixture / Product information" (marked with a red 2). The "Mixture / Product information" section includes a table with columns for "Mixture / Product name" (Disinfect now) and "Legal entity" (Disinfect now), and a "View Dossiers" button (marked with a red 5) and a "Go to source" button (marked with a red 6). Below this, the "Applicant" section (marked with a red 1) is expanded, showing sub-sections like "1.1 (Cf. 2.1) Name and address" and "1.2 (Cf. 2.1) Contact person".



- Click on 'Export' (7) and save the dossier in the folder 'IUCLID BPR SHD training' with the name '**IUCLID_dossier_active_substance_application**'.
- Now, you will need to create a second dossier: BPR Biocidal product authorisation dossier.

Note: both dossiers will be needed for the exercise on R4BP 3.

Come back to the mixture/product dataset by clicking 'Go to source' (6) and indicate the submission type as 'BPR Biocidal product authorisation'

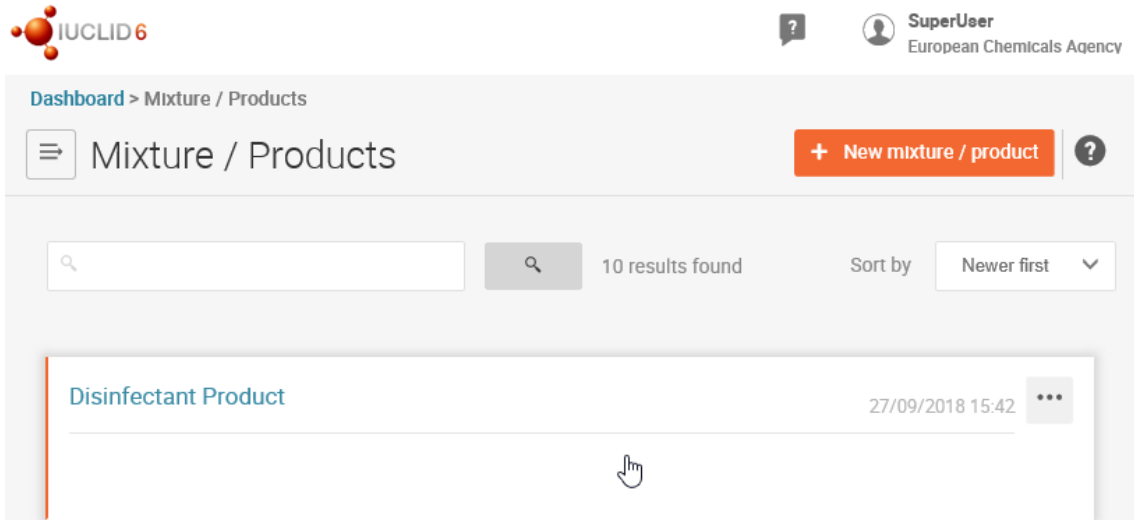


The screenshot shows a dropdown menu for "Submission Type". The menu is open, showing several options: "BPR Active substance application", "BPR Biocidal product authorisation" (highlighted with a red box and a checkmark), and "New submission type". The "BPR Biocidal product authorisation" option is the correct choice for the next step.

- Click on the button .
- Indicate dossier name 'Disinfect now' and click on .
- Open the dossier and export it to the same folder with the name '**IUCLID_dossier_product_authorisation**'.

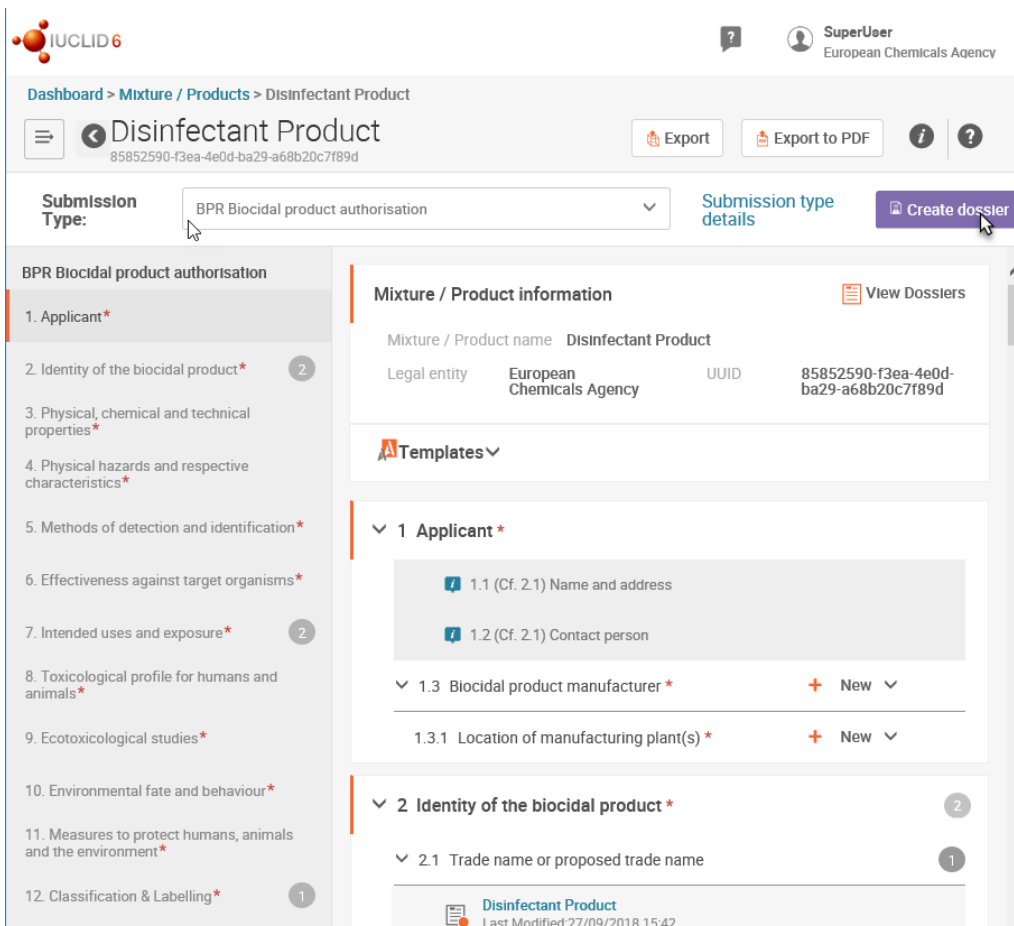
PART 4: Correct an error in a product dataset in order to successfully create a BPR dossier (validation)

1. From the list of mixtures/products select the 'Disinfectant Product' and click it to open its dataset



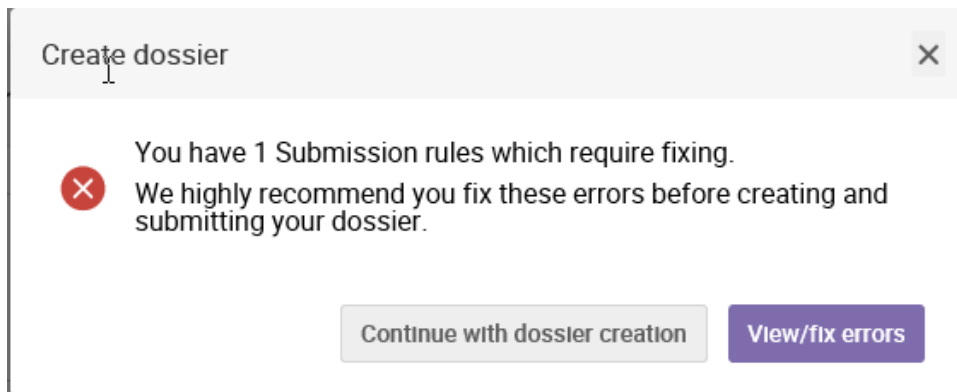
The screenshot shows the IUCLID 6 dashboard. At the top left is the IUCLID 6 logo. At the top right, the user is identified as 'SuperUser' from the 'European Chemicals Agency'. The main header reads 'Dashboard > Mixture / Products'. Below this is a search bar and a 'Mixture / Products' title. A red button labeled '+ New mixture / product' is visible. A search filter shows '10 results found' and a 'Sort by' dropdown set to 'Newer first'. A list of results is shown, with 'Disinfectant Product' selected, showing a date of '27/09/2018 15:42' and a three-dot menu icon.

2. Click 'Create dossier' button in upper right corner



The screenshot shows the 'Disinfectant Product' dataset page. The breadcrumb trail is 'Dashboard > Mixture / Products > Disinfectant Product'. The product name is 'Disinfectant Product' with a UUID of '85852590-f3ea-4e0d-ba29-a68b20c7f89d'. There are 'Export' and 'Export to PDF' buttons. The 'Submission Type' is set to 'BPR Biocidal product authorisation'. A 'Create dossier' button is highlighted with a mouse cursor. On the left is a sidebar with 12 steps of the BPR Biocidal product authorisation process. The main content area shows 'Mixture / Product information' with fields for name, legal entity (European Chemicals Agency), and UUID. Below this is a 'Templates' section and a list of 1 applicant. The applicant details include: 1.1 Name and address, 1.2 Contact person, 1.3 Biocidal product manufacturer (with a '+ New' button), and 1.3.1 Location of manufacturing plant(s) (with a '+ New' button). Section 2 'Identity of the biocidal product' is also visible, with 2.1 Trade name or proposed trade name.



3. Dossier name has been already filled as 'Dossier to be validated', so click again 'Create dossier' button in lower right corner. You will see a warning message that one submission rule requires fixing.



4. Select 'View/fix error' and read the message given.
5. Correct the error.
6. Create a new dossier. You should not see any warning message.


Note: Try to do it yourself. If any difficulty, the detailed instruction starts on the next page.

Solution to part 4:

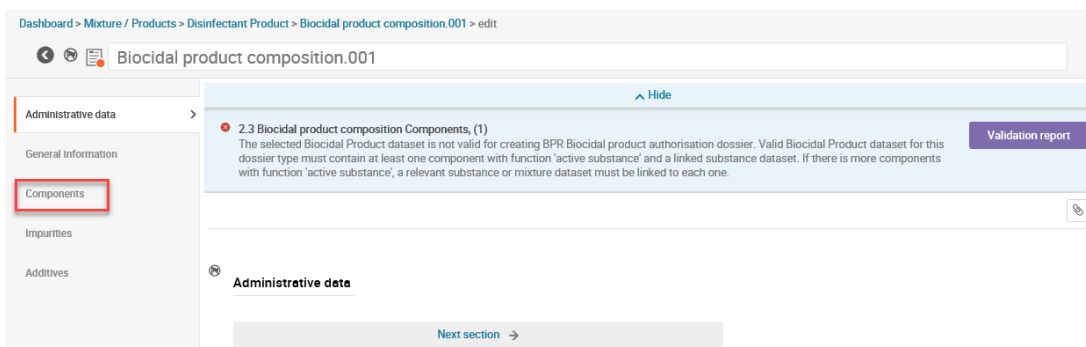
Valid biocidal product dataset must contain at least one component with function 'active substance' and a linked substance dataset. In a dataset for 'Disinfectant Product', in a section 2.3 Biocidal product composition, a component with a function 'active substance' contains a linked reference substance , and not a 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 an active substance. Therefore, a substance dataset has to be created for an active substance, and a reference substance has to be linked to its composition.

1. In the Validation assistant report click on the document which caused the error: 'Biocidal product composition.001'



2. The document will open, and you will see the repeated error message:



Select 'Components' from the menu on the left side.

3. Open the first component and then click on the link to 'hydrogen peroxide' in a field 'Name'.

Components

	+ New item
01	✎ ✕
02	✎ ✕
03	✎ ✕

Name

hydrogen peroxide ✕

4. You can see that this is a reference substance, and not a substance.

Reference substance ✎ Edit ✕

General information

Reference substance name hydrogen peroxide

Inventory

Inventory number	<ul style="list-style-type: none"> • EC 231-765-0 Name hydrogen peroxide Number 231-765-0 CAS Number 7722-84-1 Molecular formula H2O2
------------------	--

Close this reference substance by clicking on ✕.

5. Remove the link to the reference substance by clicking on ✕.

⏪ ⏴ 01

^ Hide

✖ 2.3 Biocidal product composition Components, (1)

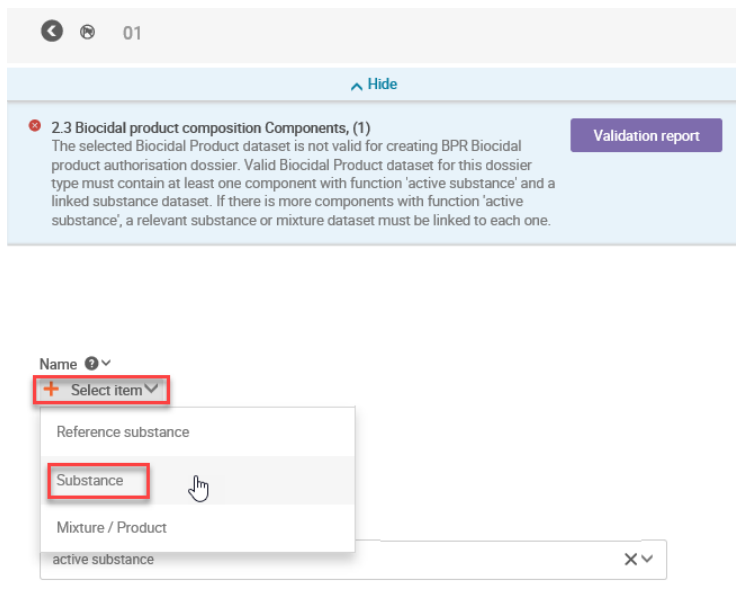
The selected Biocidal Product dataset is not valid for creating BPR Biocidal product authorisation dossier. Valid Biocidal Product dataset for this dossier type must contain at least one component with function 'active substance' and a linked substance dataset. If there is more components with function 'active substance', a relevant substance or mixture dataset must be linked to each one.

Validation report

Name

hydrogen peroxide ✕

6. Select new item - Substance





01

Hide

2.3 Biocidal product composition Components, (1)
The selected Biocidal Product dataset is not valid for creating BPR Biocidal product authorisation dossier. Valid Biocidal Product dataset for this dossier type must contain at least one component with function 'active substance' and a linked substance dataset. If there is more components with function 'active substance', a relevant substance or mixture dataset must be linked to each one.

Validation report


Name  

+ Select item

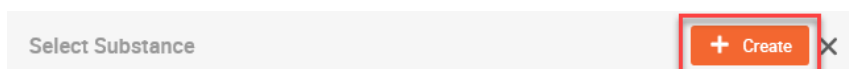
Reference substance

Substance


Mixture / Product

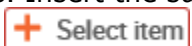
active substance 

In your IUCLID database there is no substance 'Hydrogen peroxide', therefore you need to create one. Click 'Create'

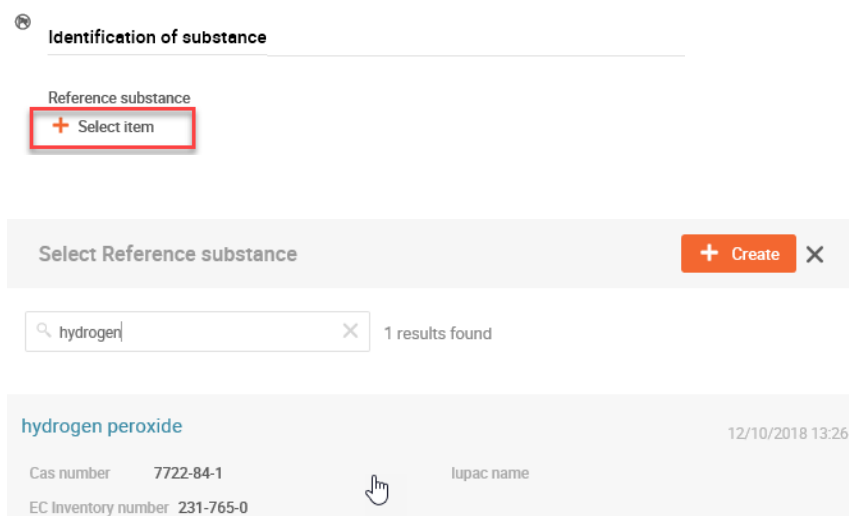


Select Substance

+ Create 

7. The sliding window for a new substance opens. Insert the substance name 'Hydrogen peroxide', add select the legal entity (click on  and on the legal entity displayed on your list).

8. Scroll down to 'Identification of substance' and add the reference substance 'hydrogen peroxide'




Identification of substance

Reference substance

+ Select item

Select Reference substance

+ Create 

hydrogen 1 results found

hydrogen peroxide 12/10/2018 13:26

Cas number 7722-84-1 lupac name

EC Inventory number 231-765-0

9. Click  and .

10. You came back to the biocidal product composition. Click on  to leave the

Edit mode, and then on  to view the document.

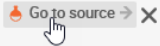
Now, the first component contains a link to the substance, however this substance follows a default '*Complete table of contents*'. You need to change it to '*BPR Active substance information*', following the steps:

a) Click on the link in the first component

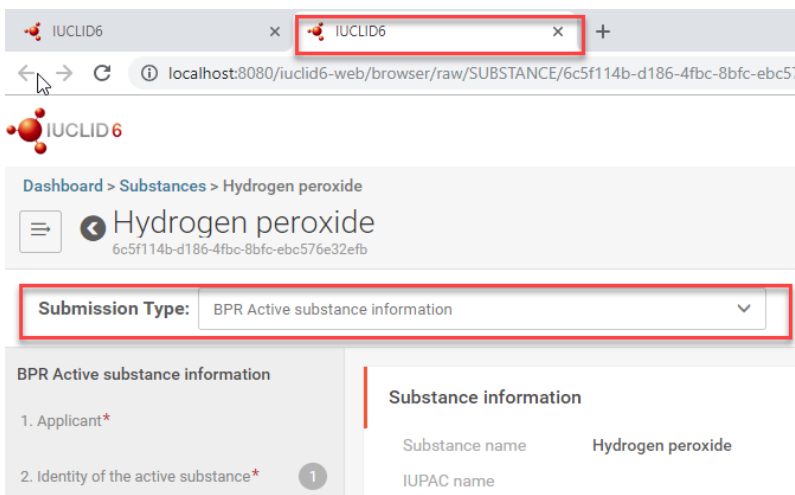
Components

Component flag	
Name	Hydrogen peroxide hydrogen peroxide 7722-84-1
Function	active substance
Typical concentration	ca. 20 % (w/w)

b) In the sliding window click on 'Go to source' button to open the active substance dataset


Substance	
Substance name	Hydrogen peroxide
Public name	

c) The active substance dataset opens in a new tab. Indicate the 'Submission type' as 'BPR Active substance information', click 'Apply' and 'Close'.



The screenshot shows a browser window with two tabs. The active tab is titled 'IUCLID6' and shows the IUCLID6 dashboard for 'Hydrogen peroxide'. The 'Submission Type' dropdown menu is highlighted with a red box and set to 'BPR Active substance information'. Below the dropdown, there are two sections: 'BPR Active substance information' and 'Substance information'. The 'Substance information' section shows 'Substance name: Hydrogen peroxide' and 'IUPAC name:'. The 'BPR Active substance information' section has two steps: '1. Applicant*' and '2. Identity of the active substance*' with a '1' in a circle next to it.

d) Close the current tab.

11. Come back to the first tab, and close the sliding window by clicking on .

12. Come back to the 'Disinfectant Product'

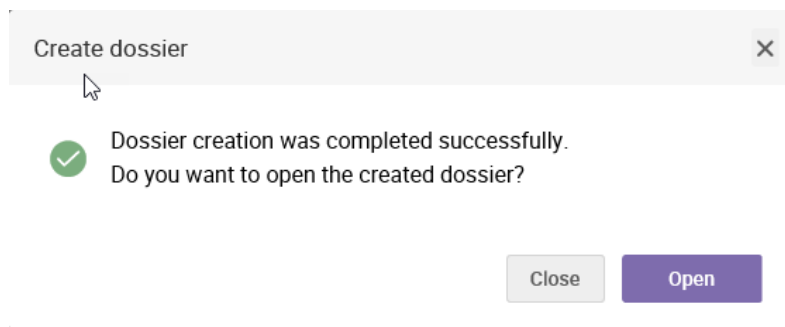
Dashboard > Mixture / Products > **Disinfectant Product** > Biocidal product composition.001

13. Come back to the 'Disinfection Product' and create a dossier.



Dashboard > Mixture / Products > **Disinfectant Product** > Biocidal product composition.001

You should see a message:



END OF THE TRAINING