

# IUCLID 6





# IUCLID 6 webinar

Version 1.3 release

*4 May 2017 / 12:00-13:00 EET*

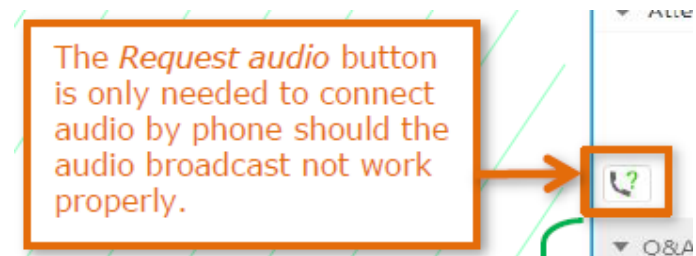
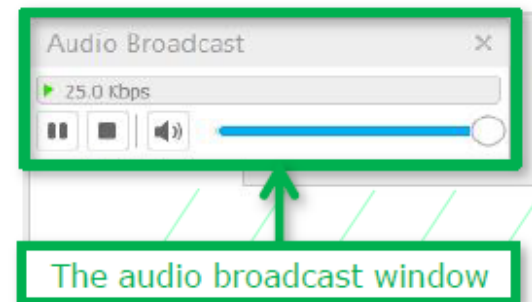
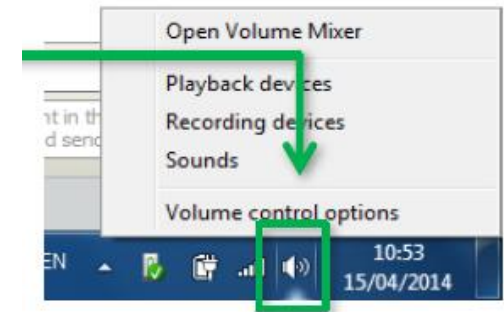


IUCLID 6 is developed by the European  
Chemicals Agency in association with the OECD



## Audio troubleshooting

- If the volume is too low, try to increase the sound volume of your computer.
- If the audio cannot be heard at all, verify that the audio broadcast window shows a green triangle and that the volume slider is not too low.
- If the problem persists, you can use a telephone for receiving audio.
  - Click the button shown above to *Request Audio*
  - Select *Use phone*, enter your phone number
  - Click on the *Call me* button



## Agenda for today

What?	Who?	When?
Welcome and introduction	François Le Goff	12pm (EEST)
Information on IUCLID 6 version 1.3 and feedback from IUCLID users		
PNEC calculator	Jesus Vazquez Rodriguez	
Report generator – advanced functions and new reports	Mark Roberts	
IUCLID Cloud Services	Tommy Hägg	
Questions and Answers session	All participants ECHA	Until 13:00

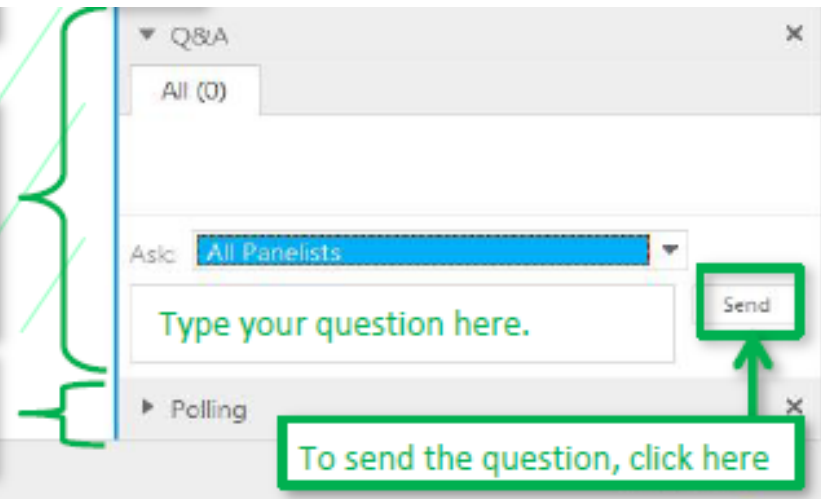
## The Q&A panel

- You can post your questions during the entire webinar
- Before the Q&A session, 5 minutes will be left to send additional questions

### The Q&A panel

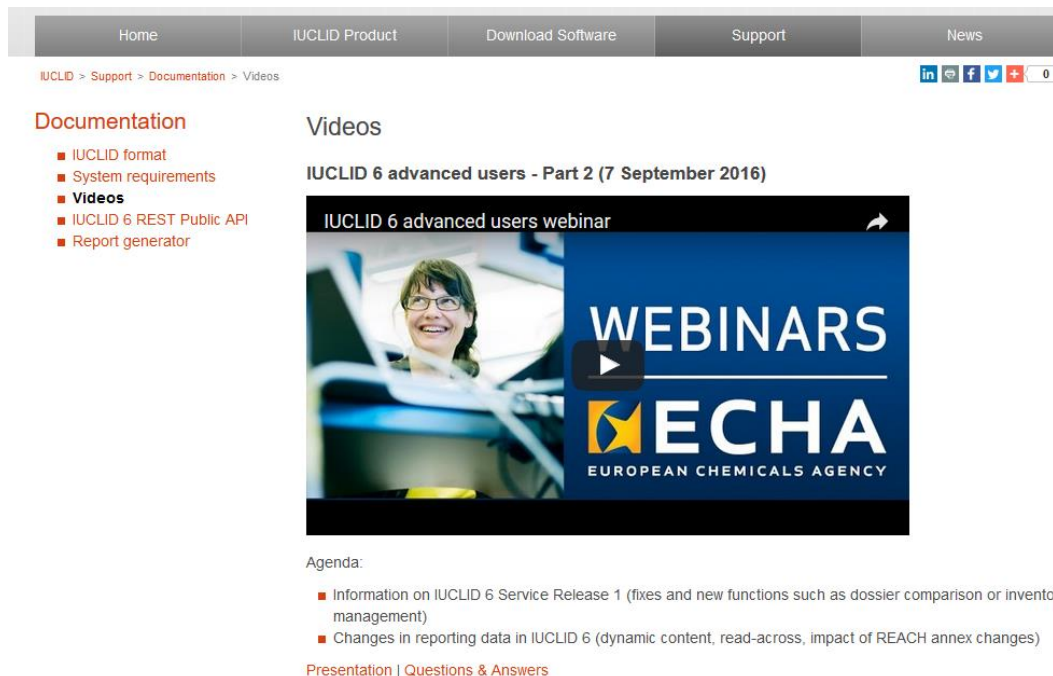
You can send questions during and after the presentations to the panellists, using the Q&A panel  
**To send a question**, select *All panelists* from the drop down menu, write your question in the lower box, and finally click *Send*.

If a poll is opened during the webinar, the polling panel will open automatically



## Recordings

- After the meeting, we will publish on the IUCLID 6 website:
  - The recording of the webinar (+ presentations)
  - Questions and answers (written document)



Home IUCLID Product Download Software Support News

IUCLID > Support > Documentation > Videos

Documentation

- IUCLID format
- System requirements
- **Videos**
- IUCLID 6 REST Public API
- Report generator

Videos

IUCLID 6 advanced users - Part 2 (7 September 2016)

IUCLID 6 advanced users webinar

WEBINARS  
ECHA  
EUROPEAN CHEMICALS AGENCY

Agenda:

- Information on IUCLID 6 Service Release 1 (fixes and new functions such as dossier comparison or inventory management)
- Changes in reporting data in IUCLID 6 (dynamic content, read-across, impact of REACH annex changes)

Presentation | Questions & Answers

# IUCLID 6 updates

## Service Release 3

- Fixes and improvements
- New features



## Version 1.3.0

### IUCLID news

28/04/2017

#### IUCLID 6 version 1.3.0 is available

**A new service release for IUCLID is available. It brings improvements and bug re-use of the dossier header and the Report manager.**

A new service release for IUCLID is available. In addition to improvements and fixes in

- PNEC calculator: helps to generate predicted no effect concentrations (PNEC) for guidance. The results are automatically stored in IUCLID.
- Dossier header re-use: when creating dossiers for submission to regulatory authorities, you can re-use dossier headers that you have previously entered for the same substance in the dossier header. You no longer need to create a new dossier header for each update.
- Report templates manager: eases generation of reports by allowing you to pre-load templates. No manual editing is needed.

This new version is compatible with previous IUCLID 6 versions. For more details about the update, please attend the webinar on Thursday 4<sup>th</sup> of May 2017. A link to register is available below.

As of today we have also launched the [IUCLID LinkedIn group](#) which will be a collaboration platform for the latest IUCLID developments and on the usage of the application. We will be posting updates regularly. You can subscribe to the group straight away.

[Download IUCLID 6](#) | [Release notes](#) | [Release presentation webinar](#) | [IUCLID LinkedIn group](#)

- As with previous updates, the installation of the new version is recommended (but optional)
- You can update from any IUCLID 6 versions with the updater
- You can migrate directly from IUCLID 5.6 to this version with the installer or the migration tool
- IUCLID 5.6 files can still be imported
- Full compatibility with previous IUCLID 6 versions / Compatible with Chesar



## Version 1.3.0 – Release notes

### IUCLID news

28/04/2017

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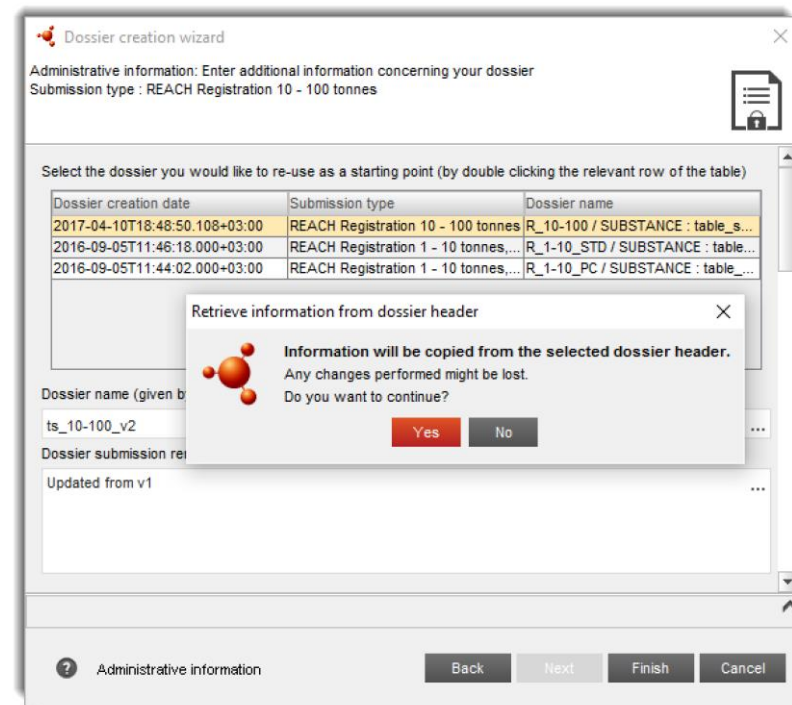
[Download IUCLID 6](#) | [Release notes](#) | [Release presentation webinar](#) | [IUCLID LinkedIn group](#)

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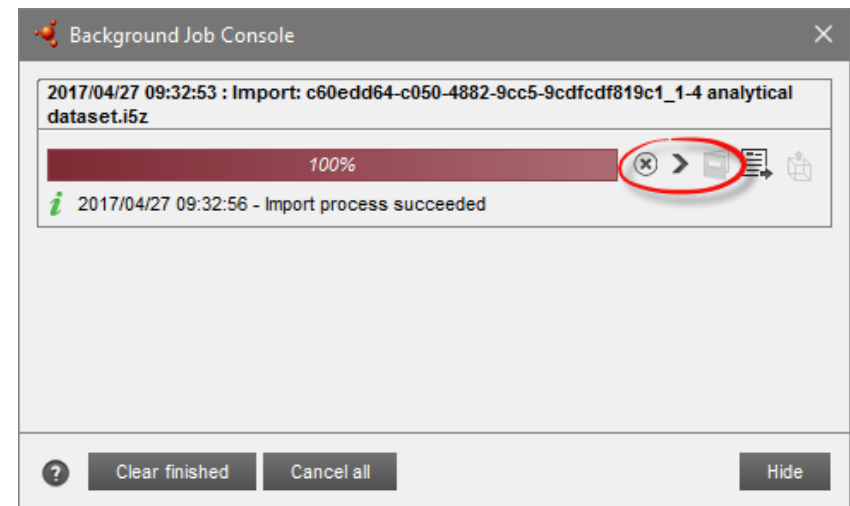
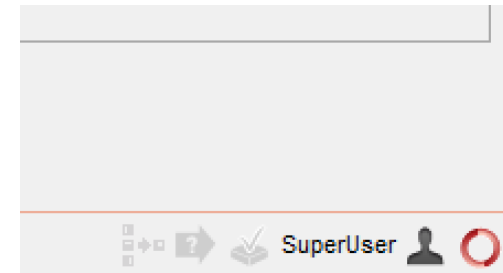
## Dossier header re-use

- New function to help filling-in the dossier header while creating a dossier update
- It gives access to previously created dossiers for the same substance
- The most recent dossiers are presented first
- You can then use the previously entered data as a starting point (e.g. justifications for confidentiality claims)



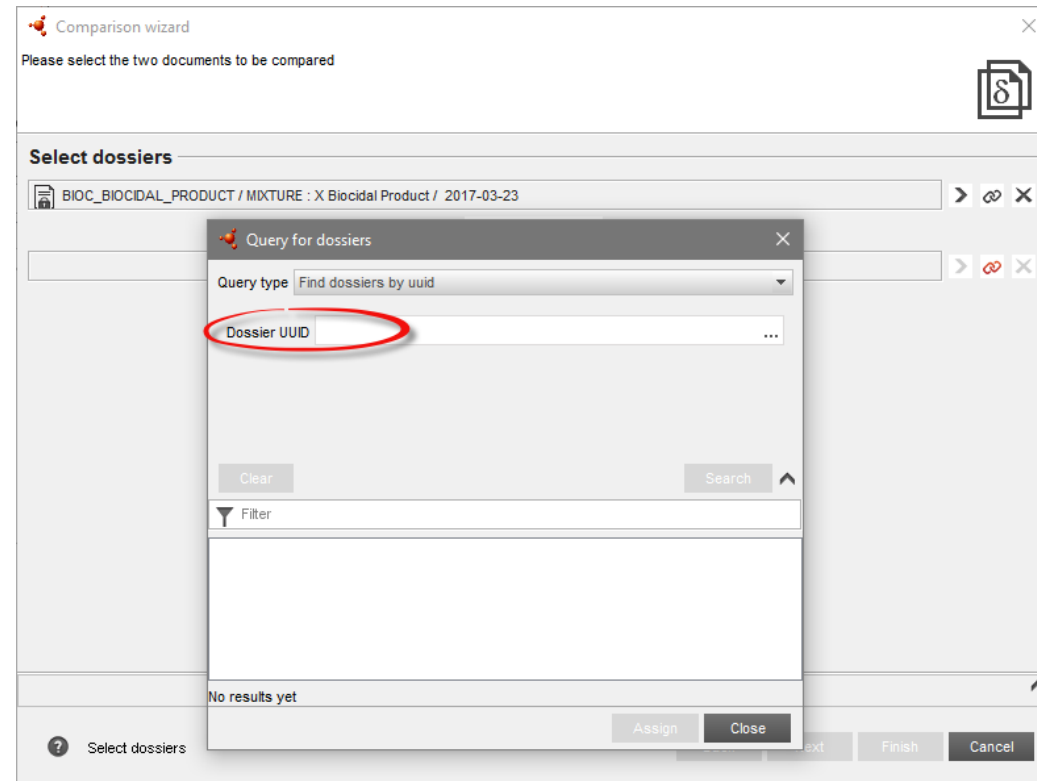
## Access a file directly after importing it

- When you import a IUCLID file, a dataset or a dossier
- Access the background jobs windows
- A link will allow you to access the imported entity directly



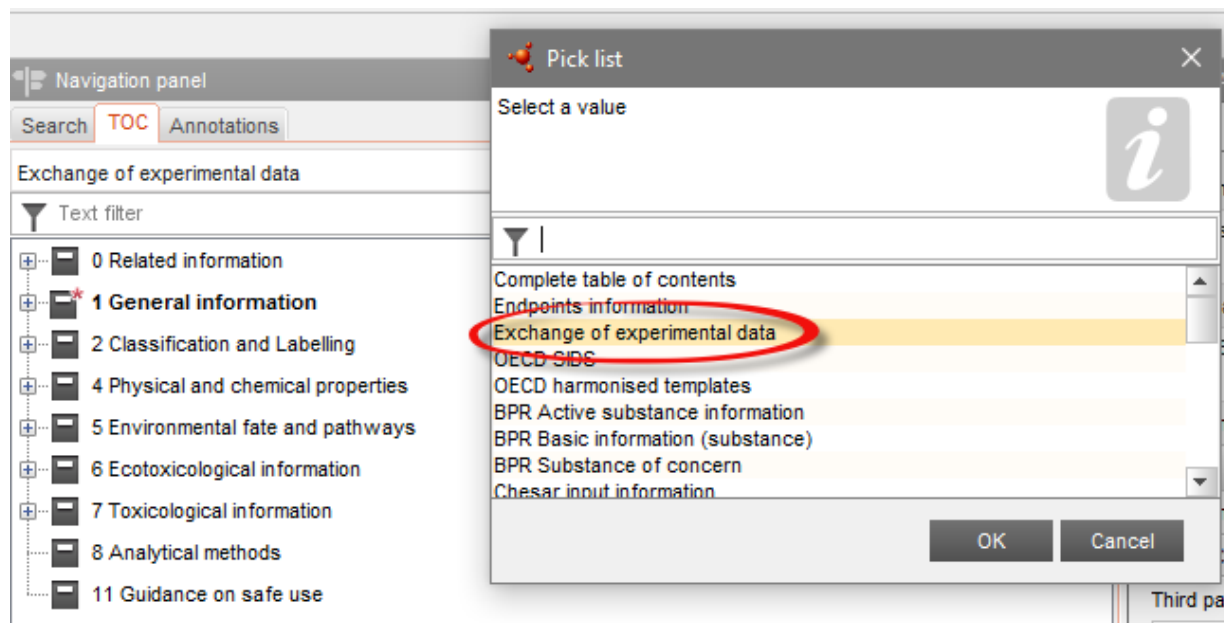
## Comparison tool

- In order to compare two dossiers you can:
  - Select two dossiers directly
  - Select one dossier and search for the second one, also using its unique identifier (UUID)



## 'Exchange of experimental data' submission type

- A new submission type has been added in order to support the 'Exchange of experimental data' outside any regulatory context. This submission type is a prototype and is subject to further validation with the IUCLID users' community. That's why the dossier creation using this submission type is not yet enabled



## Dissemination preview

- The ordering and sorting of the dissemination preview report has been improved
- All columns can now be sorted and the default sorting is done on the 'Section name' (numeric sorting)

Dissemination preview

R\_ABOVE\_1000 / SUBSTANCE : ECHA substance / ECHA Substance / 11111-11-1 / 2017-05-02

Open original document Open filtered document

Entity	Section name ^	Document name	Field	Outcome
Literature Reference		Toxicity to microorganism	Title	Not published (ineligible ...
Literature Reference		Toxicity to microorganism	Author	Not published (ineligible ...
Literature Reference		Toxicity to microorganism	Year	Published
Substance	1.1 Identification	ECHA substance		Published
Substance	1.1 Identification	ECHA substance		Filtered section 0.4 Ass...
Substance	1.1 Identification	ECHA substance	Substance name	Not published
Substance	1.1 Identification	ECHA substance	Public name	Published
Substance	1.1 Identification	ECHA substance	Manufacturer	Not published
Substance	1.1 Identification	ECHA substance	Reference substance	Published
Substance	1.1 Identification	ECHA substance	Type of substance	Published
Substance	1.1 Identification	ECHA substance	Origin	Published
Flexible Record	1.2 Composition	ECHA Substance		Published
Flexible Record	1.2 Composition	ECHA Substance	Name	Published
Flexible Record	1.2 Composition	ECHA Substance	Type of composition	Published
Flexible Record	1.2 Composition	ECHA Substance	State / form	Published
Flexible Record	1.2 Composition	ECHA Substance	Description of compositi...	Not published
Flexible Record	1.2 Composition	ECHA Substance	FLEXIBLE_RECORD/Sub...	Not published (ineligible ...
Flexible Record	1.2 Composition	ECHA Substance	FLEXIBLE_RECORD/Sub...	Published
Flexible Record	1.2 Composition	ECHA Substance	Reference substance	Published
Flexible Record	1.2 Composition	ECHA Substance	Typical concentration	Not published
Flexible Record	1.2 Composition	ECHA Substance	Concentration range	Not published
Flexible Record	1.2 Composition	ECHA Substance	Remarks	Not published

Dissemination preview report

Back Next Finish Cancel

## Dissemination preview

- The copy of the full report to Excel is now possible

Dossier	Name	R_ABOVE_1000 / SUBSTANCE : ECHA substance / ECHA Sub	Field	Published
148 Substance	1.1 Identification	ECHA substance	Public name	Published
149 Substance	1.1 Identification	ECHA substance	Manufacturer	Not published
150 Substance	1.1 Identification	ECHA substance	Reference substance	Published
151 Substance	1.1 Identification	ECHA substance	Type of substance	Published
152 Substance	1.1 Identification	ECHA substance	Origin	Published
153 Flexible Record	1.2 Composition	ECHA Substance		Published
154 Flexible Record	1.2 Composition	ECHA Substance	Name	Published
155 Flexible Record	1.2 Composition	ECHA Substance	Type of composition	Published
156 Flexible Record	1.2 Composition	ECHA Substance	State / form	Published
157 Flexible Record	1.2 Composition	ECHA Substance	Description of composition	Not published
158 Flexible Record	1.2 Composition	ECHA Substance	FLEXIBLE_RECORD/SubstanceComposition.DegreeOfPurity.Purity	Not published (ineligible for dissemination)
159 Flexible Record	1.2 Composition	ECHA Substance	FLEXIBLE_RECORD/SubstanceComposition.Constituents.Constituents[0]	Published
160 Flexible Record	1.2 Composition	ECHA Substance	Reference substance	Published
161 Flexible Record	1.2 Composition	ECHA Substance	Typical concentration	Not published
162 Flexible Record	1.2 Composition	ECHA Substance	Concentration range	Not published
163 Flexible Record	1.2 Composition	ECHA Substance	Remarks	Not published

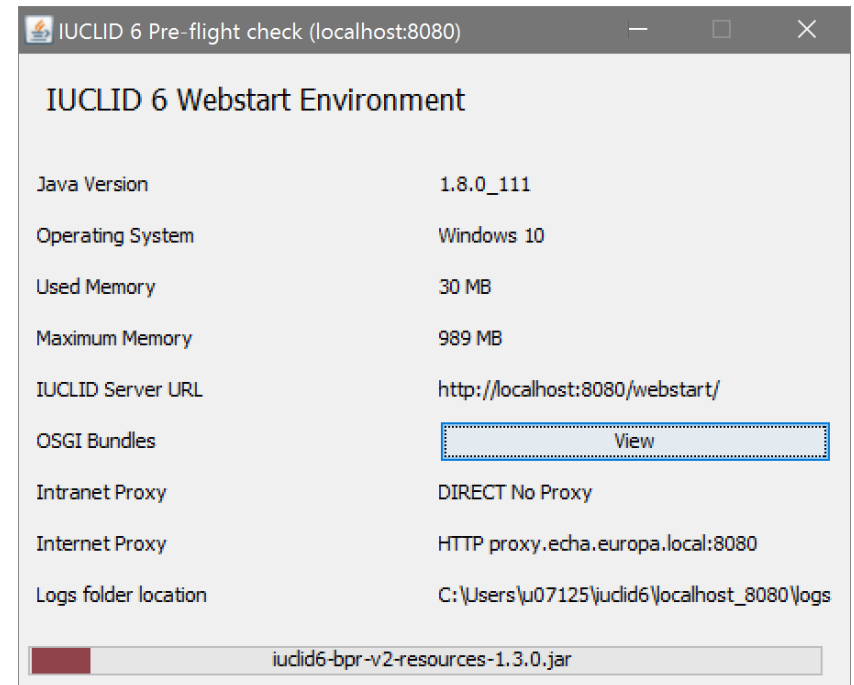
## Validation assistant

- No change to the Business Rules and Technical Completeness Check rules
- Improved quality rule QLT098 to also consider the late pre-registration number format as valid
- Quality rules (QLT) implemented for classification and labelling (section 2.1)
- First Quality rules (QLT) implemented for hazard endpoints (sections 6.3.1, 6.3.2, 6.3.3, 7.3.1, 7.3.2)



## IUCLID 6 Server – Client launch automation

- When using a Server installation the client is now launched automatically once all the files have been loaded to your computer

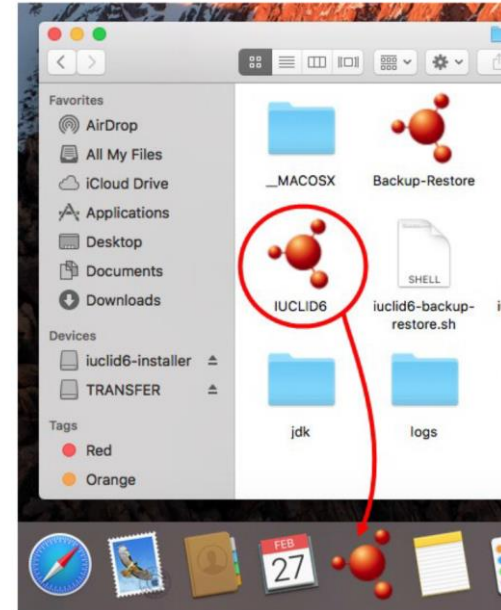


# IUCLID 6 version 1.3.0



## Mac OS installer and updater

- IUCLID 6 Desktop installer available for Mac OS X with version 1.2.0
- Now an updater is also provided for 1.3.0



## IUCLID news

27/02/2017

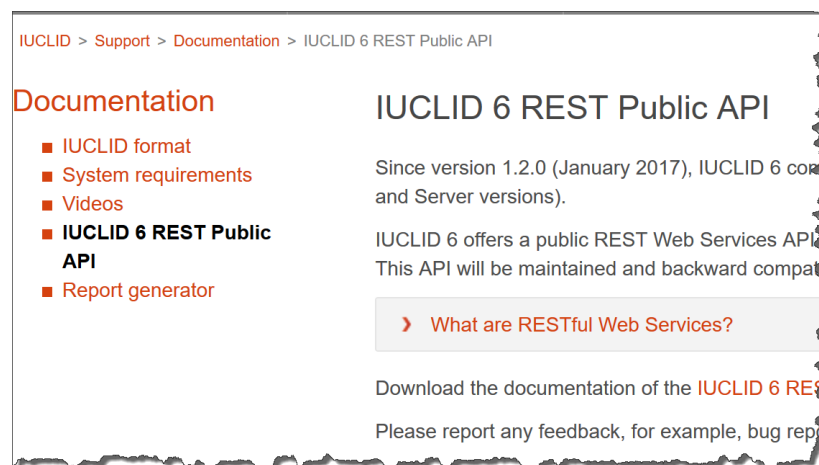
### IUCLID 6 Desktop available for Mac OS X

IUCLID 6 Desktop installer v1.2.0 has been made available for Mac OS X. The installer and the final installation of IUCLID 6 Desktop for Mac OS X both come with their own built-in installation of Java for Mac OS X. Therefore, no separate installation of Java is required. An installer and an updater will be supplied for the Mac OS X in future releases of IUCLID 6 Desktop.

[Download IUCLID 6 Desktop v1.2.0 for Mac OS X](#) | [More information](#)

## Public API

- Available since IUCLID 6 1.2.0
- Updated in version 1.3.0
  - The linking of attachments to documents is now supported
  - It is now possible to determine the type of entity (e.g. dossier, substance or mixture dataset) imported using the Public REST API import endpoint
- The documentation has been updated on the IUCLID 6 website

A screenshot of the IUCLID 6 REST Public API documentation page. The page has a breadcrumb trail: "IUCLID > Support > Documentation > IUCLID 6 REST Public API". On the left, under the heading "Documentation", there is a list of links: "IUCLID format", "System requirements", "Videos", "IUCLID 6 REST Public API" (which is bolded), and "Report generator". On the right, the main heading is "IUCLID 6 REST Public API". Below it, the text reads: "Since version 1.2.0 (January 2017), IUCLID 6 core and Server versions). IUCLID 6 offers a public REST Web Services API. This API will be maintained and backward compatible." There is a button that says "What are RESTful Web Services?". At the bottom, it says "Download the documentation of the IUCLID 6 REST Public API" and "Please report any feedback, for example, bug reports".

# Feedback from the Helpdesk



## Feedback from users

- REACH registrations and opt-out: in the case of data sharing dispute or confidential information for example
  - How does it work?
  - How to add more information, e.g. endpoint summaries

# Feedback from users



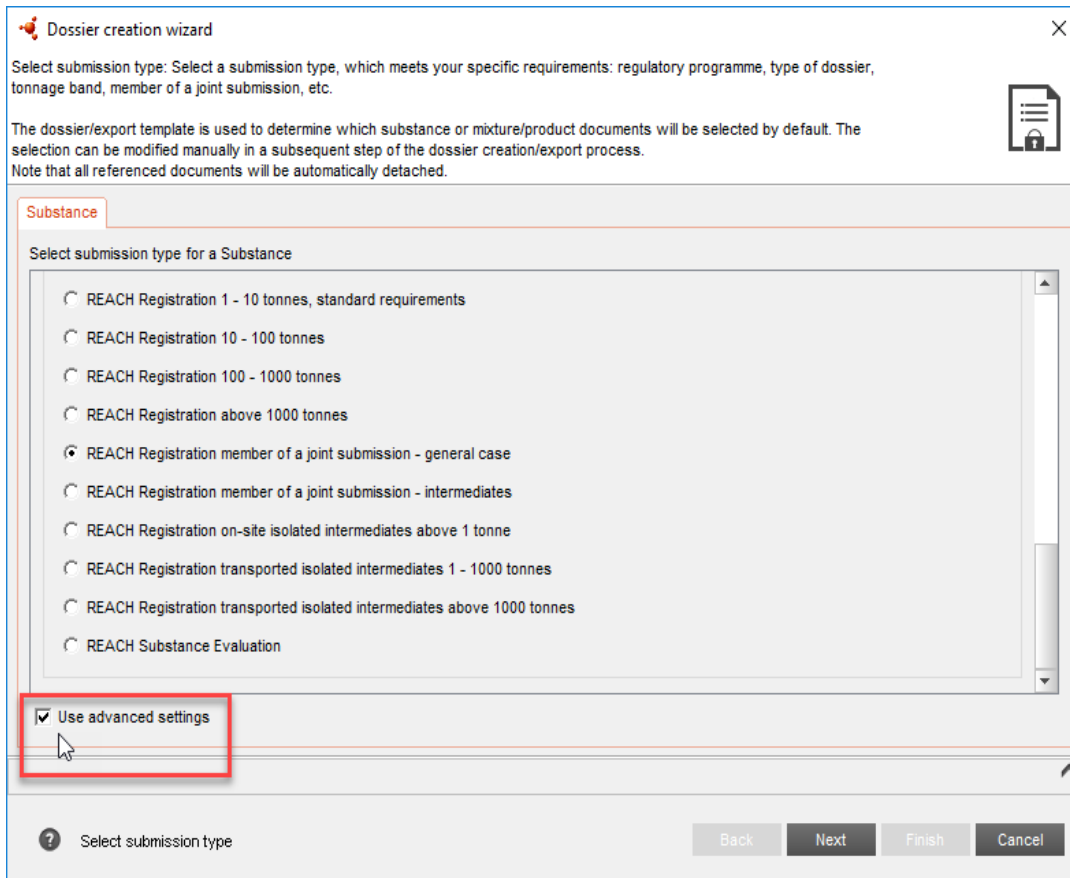
## REACH opt-outs

- Prepare your dataset
  1. Enter the data
  2. Indicate the opt-outs and the justifications under section 14

The screenshot displays the IUCLID 6 interface for REACH registration. The left panel, titled 'Navigation panel', shows a tree view of registration sections. The 'Opt-out information for REACH registration' section is highlighted in yellow. The right panel, titled 'EU\_REACH / Opt-out information', shows the 'Data selected for opt-out' section. The 'Documents' list includes 'OECD / Bioaccumulation: aquatic'. The 'Justification' field contains 'Justification for the opt-out'. The bottom right panel, titled 'Information panel', shows the 'Type' field set to 'Fixed Record', the 'UUID' field set to '5eb1aad6-1815-48d2', and the 'Dossier UUID' field.

## REACH opt-outs

- Create your REACH registration dossier as a member of a joint submission
- An opt-out is done as part of a joint submission
- Activate the advanced settings of dossier creation



**Dossier creation wizard**

Select submission type: Select a submission type, which meets your specific requirements: regulatory programme, type of dossier, tonnage band, member of a joint submission, etc.

The dossier/export template is used to determine which substance or mixture/product documents will be selected by default. The selection can be modified manually in a subsequent step of the dossier creation/export process.  
Note that all referenced documents will be automatically detached.

**Substance**

Select submission type for a Substance

- REACH Registration 1 - 10 tonnes, standard requirements
- REACH Registration 10 - 100 tonnes
- REACH Registration 100 - 1000 tonnes
- REACH Registration above 1000 tonnes
- REACH Registration member of a joint submission - general case
- REACH Registration member of a joint submission - intermediates
- REACH Registration on-site isolated intermediates above 1 tonne
- REACH Registration transported isolated intermediates 1 - 1000 tonnes
- REACH Registration transported isolated intermediates above 1000 tonnes
- REACH Substance Evaluation

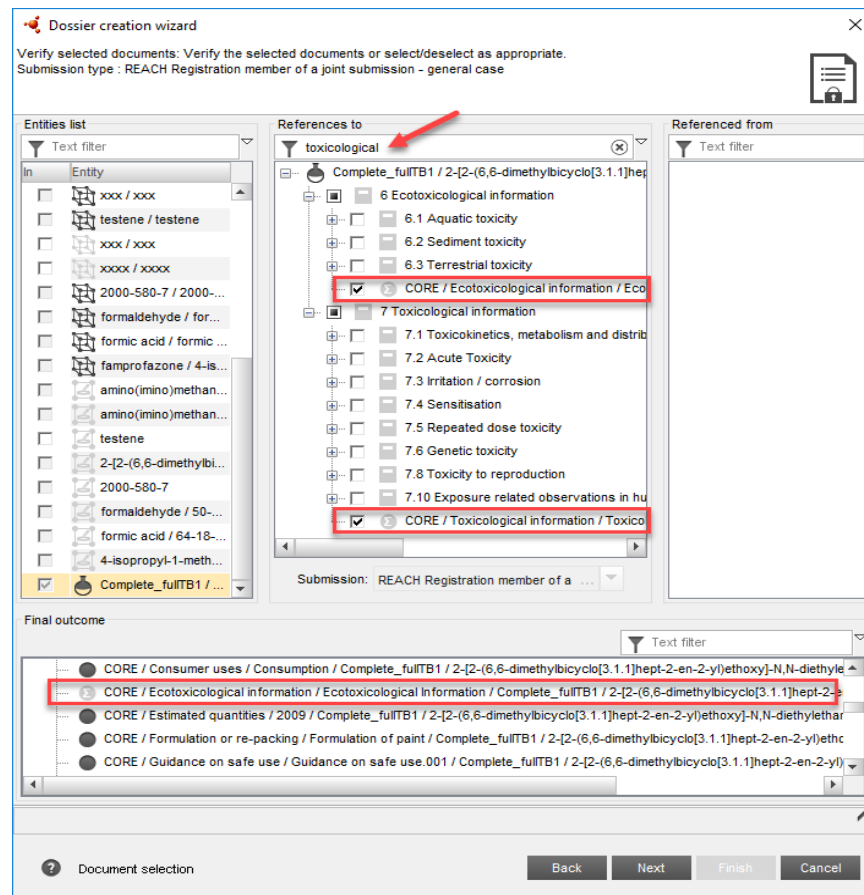
Use advanced settings

? Select submission type

Back Next Finish Cancel

## REACH opt-outs

- Manually include the appropriate documents in the dossier
- In the *Entities list*, select the substance dataset
- In the *References to* panel, use the text filter at the top to more easily locate the desired documents
- Confirm in the *Final outcome* panel that the desired selections have been indicated for inclusion.



The screenshot displays the 'Dossier creation wizard' interface. At the top, it states 'Verify selected documents: Verify the selected documents or select/deselect as appropriate. Submission type: REACH Registration member of a joint submission - general case'. The interface is divided into three main panels:

- Entities list:** A list of chemical entities with checkboxes. The entity 'Complete\_fullTB1 / ...' is selected.
- References to:** A tree view of document categories. A red arrow points to the 'toxicological' filter. Two items are highlighted with red boxes: 'CORE / Ecotoxicological information / Eco...' and 'CORE / Toxicological information / Toxico...'. Both have checkboxes that are checked.
- Final outcome:** A list of document titles. One item is highlighted with a red box: 'CORE / Ecotoxicological information / Ecotoxicological Information / Complete\_fullTB1 / 2-[2-(6,6-dimethylbicyclo[3.1.1]hept-2-en-2-yl)ethoxy]-N,N-diethyl-2-...'. Its checkbox is checked.

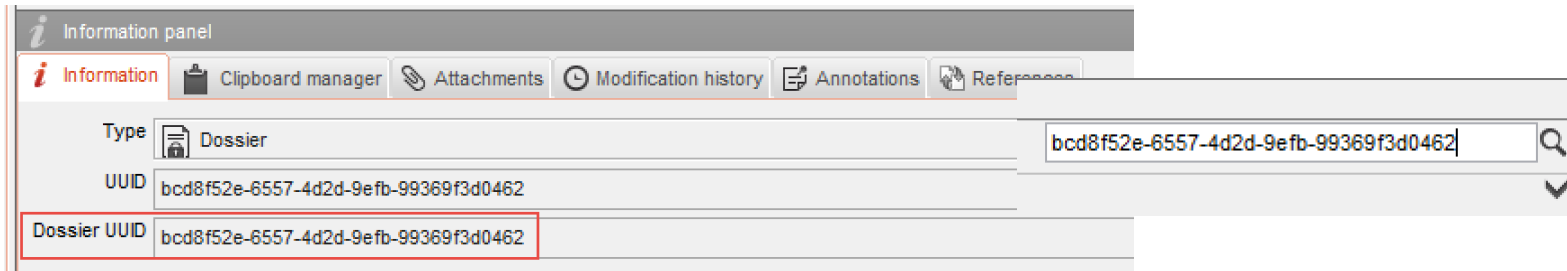
At the bottom, there are buttons for 'Back', 'Next', 'Finish', and 'Cancel', along with a 'Document selection' status indicator.



## Dossier creation and validation assistant / export

- After the dossier creation, there are two ways to retrieve it to initiate the validation assistant or to export it

1. Copy the dossier UUID and paste it to the top-right corner of IUCLID



2. Go back to the home page, go to dossier, the newly created dossier will appear first in the list



## REACH Study Results

- The non confidential data collected under REACH and available on the ECHA website are also distributed in the IUCLID format (for the study results)
  - As a Desktop installation
  - As an Oracle database that can be connected to a IUCLID Server
- Access to the data can be done using the IUCLID 6 Public API
- The use of the data is subject to specific terms and conditions

## IUCLID news

22/03/2017

### REACH study results are published

**REACH study results is a collection of non-confidential substances available to download free of charge from this website.**

REACH study results is a collection of non-confidential substance data available to download free of charge from the IUCLID 6 website. The data contains physico-chemical, ecotoxicology and toxicological information. ECHA is committed towards the goals of REACH - both in terms of improving the safe use of chemicals and the development and use of alternative methods.

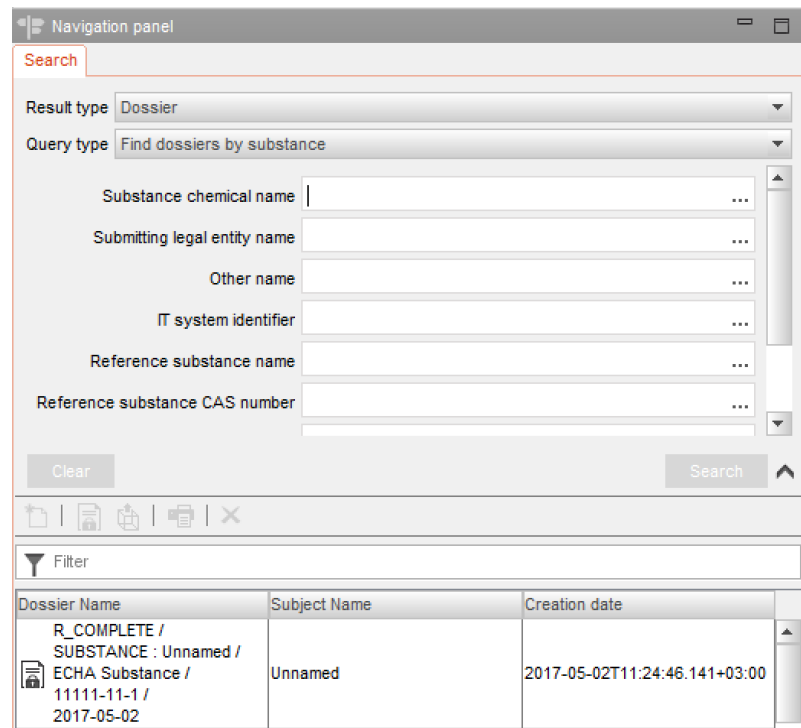
The data is derived from data that is already accessible on the ECHA website. The data is presented, and in a reduced form. On the ECHA website data may be available to download in a single file. On the ECHA website data may be available to download in a single file. [IUCLID 6 REST Public API](#).

The use of the REACH study results is subject to dedicated terms and conditions. Data may not be used for registration under the REACH Regulation.

Access the REACH study results [here](#).

## REACH Study Results

- More than 15,000 **dossiers** for the same amount of substances are available
- The basic search functions of IUCLID should be used to retrieve specific information if needed
- Comments and feedback can be sent to the ECHA Helpdesk. It will be used for future improvements.



The screenshot shows the IUCLID 6 search interface. At the top, there is a 'Navigation panel' with a 'Search' tab. Below this, the 'Result type' is set to 'Dossier' and the 'Query type' is 'Find dossiers by substance'. There are several search criteria fields: 'Substance chemical name', 'Submitting legal entity name', 'Other name', 'IT system identifier', 'Reference substance name', and 'Reference substance CAS number'. Each field has a search icon to its right. Below the search fields are 'Clear' and 'Search' buttons. A 'Filter' section is visible below the search fields. At the bottom, there is a table with the following data:

Dossier Name	Subject Name	Creation date
R_COMPLETE / SUBSTANCE : Unnamed / ECHA Substance / 11111-11-1 / 2017-05-02	Unnamed	2017-05-02T11:24:46.141+03:00

## Next IUCLID 6 update: version 2.0.0

- Planned for the end of October 2017
- Will contain fixes, improvements and new features and also update to the format of the IUCLID 6 documents
- 2018 deadline
  - REACH-IT will keep accepting dossiers generated by the new IUCLID 6 version as well as the previous one
  - The format changes will not impact the verification made to the dossiers prepared for REACH purposes
- Exchange of data
  - It will always be possible to import IUCLID 6 data from an older version to a newer one
  - We are working on a solution that should improve this situation by also allowing a version 2.0.0 user to export the data in a format that would be compatible with the previous IUCLID 6 versions

# PNEC Calculator

Jesus Vazquez Rodriguez



## What is it?

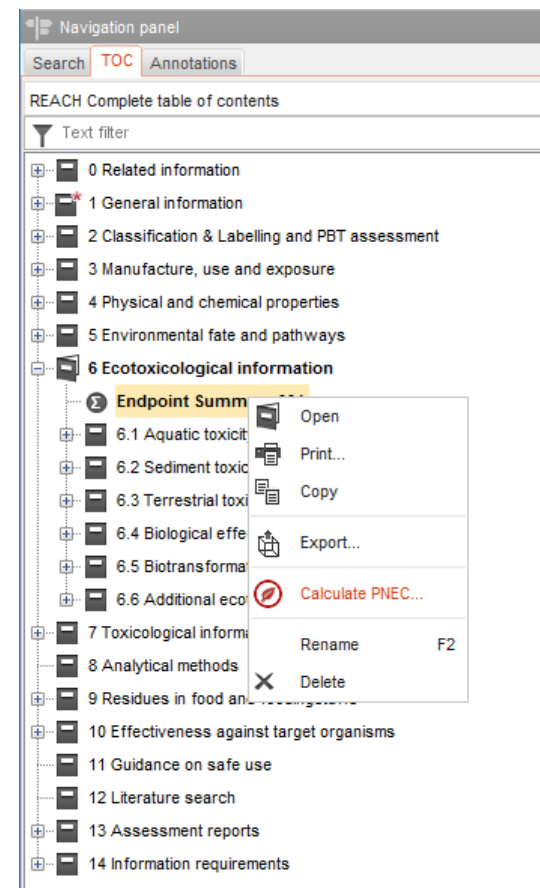
- The PNEC calculator offers you the possibility to calculate and report predicted no-effect concentrations (PNECs) in IUCLID according to ECHA Guidance on information requirements and chemical safety assessment, Chapter R.10.

## Purpose

- PNEC derivation is a key element for the risk characterisation of a chemical substance.
- The PNEC calculator allows you to derive PNECs automatically from the data already available in the **endpoint summaries** (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)) **of a substance dataset or template** and report them back in the corresponding endpoint summary under section '*6 Ecotoxicological information*'.
- Currently, the PNEC calculator only supports the **derivation of PNECs for aquatic, sediment and terrestrial environmental protection targets** according to the ECHA Guidance. Thus, the current version does not support the derivation of PNECs for microorganisms in sewage treatment plants and the PNEC<sub>oral</sub> used for the assessment of secondary poisoning.

## Overview – how it works?

- How to use it?
  - You can use the PNEC calculator by right-clicking the endpoint summary under section '*6 Ecotoxicological information*' and selecting '*Calculate PNEC*' from the displayed menu.





# PNEC calculator



## Overview – how it works?

- Outcome
  - The results (PNECs calculated according to the Guidance R10) are displayed in a tabular format by environmental protection target.
  - For each environmental protection target, the dose descriptor (effect concentration) used as starting point and the assessment factor used to address uncertainties in the extrapolation are set by the tool and displayed in the corresponding tab as read-only information.
  - For sediment and soil the type of extrapolation method used (i.e. assessment factor or equilibrium partitioning method) is also displayed.

The screenshot shows the PNEC calculator interface. At the top, there is a title bar with the text 'PNEC calculator' and a close button. Below the title bar, the main window is divided into two sections. The upper section contains a table with the following data:

Environmental compartment	PNEC Scenario
Aqua	Freshwater: 0.5 mg/L Freshwater intermittent: 0.1 mg/L Marine: 0.1 mg/L Marine intermittent: 15.0 µg/L
Sediment	Freshwater: 11.8 mg/kg sediment dw Marine: 2.36 mg/kg sediment dw
Soil	Soil: 3 mg/kg soil dw

The lower section of the interface is a configuration panel with tabs for 'Aqua', 'Sediment', and 'Soil'. The 'Aqua' tab is active and shows settings for four categories: 'Freshwater', 'Freshwater, intermittent', 'Marine', and 'Marine, intermittent'. Each category has a 'Dose descriptor' dropdown menu, an 'Assessment factor' input field, and a 'Justification' dropdown menu. The 'Assessment factor' values are 10.0 for Freshwater, 100.0 for Freshwater, intermittent, 100.0 for Marine, and 1000.0 for Marine, intermittent. The 'Justification' for all categories is 'Default (PNEC calculator plug-in)'. At the bottom of the window, there is a footer with a help icon, the text 'PNEC calculator', and buttons for 'Edit', 'Print', 'Finish', and 'Cancel'.

# PNEC calculator



## Overview – how it works?

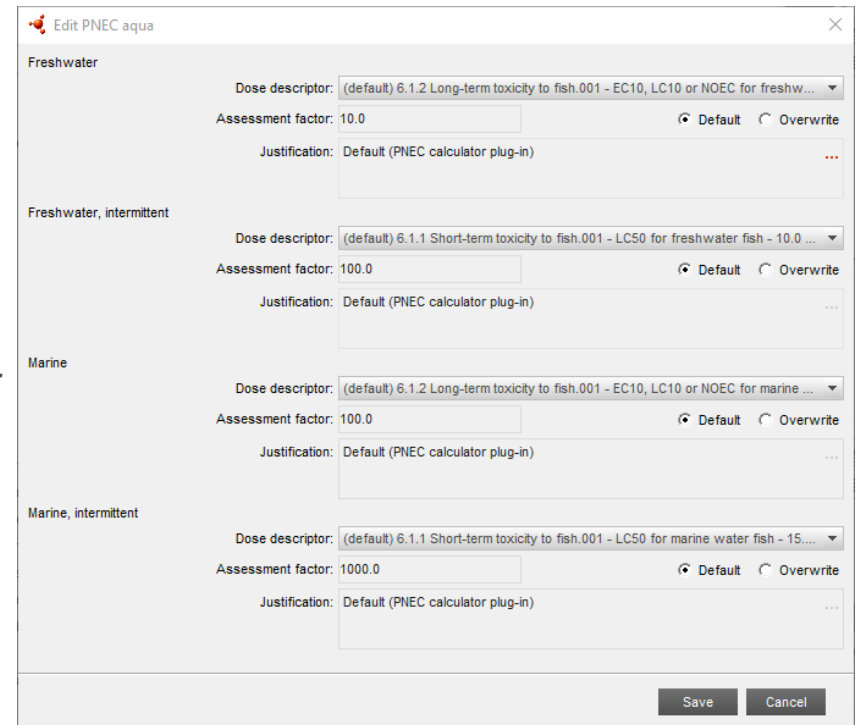
- Functionalities
  - **Edit button** enables an edit pop-up window.
  - **Print button** generates a report in a .rtf format containing the derived PNECs information as in section 7.5 of the CSR.
  - **Finish button** closes the calculator after saving the results in the corresponding endpoint summary under section '6 *Ecotoxicological information*'.
  - **Cancel button** closes the calculator without any further action.

The screenshot shows the PNEC calculator interface. At the top, there is a table with two columns: 'Environmental compartment' and 'PNEC Scenario'. The table lists four compartments: Aqua, Sediment, Soil, and Marine. The Aqua compartment is highlighted in yellow and has a sub-table with four rows: Freshwater (0.5 mg/L), Freshwater intermittent (0.1 mg/L), Marine (0.1 mg/L), and Marine intermittent (15.0 µg/L). The Sediment compartment has two rows: Freshwater (11.8 mg/kg sediment dw) and Marine (2.36 mg/kg sediment dw). The Soil compartment has one row: Soil (3 mg/kg soil dw).

Below the table, there are tabs for 'Aqua', 'Sediment', and 'Soil'. The 'Aqua' tab is selected, and it shows a list of compartments: 'Freshwater', 'Freshwater, intermittent', 'Marine', and 'Marine, intermittent'. Each compartment has a 'Dose descriptor' dropdown menu, an 'Assessment factor' input field, and a 'Justification' dropdown menu. The 'Freshwater' compartment has a dose descriptor of '(default) 6.1.2 Long-term toxicity to fish.001 - EC10, LC10 or NOEC for fres...', an assessment factor of 10.0, and a justification of 'Default (PNEC calculator plug-in)'. The 'Freshwater, intermittent' compartment has a dose descriptor of '(default) 6.1.1 Short-term toxicity to fish.001 - LC50 for freshwater fish - 1...', an assessment factor of 100.0, and a justification of 'Default (PNEC calculator plug-in)'. The 'Marine' compartment has a dose descriptor of '(default) 6.1.2 Long-term toxicity to fish.001 - EC10, LC10 or NOEC for mari...', an assessment factor of 100.0, and a justification of 'Default (PNEC calculator plug-in)'. The 'Marine, intermittent' compartment has a dose descriptor of '(default) 6.1.1 Short-term toxicity to fish.001 - LC50 for marine water fish - ...', an assessment factor of 1000.0, and a justification of 'Default (PNEC calculator plug-in)'. At the bottom of the interface, there are buttons for 'Edit', 'Print', 'Finish', and 'Cancel'.

## Overview – how it works?

- Edit mode
  - Allows the user to:
    - select a different dose descriptor as starting point,
    - use non-default assessment factors,
    - use another extrapolation method (for sediment and soil).
  - Any modification from default requires the user to provide a justification.



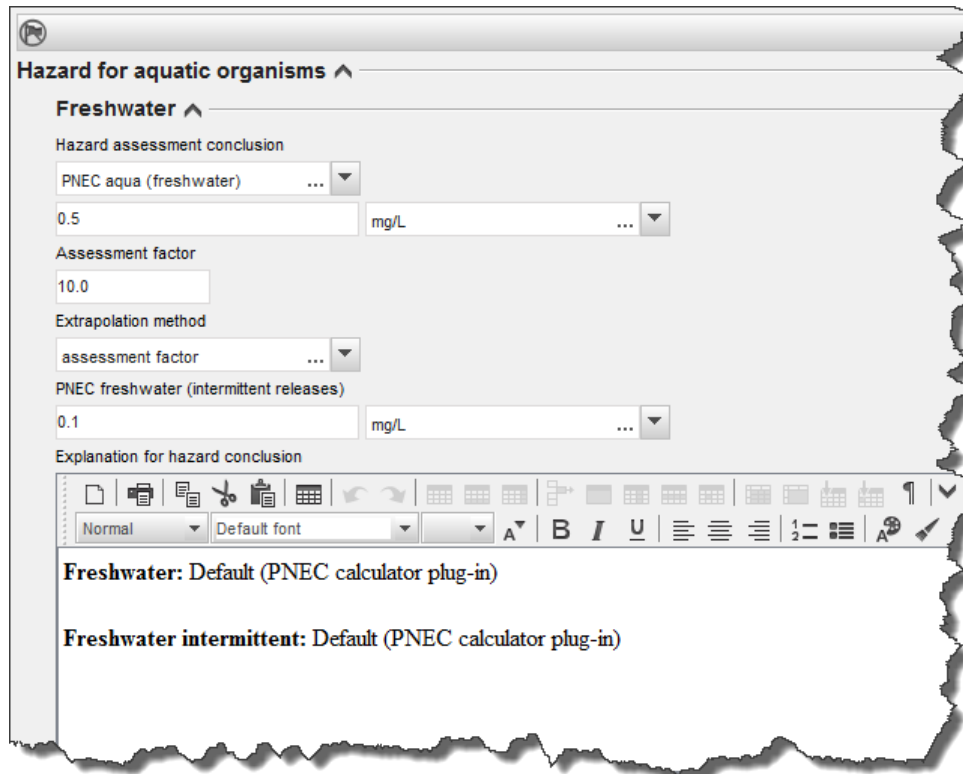
The screenshot shows the 'Edit PNEC aqua' dialog box with the following configuration:

Category	Dose descriptor	Assessment factor	Justification
Freshwater	(default) 6.1.2 Long-term toxicity to fish.001 - EC10, LC10 or NOEC for freshw...	10.0	Default (PNEC calculator plug-in)
Freshwater, intermittent	(default) 6.1.1 Short-term toxicity to fish.001 - LC50 for freshwater fish - 10.0 ...	100.0	Default (PNEC calculator plug-in)
Marine	(default) 6.1.2 Long-term toxicity to fish.001 - EC10, LC10 or NOEC for marine ...	100.0	Default (PNEC calculator plug-in)
Marine, intermittent	(default) 6.1.1 Short-term toxicity to fish.001 - LC50 for marine water fish - 15.0 ...	1000.0	Default (PNEC calculator plug-in)

Buttons: Save, Cancel

## Overview – how it works?

- Reporting in IUCLID
  - It is done in the corresponding endpoint summary under section ‘6 *Ecotoxicological information*’ from which the PNEC calculator was started.



The screenshot displays the PNEC calculator interface for freshwater. The main window is titled "Hazard for aquatic organisms" and is expanded to show "Freshwater". The "Hazard assessment conclusion" section includes a dropdown menu set to "PNEC aqua (freshwater)", a text input field containing "0.5", and a unit dropdown menu set to "mg/L". Below this, the "Assessment factor" is set to "10.0" in a text input field. The "Extrapolation method" is set to "assessment factor" in a dropdown menu. The "PNEC freshwater (intermittent releases)" section shows a text input field with "0.1" and a unit dropdown menu set to "mg/L". At the bottom, there is a text area for the "Explanation for hazard conclusion" with a rich text editor toolbar. The explanation text reads: "Freshwater: Default (PNEC calculator plug-in)" and "Freshwater intermittent: Default (PNEC calculator plug-in)".

# DNEL Calculator

Feedback from users



## Discrepancy between the standard respiratory volumes used by the DNEL calculator for the general population and the values in ECHA Guidance, Chapter R.8

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. For the latter, ECHA Guidance R.8 (version 2.1, November 2012) states on p. 10 that “*the body weights to be used in the calculations are 60 and 70 kg for the general population and for workers, respectively*”.

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.

## Discrepancy between the standard respiratory volumes used by the DNEL calculator for the general population and the values in ECHA Guidance, Chapter R.8

### Example:

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

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

- For workers (70 kg)

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

- For general population (60 kg)

$$\text{sRV}(\text{human}, 8\text{h}) = 6.7 / 60 \text{ kg} = 0.1117 \text{ m}^3/\text{kg bw}/8\text{h}$$

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

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

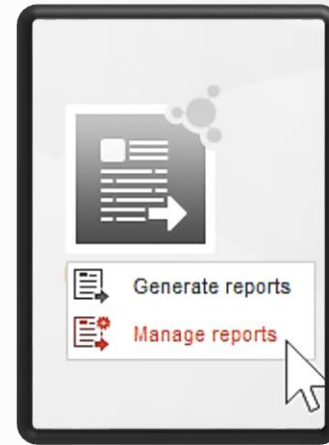
$$\text{sRV}(\text{rat}, 8\text{h}) = \text{sRV}(\text{human}, 8\text{h}) \times \text{allometric scaling factor} = 0.1117 \times 4 = 0.45 \text{ m}^3/\text{kg bw}/8\text{h} \text{ for general population}$$

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

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

# Report Generator

Mark Roberts



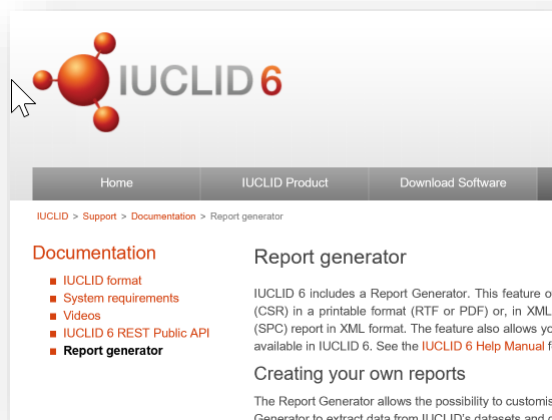


## The IUCLID Report Generator - what's new?

- Manage Reports (new feature of the report generator)



- New templates available to store in  **Manage reports** and use with the  **Report generator...**



### Report templates

#### Available report templates

Report template	Status
<a href="#">REACH Chemical Safety Report (CSR) - 2 May 2017</a>	Included in IUCLID 6
<a href="#">BPR Summary of Product Characteristics (SPC) - 27 October 2016</a>	Included in IUCLID 6
<a href="#">List of confidentiality claims in a BPR dossier - 2 May 2017</a>	<i>Under testing</i>
<a href="#">List of literature references - 2 May 2017</a>	<i>Under testing</i>
<a href="#">List of attachments</a>	<i>Under development</i>
<a href="#">List of annotations</a>	<i>Under development</i>

## Manage reports – what is it used for?

### The Manage reports feature allows you to:

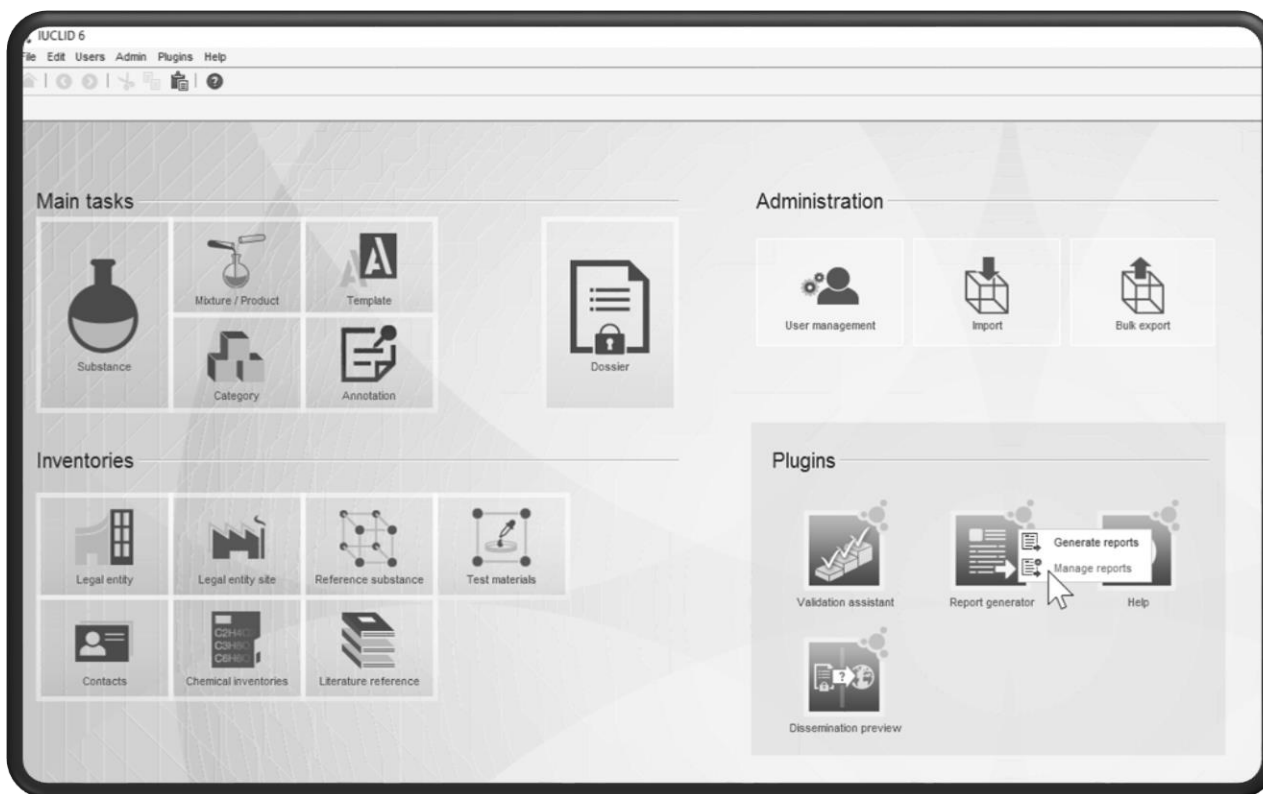
- **Upload and Store report templates in your own IUCLID installation and use these with the report generator**
- **Further customise your saved report:**
  - Select which outputs your report template supports, for example a TXT or DOC file,
  - Select the stylesheets you wish to have available to use with your report
  - Select if your report is applicable to Substances and/or Mixtures
  - Select what submission types the report is relevant for, for example, the BPR Biocidal Product Authorisation, a REACH Registration 10 to 100 tonnes etc.

# Report Generator



## How to store and further customise your report templates

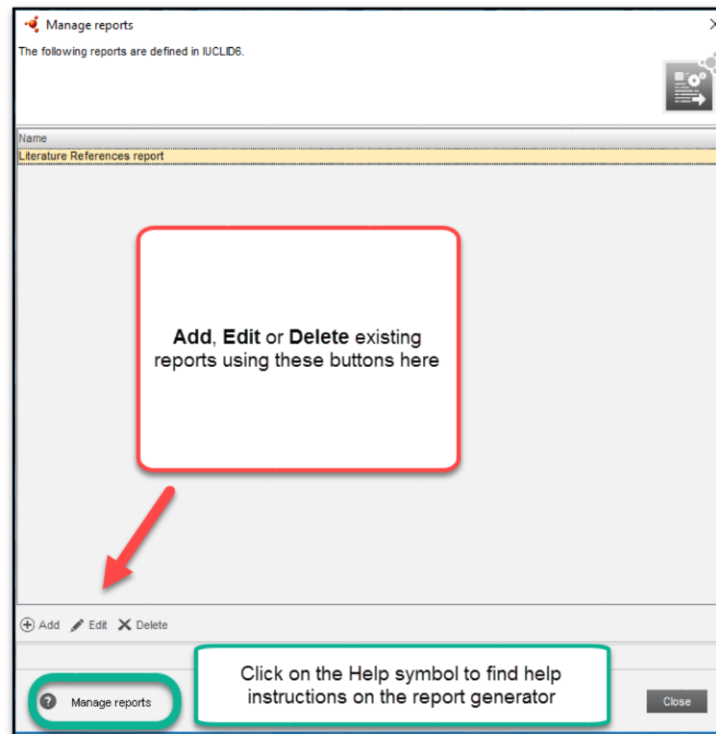
- Go to the IUCLID dashboard
- Left-click on the 'Report generator' icon
- Select 'Manage reports'



## How to store and further customise your report templates

A 'Manage reports' window is opened allowing you to:

- Add a report
- Edit a report
- Delete a report



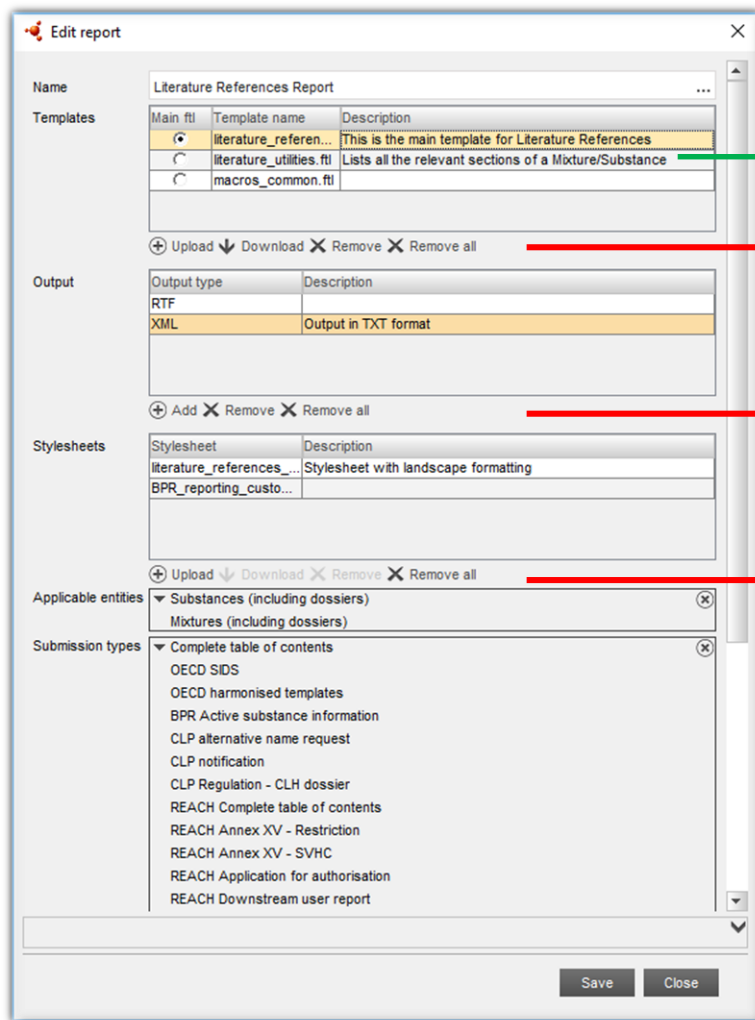
## How to store and further customise your report templates

When adding a report, fill out the following information to further customise your report

- **Name** (Mandatory field): a recognisable name which you want to give to your report
- **Templates** (Mandatory field): upload here the relevant report templates
- **Output** (Mandatory field): select one or more output types which the report can be generated with
- **Stylesheets**: upload one or more stylesheets which the report can use to modify the report layout
- **Applicable entities**: select whether your report is applicable to a Substance (used for REACH and the Biocidal Products Regulation) and/or Mixture (used for the Biocidal Products Regulation)
- **Submission types**: select which submission types are relevant for your report, for example, REACH Registration 10-100 tonnes

# Report Generator

## Editing or adding your report templates

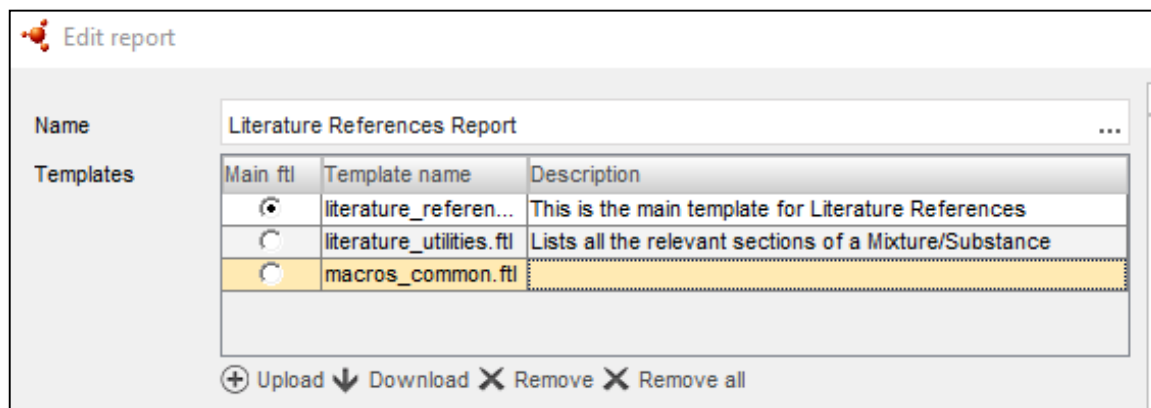


Make short comments about your uploaded files

Upload, download and remove your files

## Editing or adding your report templates

A 'Main template' is uploaded and is indicated by the marked checkbox in column 'Main.ftl'.



Additional templates are usually uploaded alongside the Main template to help shorten the length and complexity of the Main template or to re-use code which is repeatedly used by the Main template, saving time for the person writing the template and reducing the risk of errors when generating the report.

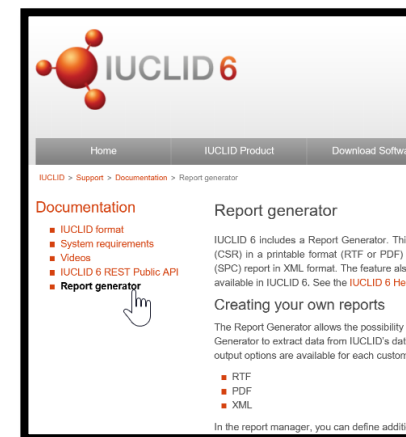
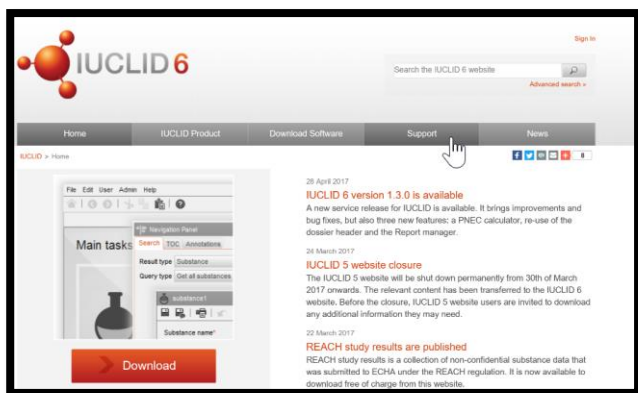
For example, a 'utilities' template in the example above lists all the relevant sections in a Substance and Mixture which I wish the Main template to include in the report.

# Report Generator



## Downloading reports from the IUCLID 6 website

For this release of IUCLID 6, we have published some report templates which you can store and use with the Report generator.



Report template	Status
REACH Chemical Safety Report (CSR) - 2 May 2017	Included in IUCLID 6
BPR Summary of Product Characteristics (SPC) - 27 October 2016	Included in IUCLID 6
List of confidentiality claims in a BPR dossier - 2 May 2017	Under testing
List of literature references - 2 May 2017	Under testing
List of attachments	Under development
List of annotations	Under development

You can re-use any of these reports to create and modify your own report templates



# Report Generator



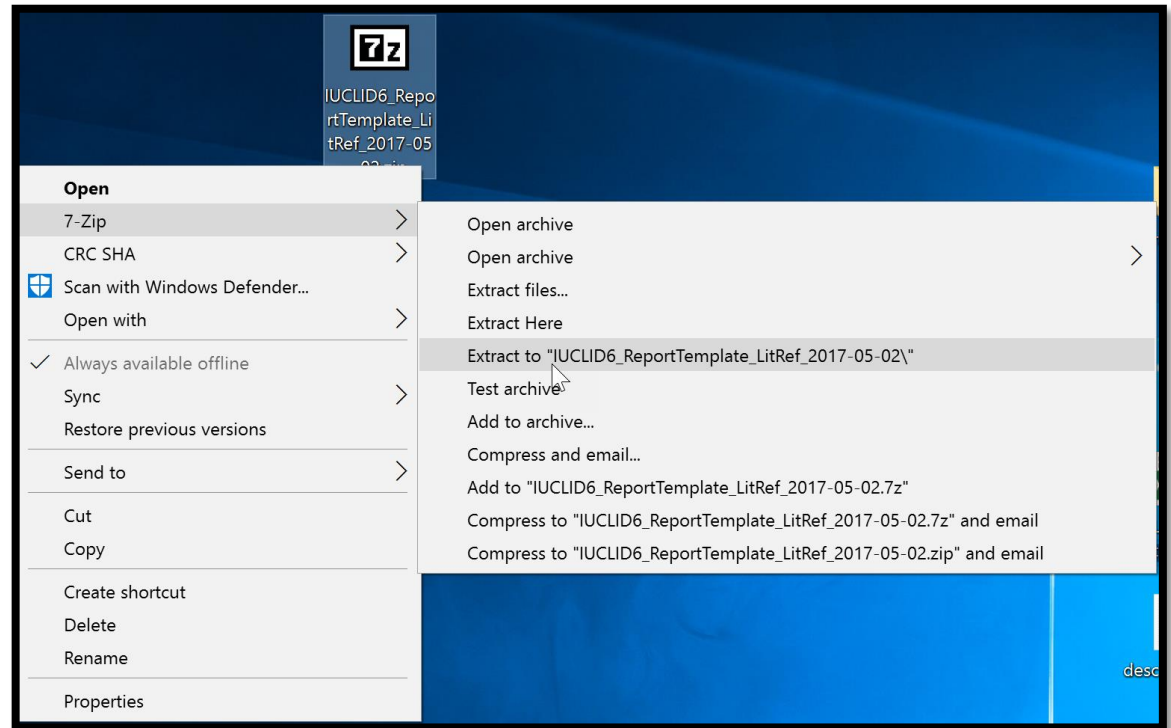
## Downloading reports from the IUCLID 6 website

Click on the report you wish to download and 'Save as'.

A Zip file will be saved in the Directory where you have chosen to save the file.

Extract the Zip folder like so:

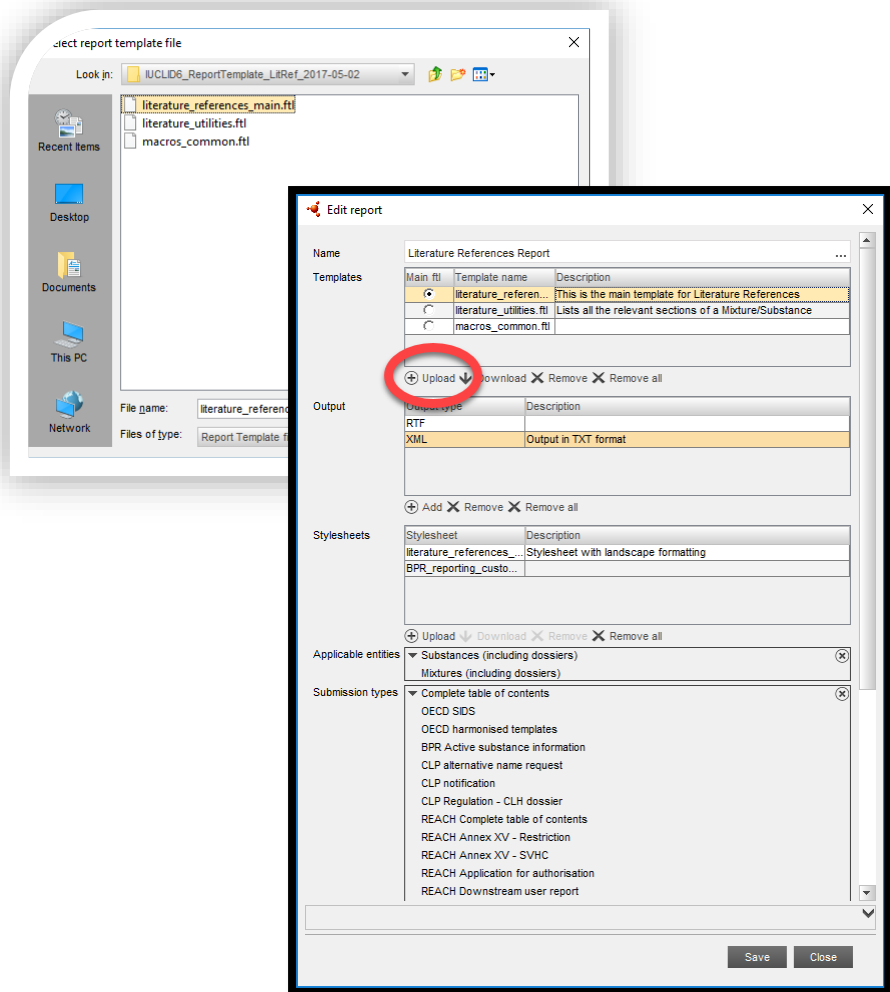
You then have a folder from which you can upload your report templates



# Report Generator



## Downloading reports from the IUCLID 6 website



Now I can add a report and upload my templates into the Manage reports tool

How you choose to customise the report will be reflected in the options presented to you when generating the report

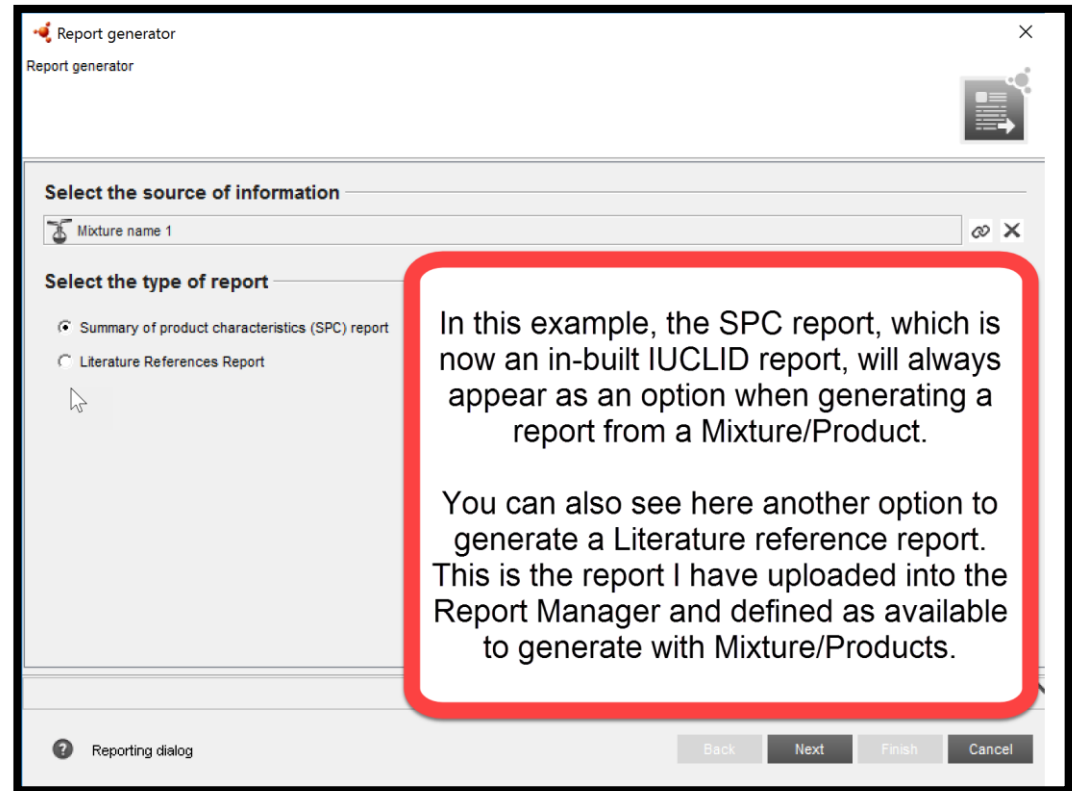
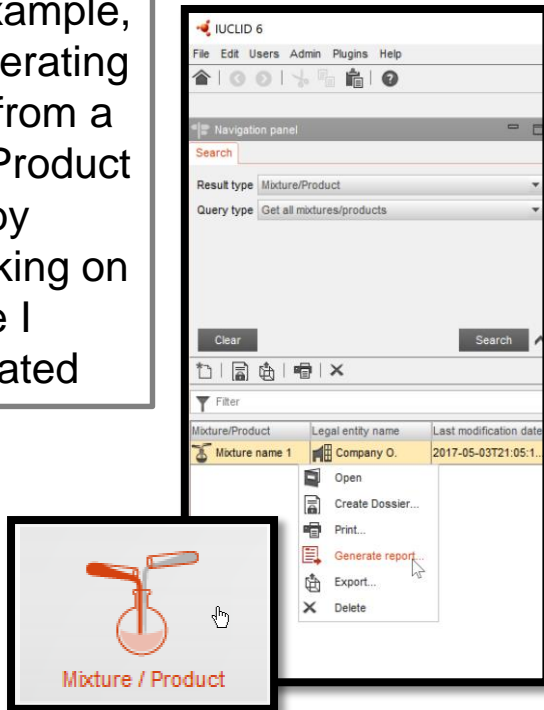
# Report Generator



Generating a report – how does it look like?

**Generate a report as usual from a dataset or dossier**

In this example, I am generating a report from a Mixture/Product dataset by right-clicking on a Mixture I have created



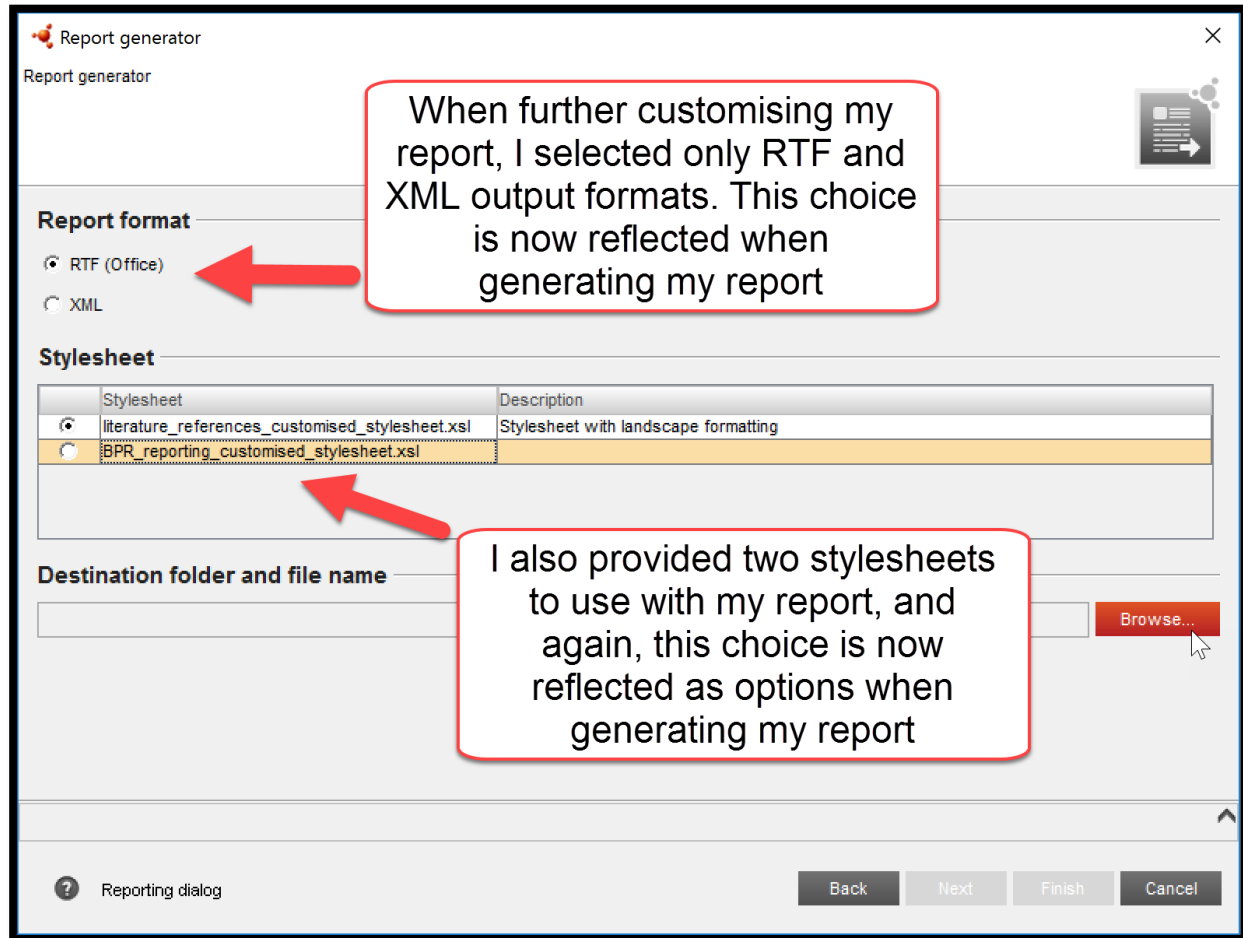
**First step of the Report generator wizard**

# Report Generator

## Generating a report – how does it look like?

Second and final step of the Report generator wizard

When you have selected the desirable options, choose where you wish to save your report, as normal



Report generator

Report generator

**Report format**

RTF (Office)

XML

**Stylesheet**

Stylesheet	Description
<input checked="" type="radio"/> literature_references_customised_stylesheet.xsl	Stylesheet with landscape formatting
<input type="radio"/> BPR_reporting_customised_stylesheet.xsl	

**Destination folder and file name**

Browse...

Reporting dialog

Back Next Finish Cancel

When further customising my report, I selected only RTF and XML output formats. This choice is now reflected when generating my report

I also provided two stylesheets to use with my report, and again, this choice is now reflected as options when generating my report

# Report Generator

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## Relevant links

IUCLID 6 webpage: <https://iuclid6.echa.europa.eu/>

IUCLID 6 Report generator webpage: <https://iuclid6.echa.europa.eu/reports>

FreeMarker help: <http://freemarker.org/docs/index.html>

DocBook help: <http://tdg.docbook.org/tdg/5.2/ch01.html>

# IUCLID Cloud Services

Tommy Hägg



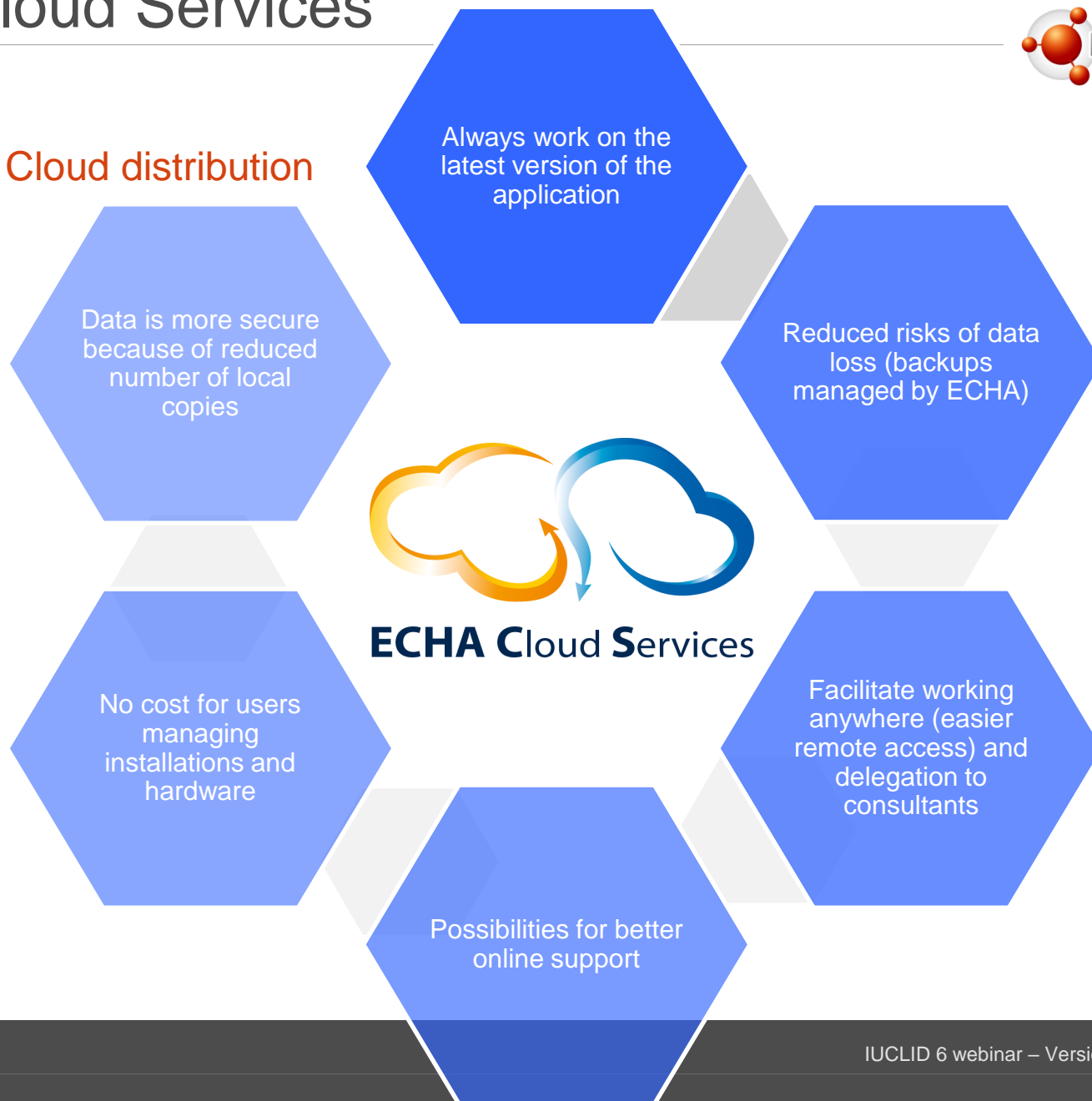
**ECHA** Cloud **S**ervices



## ECHA Cloud Services

- New, simpler way of distributing IT applications
- We manage the application for you
- Secure private cloud where only you have access to your data
- Access with the same user account you use for REACH-IT
- The first services launched focus on IUCLID 6 and the functionalities are prioritised for the needs of small and medium-size enterprises (SMEs)
- Start from <https://ecs.echa.europa.eu> and login with your ECHA Account

## Benefits with Cloud distribution





## IUCLID Cloud for SMEs

The logo for IUCLID 6 SME, featuring a stylized molecular structure with three orange spheres and a white sphere, followed by the text "IUCLID 6" in a bold, sans-serif font, and "SME" in a smaller font below it, all enclosed in a rounded rectangular border.

- To be released in summer 2017
- Trial release available already now. New features will be added on monthly bases
- Aimed for SMEs to prepare registration dossiers for REACH 2018 deadline
- Works fully in a web browser
- No need to install anything locally
- You can allow others to access your IUCLID database with their own ECHA accounts

# Questions and answers

*Please continue to send your questions for the next 5 minutes, using the Q&A panel*



# Questions and answers



## News and next events

- Roadmap 2018 Spring school

2017

› **REACH 2018 Spring School - Day 5: Submit your registration**

19 May 2017

11:00 - 15:00 EET, GMT +2

› **REACH 2018 Spring School - Day 4: Prepare your registration as a IUCLID dossier**

18 May 2017

11:00 - 13:30 EET, GMT +2

› **REACH 2018 Spring School - Day 3: Getting your chemical safety assessment done**

17 May 2017

11:00 - 13:30 EET, GMT +2

› **REACH 2018 Spring School - Day 2: Get organised with co-registrants and assess hazards and risks**

16 May 2017

11:00 - 15:30 EET, GMT +2

› **REACH 2018 Spring School - Day 1: Know your portfolio and find your co-registrants**

15 May 2017

11:00 - 15:30 EET, GMT +2

## News and next events

- Video tutorials
  - In the context of the 2018 roadmap
  - Series of video tutorials on IUCLID functions
  - Four videos will be available for the Spring School in May
    - How to **install** IUCLID 6 Desktop
    - How to run the **Validation assistant** in IUCLID 6
    - How to **update** IUCLID 6 Desktop
    - How to **backup** and restore IUCLID 6

## News and next events

- **LinkedIn** group

<https://www.linkedin.com/groups/12043483>

- Platform to exchange, discuss and provide feedback on the use of IUCLID and on future evolutions of the product
- Join now to be involved in the development of our database



# Future updates



## Planned releases

- More information on the planned IUCLID 6 releases can be found on the IUCLID 6 website
- <https://iuclid6.echa.europa.eu/project-iuclid-6#ServiceRelease>

The screenshot shows the IUCLID 6 website interface. At the top left is the IUCLID 6 logo. To the right is a search bar with the text "Search the IUCLID 6 website" and a magnifying glass icon. Below the search bar is a navigation menu with links for "Home", "IUCLID Product", "Download Software", "Support", and "News". In the top right corner, there is a "Sign In" link and a social media sharing bar with icons for Facebook, Twitter, LinkedIn, and a share icon, along with a "5" notification badge.

The main content area is titled "IUCLID Product" and contains a sub-section "IUCLID 6 maintenance and service releases". The text below this section states: "After the release of IUCLID 6 to the public, service and maintenance releases are prepared in order to fix reported issues and to provide improvements and new features requested by the users. Under this section the current planning and scope for the future releases are made available for information only and are subject to change (updated on 5 September 2016)."

The planned releases are listed as follows:

- 21<sup>st</sup> June 2016 (maintenance release)
  - Compatibility with Chesar 3
  - Performance improvements for performance issues detected in dossier creation
- October 2016 (maintenance release (v. 4), can include for example:
  - Other user requirements currently not prioritised
    - LDAP connectivity
    - Spell checker
    - Attachments versioning
    - Announcements for IUCLID system administrators
    - Link to email server (e.g. for resetting passwords)



*Thank you for your participation*

[echa.eu](http://echa.eu)

[iuclid6.echa.europa.eu](http://iuclid6.echa.europa.eu)

[oecd.org/ehs/templates](http://oecd.org/ehs/templates)



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

