



IUCLID 6



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





REACH Stakeholder's IT Tools training

30 January 2018



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Chemicals Agency in association with the OECD



Introduction to IUCLID



What is IUCLID? A multi-purpose tool



International Uniform Chemical Information Database

- A key application to **prepare**, **store** and **exchange data** on chemicals in a harmonised format.
- REACH Article 111: a dossier must be in IUCLID format and ECHA should work with the OECD towards the **maximum harmonisation** of the IUCLID data format

IUCLID is used by regulatory authorities and the chemical industry to fulfil their respective obligations under the REACH, CLP and the BPR regulations

Article 111

Formats and software for submission of information to the Agency

The Agency shall specify formats and make them available free of charge, and software packages and make them available on its website for any submissions to the Agency. Member States, manufacturers, importers, distributors or downstream users shall use these formats and packages in their submissions to the Agency pursuant to this Regulation. In particular, the Agency shall make available software tools to facilitate the submission of all information relating to substances registered in accordance with Article 12(1).

For the purposes of registration, the format of the technical dossier referred to in Article 10(a) shall be IUCLID. The Agency shall coordinate the further development of this format with the Organisation for Economic Cooperation and Development to ensure maximum harmonisation.

From where IUCLID 6 is downloaded?



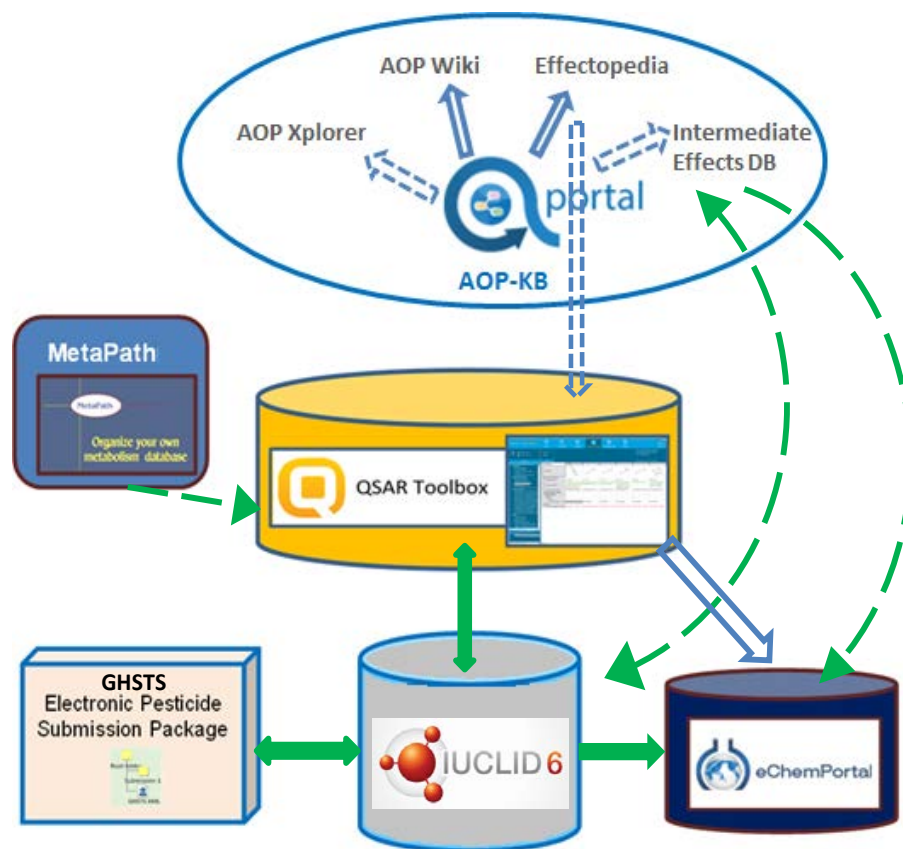
International cooperation

Organisation for Economic Co-operation and Development (OECD)

A global outreach

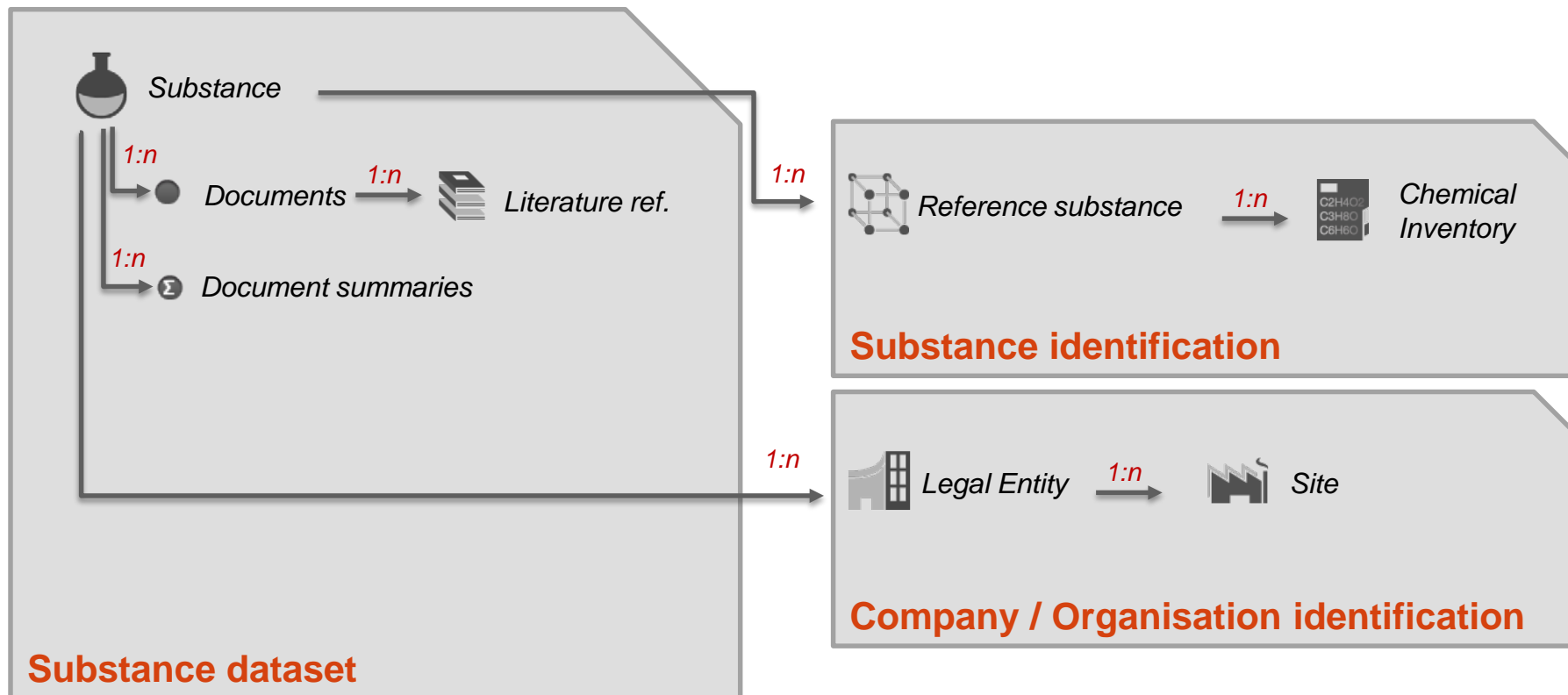


OECD 4



IUCLID entities (type of information)

Main entities and relationships (Substance)



 Attachments can be added to all entities and documents

 Annotations can be linked to all entities and documents

Information managed in IUCLID



- Substance identity

- Substance identification
- Composition(s)

+ 0 Related information

- 1 General information

1.1 Identification

+ 1.2 Composition

+ 1.3 Identifiers

+ 1.4 Analytical information

- Classification and Labelling

+ 2 Classification & Labelling and PBT assessment

- Use and exposure

- 3 Manufacture, use and exposure

+ 3.1 Technological process

+ 3.2 Estimated quantities

+ 3.3 Sites

+ 3.4 Information on mixtures

+ 3.5 Life Cycle description

+ 3.6 Uses advised against

+ 3.7 Exposure Scenarios, exposure and risk assessment

- Study and endpoint summaries

+ 4 Physical and chemical properties

+ 5 Environmental fate and pathways

+ 6 Ecotoxicological information

+ 7 Toxicological information

+ 8 Analytical methods

- Assessment reports

+ 11 Guidance on safe use

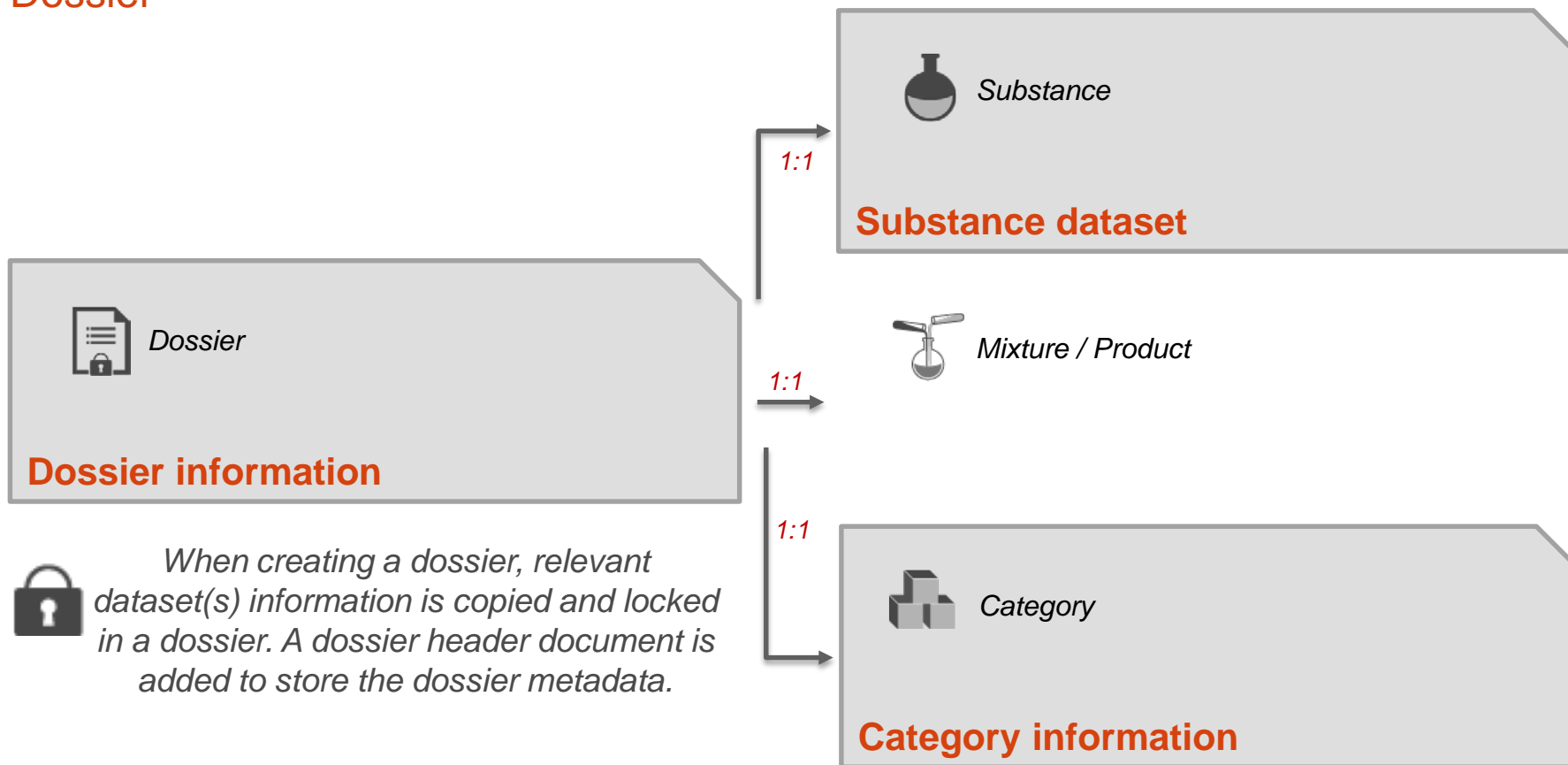
+ 12 Literature search

- 13 Assessment reports

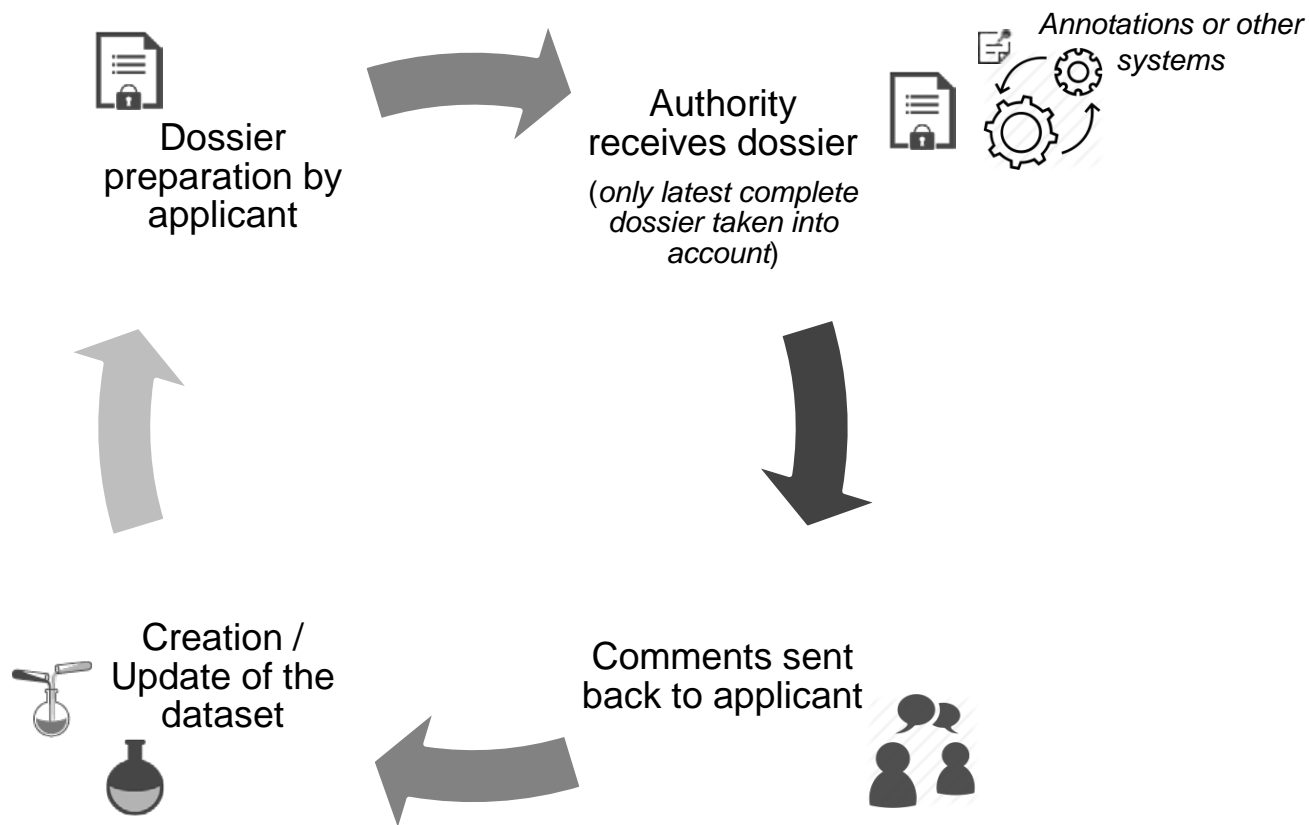
● Assessment reports.001

IUCLID entities (type of information)

Dossier



ECHA's approach



IUCLID 6 standard user interface



Main screen

The screenshot shows the IUCLID 6 main screen with three numbered callouts:

- 1. Navigation panel:** Located on the left, it includes a search bar, filters for result and query types, a search button, and a table of search results.
- 2. Data view and entry:** Located in the top right, it displays the details for a selected substance, including fields for substance name, public name, legal entity flags, legal entity, and third party flags.
- 3. Information panel:** Located at the bottom right, it provides additional information about the selected substance, including a list of categories.

Chemical name	Legal entity name	Reference subst.	Last modification
substance_1	user_manual	butanone / butan-2-one / 78-93-3 / 201-159-0	2016-06-26T18:2...
substance_2	legal_entity_two	potassium chloride / potassium chloride / 7447-40-7 / 231-211-6	2016-06-26T18:2...
substance_one	user_manual		2016-06-30T18:1...

1. Navigation panel
2. Data view and entry
3. Information panel

IUCLID: 3 ways to create a registration dossier



REACH-IT Online

- For members of joint submissions only
- Agree with all information submitted on your behalf by the lead registrant
- The simplified dossier creation wizard in REACH-IT guides you through this process by showing you which data you need to provide



IUCLID Cloud for SMEs

- Simplified web version of IUCLID for SME companies
- Maintained, backed-up, updated and hosted for free by ECHA
- Build all different REACH dossiers
- Easy access of data by company and consultant
- Logical choice for SMEs



IUCLID 6 Download

- For large companies
- Full set of functionalities for data management
- Installed and maintained locally by users
- Desktop version easy to install
- Server version available for multi-user companies



Questions and Answers

- Questions have been received during the event
- They will be covered during this session
- Please ask the most important questions now



- IUCLID user interface and Help
- Reporting data in IUCLID
 - Dynamic content validation*
 - Substance identity
 - Read across
 - Waivers
 - PNEC calculator*
 - DNEL calculator*
 - Opt-out
 - Changes between IUCLID 5 and IUCLID 6
- IUCLID features
 - Validation assistant
 - Print*
 - Report generator* / CSR
 - Fee calculator*
 - Dissemination preview
 - Dossiers comparison*
 - Inventory management*
 - IUCLID versions compatibility
 - Integration with other tools
- Where to find more information

** Only in IUCLID 6 Desktop and Server*

IUCLID user interface and Help



File Edit User

Search by UUID

Main tasks

- Substance
- Mixture / Product
- Template
- Category
- Annotation
- Dossier

Create new or modify your existing substances here

Create a template to reuse same endpoint data in different datasets.

View your dossiers

Administration

- My account
- Import
- Bulk export

Import files: LE, substance datasets, reference substances

Inventories

- Legal entity
- Legal entity site
- Reference substance
- Contacts
- Chemical inventories
- Literature reference

Store chemical information on particular chemicals once in the database and link it from there to any IUCLID section.

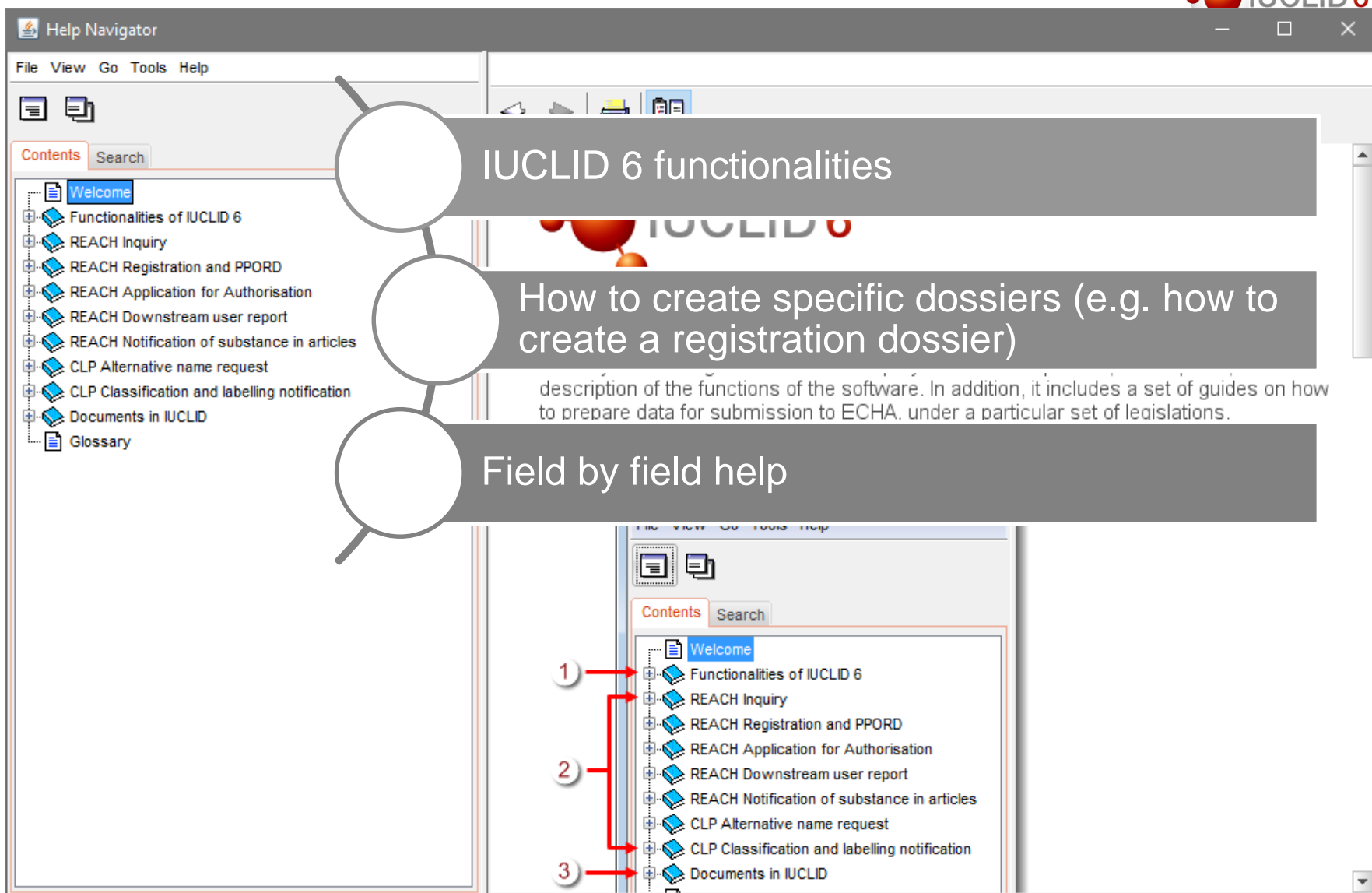
Validate the substance datasets and also the final dossiers in order to minimize the risk for errors

Plugins

- Validation assistant
- Dissemination preview
- Fee calculator
- Help

View what information will be published on the ECHA website

Embedded Help System (press F1)



The screenshot shows the 'Help Navigator' window with a menu bar (File, View, Go, Tools, Help) and a toolbar. The 'Contents' tab is active, displaying a tree view of help topics. Three callouts are overlaid on the window:

- IUCLID 6 functionalities**: A callout pointing to the 'Functionalities of IUCLID 6' item in the tree.
- How to create specific dossiers (e.g. how to create a registration dossier)**: A callout pointing to the 'REACH Registration and PPORD' item in the tree.
- Field by field help**: A callout pointing to the 'Documents in IUCLID' item in the tree.

The main content area shows a preview of the 'Functionalities of IUCLID 6' page, featuring the IUCLID 6 logo and a description of the software's functions and guides.

description of the functions of the software. In addition, it includes a set of guides on how to prepare data for submission to ECHA, under a particular set of legislations.

The bottom part of the image shows a zoomed-in view of the 'Contents' list with three red arrows and numbered circles (1, 2, 3) pointing to the following items:

1. Functionalities of IUCLID 6
2. REACH Inquiry
3. Documents in IUCLID

Embedded Help System (F1)

A screenshot of the IUCLID 6 Help Navigator application. The window is titled "Help Navigator" and has a menu bar with "File", "View", "Go", "Tools", and "Help". Below the menu bar are icons for a list and a document. The main area is split into two panes. The left pane, titled "Contents", shows a hierarchical table of contents. The right pane displays a manual page with a blue header "MANUAL" and the main title "How to prepare registration and PPORD dossiers".

Help Navigator

File View Go Tools Help

Contents Search

- Welcome
- Functionalities of IUCLID 6
- REACH Inquiry
 - REACH Registration and PPORD
 - Changes to this document
 - Table of Contents
 - Table of Figures
 - Table of Tables
 - 1. Introduction
 - 2. Legal entity
 - 3. Legal entity site
 - 4. Contact
 - 5. Chemical inventories
 - 6. Reference substance
 - 7. Literature reference
 - 8. Test material
 - 9. How to create a Substance dataset
 - 10. How to create a Dossier
 - 11. How to export a Dossier
 - 12. Submit Dossier
 - 13. Update Dossier
 - Annex 1. Overview of the business rules checks per
 - Annex 2. Overview of the completeness check perfc
 - Annex 3. Overview of endpoints and information req
 - Annex 4. Minimum information required for updating a
 - Annex 5. The assessment entity in IUCLID
 - Annex 6. Overview of tonnage fields in IUCLID

MANUAL

How to prepare registration and PPORD dossiers

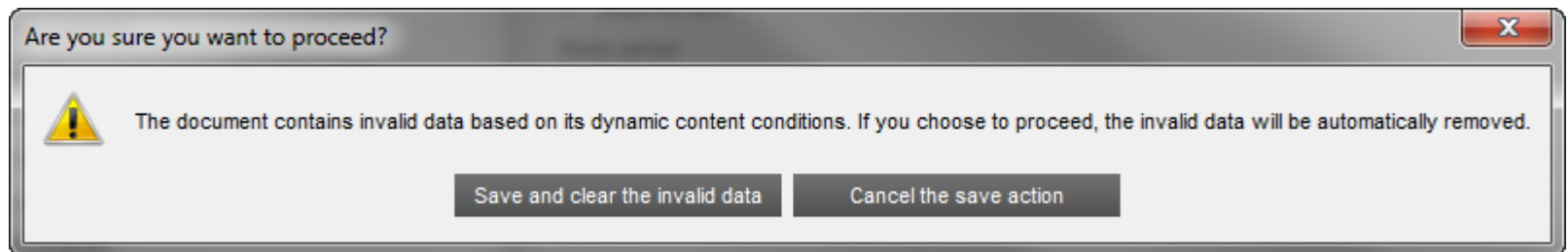
Reporting data in IUCLID

Dynamic content validation



Dynamic content validation (1)

- **What?**
 - When the user makes selections in a field that is subject to dynamic content validation, this causes the incompatible fields to become inactive
- **Why?**
 - To support the user in not entering conflicting information in the application.
- **How?**
 - When the user makes selections in a field that is subject to dynamic content validation, the incompatible fields become inactive
 - If the document was migrated from IUCLID 5 and already contains incompatible information, the conflicting content is shown highlighted in orange. If the user tries to save the document, an information message is displayed. The conflicting information must be corrected before saving is allowed.



Dynamic content validation (2)

- **Where?**
- Section 2.1 – GHS:
 - The field ‘Reason for no classification’ is inactive if any of the fields ‘Hazard category’ and ‘Hazard statement’ are filled in, and vice versa.
 - Already in IUCLID 5

Health hazards

	Hazard category	Hazard statement	Reason for no classification
Acute toxicity - oral	<input type="text"/>	<input type="text"/>	data lacking
Acute toxicity - dermal	<input type="text"/>	<input type="text"/>	data lacking
Acute toxicity - inhalation	<input type="text"/>	<input type="text"/>	data lacking
Skin corrosion/irritation	<input type="text"/>	<input type="text"/>	data lacking
Serious eye damage/ eye irritation	Eye Irrit. 2	H320: Causes eye i	

IUCLID 5

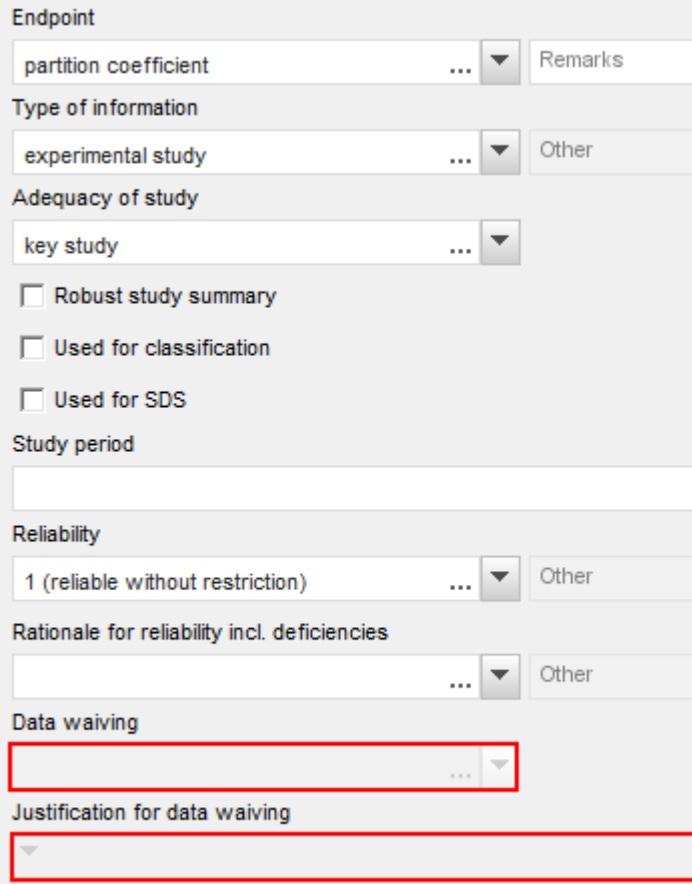
Health hazards ^

	Hazard category	Hazard statement	Reason for no classification
Acute toxicity - oral	data lacking ...
Acute toxicity - dermal	data lacking ...
Acute toxicity - inhalation	data lacking ...
Skin corrosion / irritation	data lacking ...
Serious eye damage / eye irrit...	Eye Irrit. 2	H320: Causes eye irrita...	...

IUCLID 6

Dynamic content validation (3)

- **Where?**
- Endpoint study record – Administrative data:
 - When a new endpoint study record is created, and is indicated as a study, the fields that are relevant for reporting a data waiving are not available, and vice versa



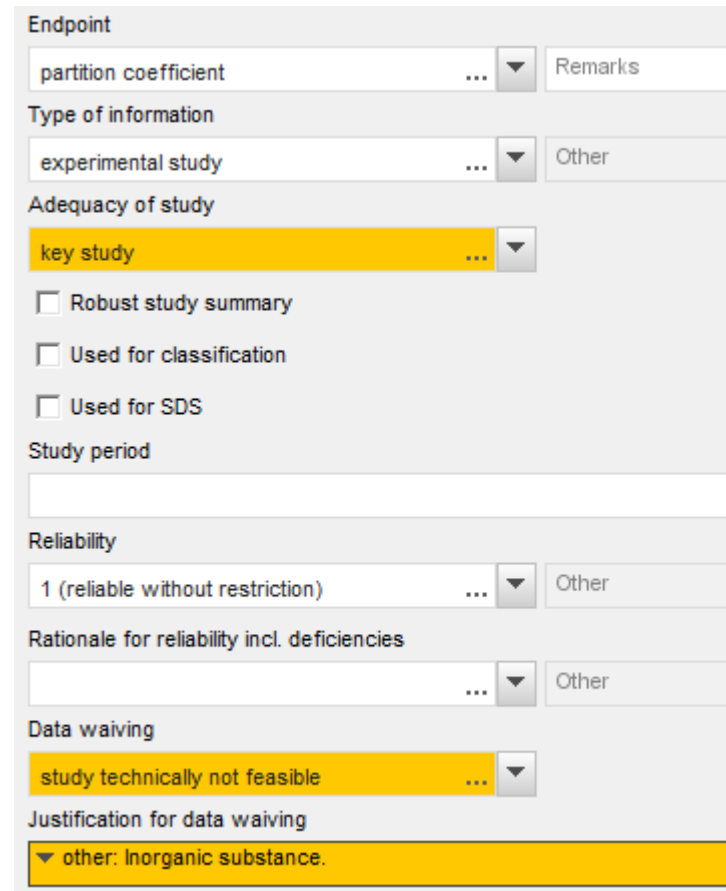
The screenshot shows the 'Endpoint' form in IUCLID 6. The form is divided into several sections:

- Endpoint:** A dropdown menu with 'partition coefficient' selected and a 'Remarks' field.
- Type of information:** A dropdown menu with 'experimental study' selected and an 'Other' field.
- Adequacy of study:** A dropdown menu with 'key study' selected and three checkboxes: 'Robust study summary', 'Used for classification', and 'Used for SDS', all of which are unchecked.
- Study period:** An empty text input field.
- Reliability:** A dropdown menu with '1 (reliable without restriction)' selected and an 'Other' field.
- Rationale for reliability incl. deficiencies:** An empty text input field and an 'Other' field.
- Data waiving:** A dropdown menu with a red box around it.
- Justification for data waiving:** A text input field with a red box around it.

IUCLID 6: Section 4.7, new endpoint study record

Dynamic content validation (4)

- **Where?**
- Endpoint study record – Administrative data:
 - When an endpoint study record has been migrated from IUCLID 5 and contains conflicting information in fields with dynamic content validation, the fields that contain inconsistent information are highlighted in orange.
 - The conflicting information needs to be amended before saving of new information is possible in this document.

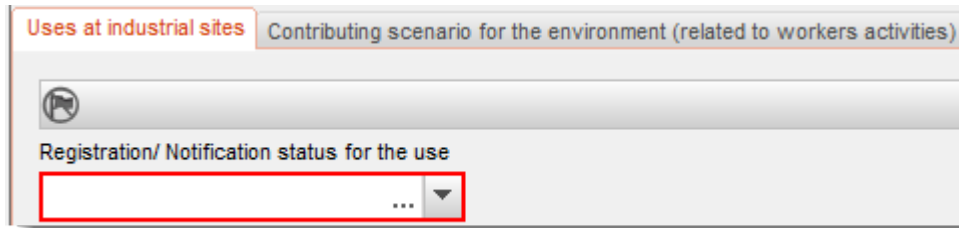


Endpoint	partition coefficient	Remarks
Type of information	experimental study	Other
Adequacy of study	key study	
	<input type="checkbox"/> Robust study summary	
	<input type="checkbox"/> Used for classification	
	<input type="checkbox"/> Used for SDS	
Study period		
Reliability	1 (reliable without restriction)	Other
Rationale for reliability incl. deficiencies		Other
Data waiving	study technically not feasible	
Justification for data waiving	other: Inorganic substance.	

IUCLID 6: Section 4.7, migrated endpoint study record

Dynamic content validation (5)

- **Where?**
- Section 3.5.X – Use and exposure information:
 - The field ‘Registration/notification status for the use’ conditions the availability of the fields in each use record.

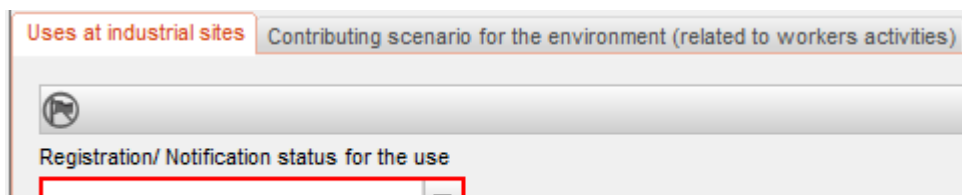


The screenshot shows a software interface with two tabs at the top: 'Uses at industrial sites' (selected) and 'Contributing scenario for the environment (related to workers activities)'. Below the tabs is a grey header bar with a flag icon. Underneath, the text 'Registration/ Notification status for the use' is displayed above a dropdown menu. The dropdown menu is currently empty and has a red border around it.

*IUCLID 6: Section 3.5.3 –
Uses at industrial sites*

Dynamic content validation (6)

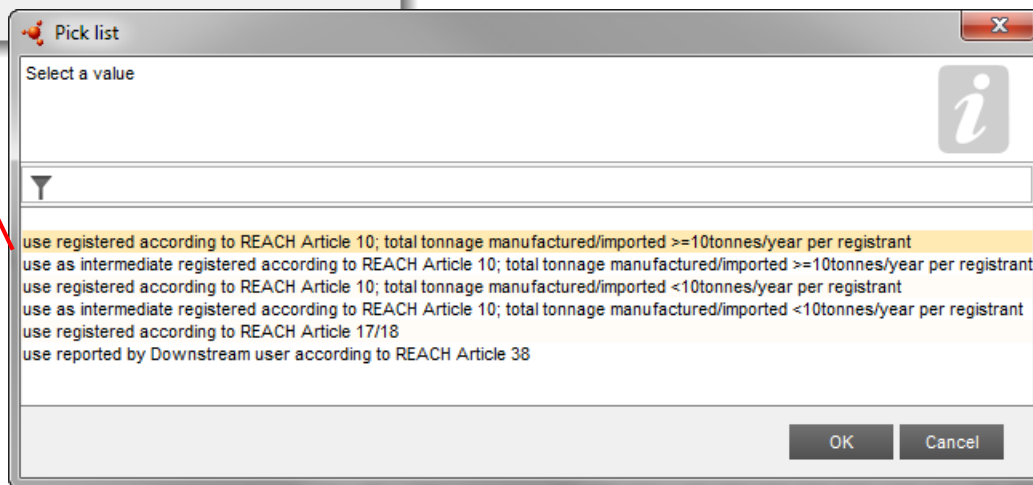
- **Where?**
- Section 3.5.X – Use and exposure information:
 - The field ‘Registration/notification status for the use’ conditions the availability of the fields in each use record.



Uses at industrial sites Contributing scenario for the environment (related to workers activities)

Registration/ Notification status for the use

*IUCLID 6: Section 3.5.3 –
Uses at industrial sites*



Pick list

Select a value

use registered according to REACH Article 10; total tonnage manufactured/imported >=10tonnes/year per registrant

use as intermediate registered according to REACH Article 10; total tonnage manufactured/imported >=10tonnes/year per registrant

use registered according to REACH Article 10; total tonnage manufactured/imported <10tonnes/year per registrant

use as intermediate registered according to REACH Article 10; total tonnage manufactured/imported <10tonnes/year per registrant

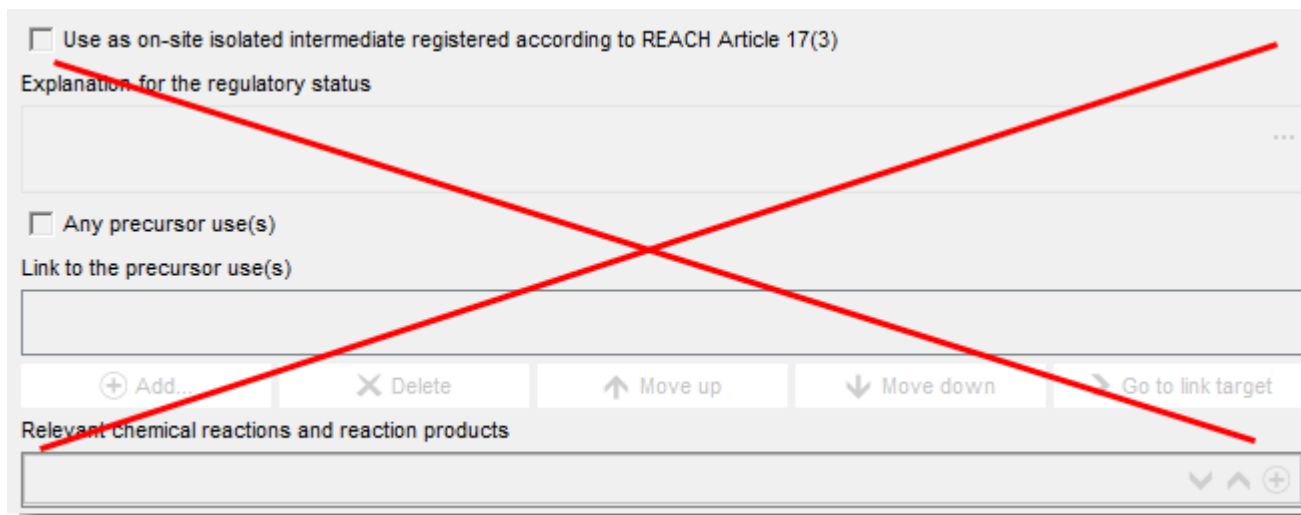
use registered according to REACH Article 17/18

use reported by Downstream user according to REACH Article 38

OK Cancel

Dynamic content validation (7)

- **Where?**
- Section 3.5.3 – Uses at industrial sites:
 - **use registered according to REACH Article 10; total tonnage manufactured/imported ≥ 10 tonnes/year per registrant.**
 - Fields for reporting information on intermediates are inactive



Use as on-site isolated intermediate registered according to REACH Article 17(3)

Explanation for the regulatory status

Any precursor use(s)

Link to the precursor use(s)

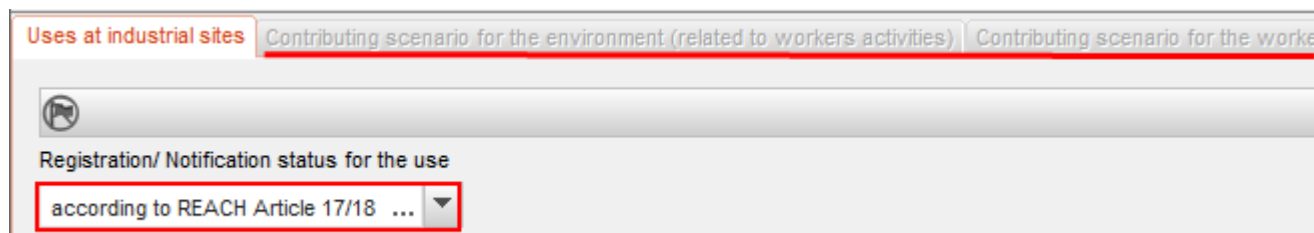
+ Add... X Delete ↑ Move up ↓ Move down → Go to link target

Relevant chemical reactions and reaction products

IUCLID 6: Section 3.5.3 – Uses at industrial sites

Dynamic content validation (8)

- **Where?**
- Section 3.5.3 – Uses at industrial sites:
 - **use registered according to REACH Article 17/18.**
 - Tabs for reporting contributing scenarios for workers and the environment are inactive
 - Fields for reporting information on intermediates are active

A screenshot of the IUCLID 6 software interface. At the top, there are three tabs: 'Uses at industrial sites' (highlighted in red), 'Contributing scenario for the environment (related to workers activities)', and 'Contributing scenario for the worke'. Below the tabs is a grey bar with a lock icon and the text 'Registration/ Notification status for the use'. A dropdown menu is open, showing the selected option 'according to REACH Article 17/18 ...' with a downward arrow.

IUCLID 6: Section 3.5.3 – Uses at industrial sites

Reporting data in IUCLID

Substance Identity



Tips based on experience – Substance ID



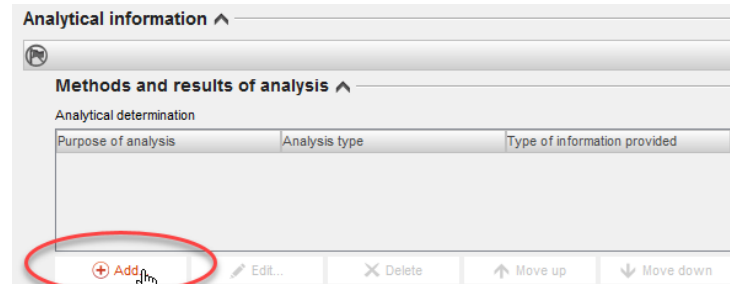
- IUCLID section 1.4 'Analytical Information'
 - 'Identification' and 'Quantification' should be provided with attachment in 'Analytical determination' table

The screenshot displays the IUCLID software interface. On the left, a navigation pane shows a tree structure of sections, with '1.4 Analytical Information' highlighted in red. The main window shows the 'Analytical information' section, which is expanded to show 'Methods and results of analysis'. This section contains a table with the following columns: 'Purpose of analysis', 'Analysis type', 'Type of information provided', 'Attached method(s)', 'Substance to be tested', 'Last location', and 'Remarks'. Below the table, there are buttons for 'Add', 'Edit', 'Delete', 'Print all', and 'Print sheet'. The 'Add' button is highlighted with a red box. Below the table, there is a section for 'Optical activity' and 'Remarks'. At the bottom of the window, there is an 'Information area' showing details for the substance, including 'Type: Particle flaked', 'UID: 9387395-3c7e-3e64-891e-2d60c4932199', and 'Dossier ID: 101'.

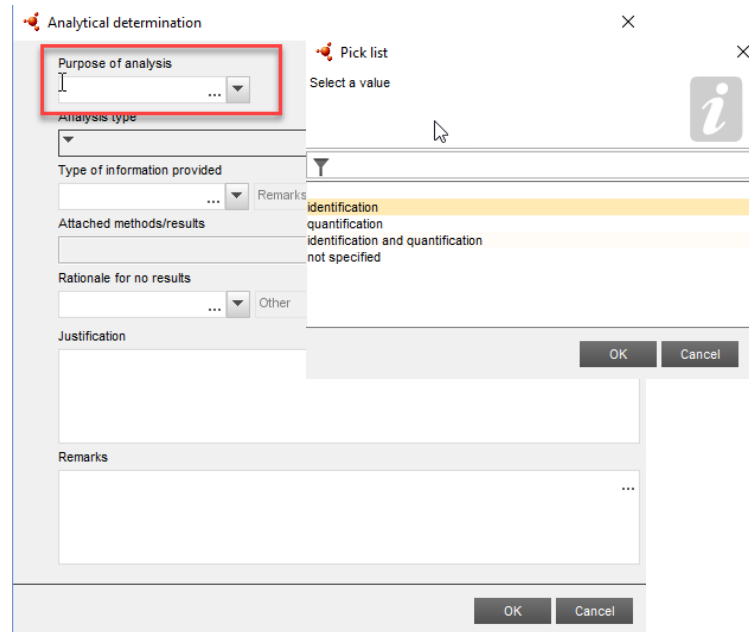
Tips based on experience – Substance ID



- Add row



- 'Purpose of the analysis' picklist



Tips based on experience – Substance ID



'Identification' and 'Quantification'

Analytical information ^

Methods and results of analysis ^

Analytical determination

Purpose of analysis	Analysis type	Type of information provided	Attached methods/results	Rationale for no results
identification	chromatography – other, chromatography – HPLC	methods and results	Report_gen_01.pdf / 285.451 KB / application/pdf	
quantification	titration	methods and results	Report_gen_01.pdf / 285.451 KB / application/pdf	

+ Add... Edit... X Delete ↑ Move up ↓ Move down

'Identification and Quantification'

Analytical information ^

Methods and results of analysis ^

Analytical determination

Purpose of analysis	Analysis type	Type of information provided	Attached methods/results	Rationale for no results
identification and quantification	IR, chromatography – IC	methods and results	Report_gen_01.pdf / 285.451 KB / application/pdf	

+ Add... Edit... X Delete ↑ Move up ↓ Move down

Tips based on experience – Substance ID



- IUPAC name should be provided
 - Section 1.1 reference substance
 - If unavailable then chemical name in same field

Identification of substance ^

Reference substance flags

Reference substance

water / water / 7732-18-5 / 231-791-2

Inventory	Inventory number	Inventory name
EC Inventory	231-791-2	water
CAS number	CAS name	
7732-18-5		
IUPAC name		
water		

Tips based on experience – Substance ID



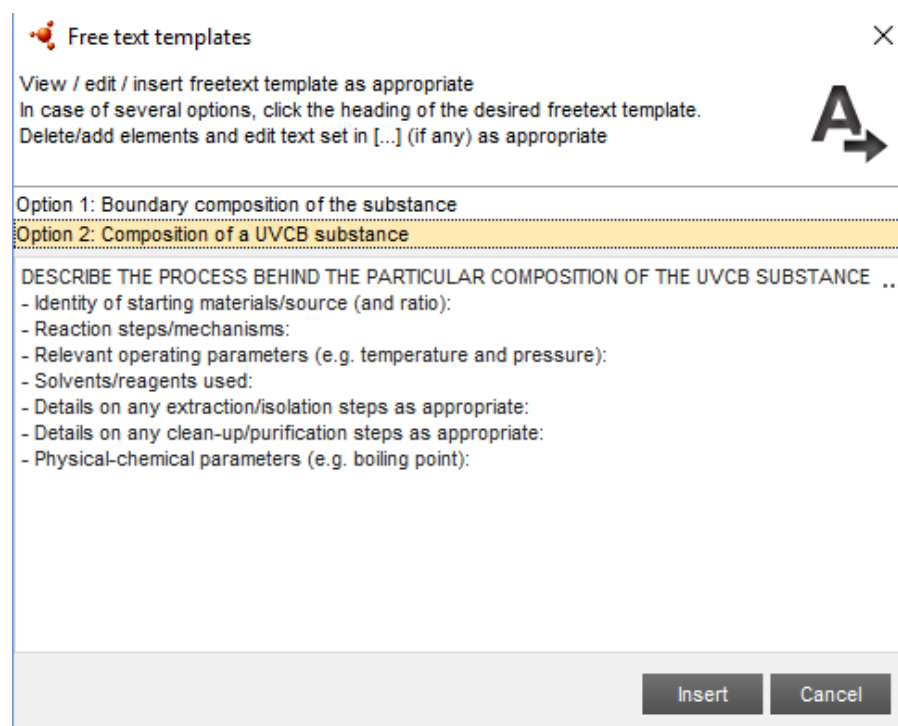
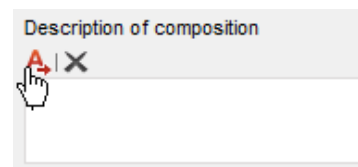
- UVCB substances:
 - Manufacturing process description should be provided for the **registered substance**
 - IUCLID section 1.2

The screenshot displays the IUCLID 6 web interface for a substance record. The left-hand navigation panel shows a tree structure of sections, with '1.2 Composition' selected and highlighted. The main content area shows the 'General Information' section, which includes fields for 'Name', 'Standard composition', 'Type of composition', and 'State / form'. The 'Type of composition' dropdown menu is set to 'legal entity composition of the substance'. Below this, the 'Description of composition' text area contains the text 'Manufacturing process description'. The interface also shows an 'Attached description' section with a table for 'Attached document' and 'Remarks', and a 'Justification for deviations' section. At the bottom, there is a 'Related composition(s)' section.

Tips based on experience – Substance ID



- UVCB substances:
 - Use the Text template
 - Address all the points



Tips based on experience – Substance ID



- UVCB substances
 - Breakdown of the composition should be provided for the **registered substance** in IUCLID section 1.2 'Composition'
 - If it cannot be provided constituent by constituent, the group of constituents should be provided at least

Constituents ^

labeltalol / 2-hydroxy-5-{1-hydroxy-2-[(1-methyl-3-phenylpropyl)amino]ethyl}benzamide / 36894-69-6 / 253-258-3, ca. 99.9 % (w/w), >= 99.7 - <= 100.0 % (w/w)

Reference substance

labeltalol / 2-hydroxy-5-{1-hydroxy-2-[(1-methyl-3-phenylpropyl)amino]ethyl}benzamide / 36894-69-6 / 253-258-3

Inventory	Inventory number	Inventory name
EC Inventory	253-258-3	labeltalol
CAS number	CAS name	
36894-69-6		
IUPAC name		
2-hydroxy-5-{1-hydroxy-2-[(1-methyl-3-phenylpropyl)amino]ethyl}benzamide		

Typical concentration

ca. 99.9 % (w/w)

Concentration range

>= 99.7 <= 100.0 % (w/w)

Remarks

Tips based on experience – Substance ID



- UVCB substances:
 - In exceptional cases where the nature of substance does not allow identification of any separate constituents, a justification should exist under the highlighted field

A screenshot of the IUCLID 6 web interface. The browser address bar shows the URL: CORE / Composition / Standard composition / Complete_fullTB1 / myrtecaine / 2-[2-(6,6-dimethylbicyclo[3.1.1]hept-2-en-2-yl)ethoxy]-N,N-diethylet... IUCLID. The page title is 'General Information ^'. The form contains several fields: 'Name' (Standard composition), 'Type of composition' (legal entity composition of the substance), 'State / form', and 'Description of composition'. Below these is an 'Attached description' table with columns for 'Attached document' and 'Remarks'. A table with one row is visible, containing the text 'Tips based on experience - Sub...'. At the bottom, there is a 'Justification for deviations' field, which is highlighted with a red rectangular border. Above this field are buttons for '+ Add...', 'Edit...', 'Delete', 'Move up', and 'Move down'.

Reporting data in IUCLID

Read across



Reporting of read-across information (1)

- **Background:**

- In IUCLID 5, read-across information was reported differently, depending on whether a grouping/category approach, or analogue approach was used.
- Read-across is one of the main areas where the quality of the provided information has been a concern.
- Decision to streamline the reporting approach to support clarity of information.

- **IUCLID 6:**

- Read-across is always reported as a source-target structure.
- Important change: endpoint-specific read-across justification must be provided in the target record.

Reporting of read-across information (2)

1. Category approach:

- Source information, i.e. the experimental data from the group of substances, is provided in the category member substance datasets.
- Target information, i.e. the outcome of the read-across, is provided as an endpoint study record in the substance dataset of the registered substance, with the 'Type of information' set to "read-across based on grouping of substances (category approach)".
- Similar to IUCLID 5 approach, but limited target record information to be provided compared to a normal endpoint study record; only fields that reflect the read-across exercise are to be filled in; not fields related to experimental setup (available in source data).

Reporting of read-across information (3)

2. Analogue / supporting substance approach:

- Source and target information to be provided in the substance dataset of the registered substance in separate records.
- Source data are reported as a normal experimental study record, filled in according to the instructions for a robust study summary. The test material information identifies the substance on which the test was done.
- Target data are reported as a separate endpoint study record with ‘Type of information’ field set to “read-across from supporting substance (structural analogue or surrogate)”.
- The information to be provided is limited in comparison to a normal endpoint study record; only fields that reflect the read-across exercise are to be filled in; not fields related to experimental setup (available in source record).

Reporting of read-across information (4)

2. Analogue / supporting substance approach:

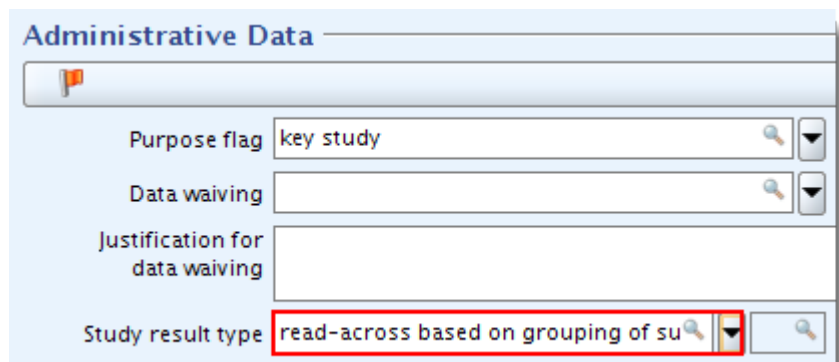
	Endpoint study record	Source record	Target record
i	Administrative data	X	X
	Endpoint	X	X
	Type of information	X	X
	Adequacy of study	X	X
	Robust study summary		
	Used for classification	X	X
	Used for SDS		
	Study period	X	
	Reliability	X	
	Rationale for reliability incl. deficiencies	X	
	Data waiving		
	Justification for data waiving		
	Justification for type of information		X
	Attached justification		X
	Cross-reference		X
ii	Data source	X	
iii	Materials and methods	X	
iv	Test materials	X	X
v	Result and discussion	X	X
vi	Overall remarks, attachments	X	X
vii	Applicant's summary and conclusion	X	X

X = relevant chapters/fields; X = subject to completeness check

Reporting of read-across information (5)

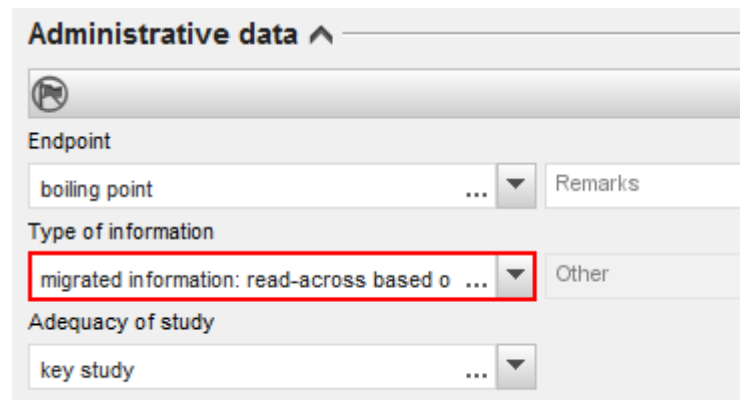
Migration from IUCLID 5 to IUCLID 6:

- Migration from IUCLID 5 was done adding the tag “migrated information” to the ‘Type of information’ field, and such records are checked at completeness check as normal experimental study records (one complete record required).
- Strongly recommended, for the benefit of clarity and data quality, to move to the new approach whenever possible.



The screenshot shows the 'Administrative Data' section of the IUCLID 5 interface. It features a light blue header with a flag icon. Below the header are four input fields: 'Purpose flag' with the value 'key study', 'Data waiving', 'Justification for data waiving', and 'Study result type' with the value 'read-across based on grouping of su'. The 'Study result type' field is highlighted with a red border.

IUCLID 5: read-across record



The screenshot shows the 'Administrative data' section of the IUCLID 6 interface. It features a grey header with an upward arrow icon. Below the header are four input fields: 'Endpoint' with the value 'boiling point', 'Type of information' with the value 'migrated information: read-across based o', 'Adequacy of study' with the value 'key study', and a 'Remarks' field. The 'Type of information' field is highlighted with a red border.

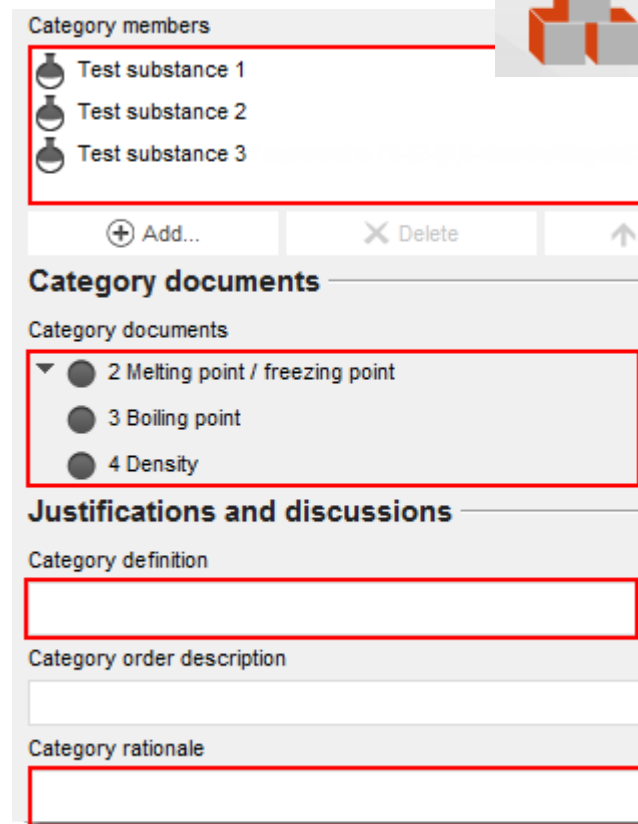
IUCLID 6: migrated read-across record

Reporting of read-across information (6)

Migrated data – checklist for category approach:

- Category object exists, and contains the full documentation of the category definition and rationale behind the grouping.
- Category member datasets contain the source data used in the read-across.
- As in IUCLID 5.

Source data: category and its members



The screenshot displays the IUCLID 6 interface for a category. It is divided into several sections:

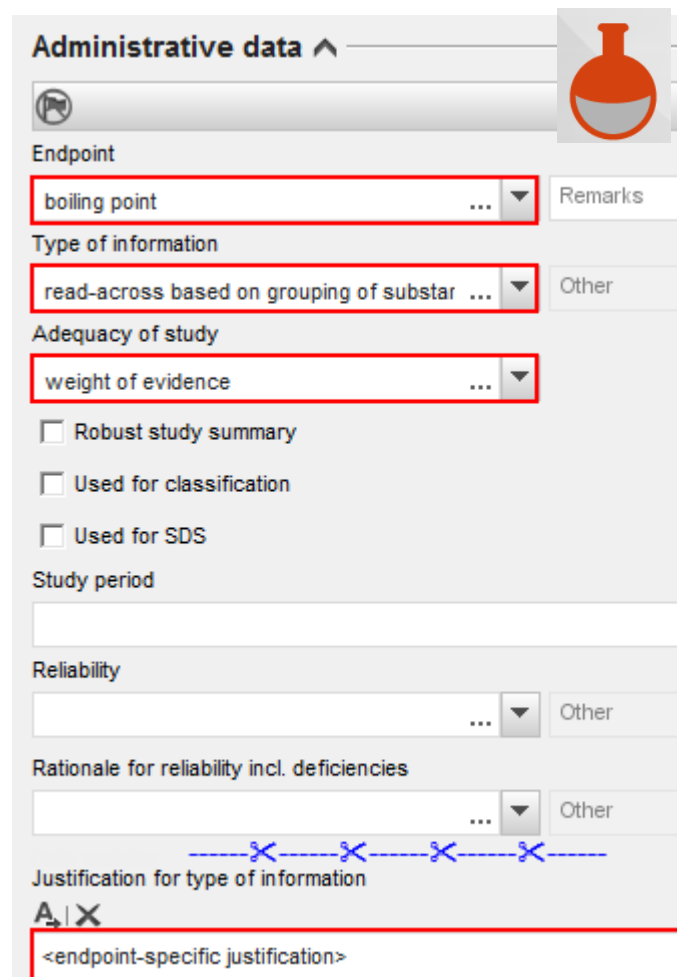
- Category members:** A list of three test substances: "Test substance 1", "Test substance 2", and "Test substance 3". Each entry is preceded by a flask icon. Below the list are buttons for "Add...", "Delete", and an upward arrow.
- Category documents:** A section containing a list of documents: "2 Melting point / freezing point", "3 Boiling point", and "4 Density". Each document has a radio button next to it.
- Justifications and discussions:** A section with three text input fields:
 - Category definition:** An empty text box.
 - Category order description:** An empty text box.
 - Category rationale:** An empty text box.

Reporting of read-across information (7)

Migrated data – checklist for category approach:

- In the target endpoint study record of the registered substance dataset:
 - Set the ‘Type of information’ to “read-across based on grouping of substances (category approach)”
 - Set the ‘Adequacy of study’ to the appropriate value depending on how you use the read-across to fulfil the information requirement (typically “key study” or “weight-of-evidence”)
 - Leave empty the fields that relate to the experimental setup and the validity of the source information (provided in source data)
 - Add the endpoint-specific justification in the field ‘Justification for type of information’.

Target data: read-across record in substance dataset of registered substance



Administrative data ^

Endpoint
boiling point ...

Type of information
read-across based on grouping of substar ...

Adequacy of study
weight of evidence ...

Robust study summary
 Used for classification
 Used for SDS

Study period

Reliability
... Other

Rationale for reliability incl. deficiencies
... Other

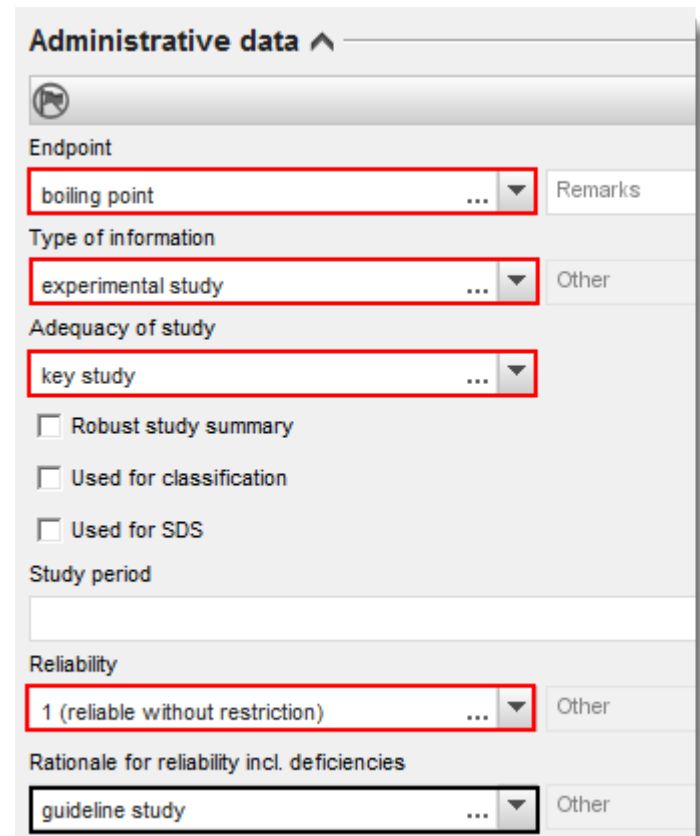
Justification for type of information
A | X
<endpoint-specific justification>

Reporting of read-across information (8)

Migrated data – checklist for analogue approach:

- Split the read-across information into source and target data.
- The source record
 - Set the ‘Type of information’ to “experimental study”
 - Set the ‘Adequacy of study’ to “key study”
 - Fill in the source record as a normal experimental study record; should reflect a standalone study summary on the source material.
 - Ensure that all the information provided reflects the source data.

Source data: experimental study



The screenshot shows the 'Administrative data' form in IUCLID 6. The form is titled 'Administrative data' with an upward arrow. It contains several sections with dropdown menus and checkboxes. The following table summarizes the data entered in the form:

Field	Value	Remarks/Other
Endpoint	boiling point	Remarks
Type of information	experimental study	Other
Adequacy of study	key study	
Robust study summary	<input type="checkbox"/>	
Used for classification	<input type="checkbox"/>	
Used for SDS	<input type="checkbox"/>	
Study period		
Reliability	1 (reliable without restriction)	Other
Rationale for reliability incl. deficiencies	guideline study	Other

Data reporting in IUCLID 6



Reporting of read-across information (9a)

Migrated data – checklist for analogue approach:

– The target record

- Set the 'Type of information' to "read-across from supporting substance (structural analogue or surrogate)"
- Set the 'Adequacy of study' to the appropriate value depending on how you use the read-across to fulfil the information requirement (typically "key study" or "weight-of-evidence")
- Leave empty the fields that relate to the reliability of the source information (provided in source data)
- Add the endpoint-specific justification in the field 'Justification for type of information'.
- Under 'Cross-reference', link to the endpoint study record which contains the source data.

Target data: read-across record

Administrative data ^

Endpoint
boiling point ... Remarks

Type of information
read-across from supporting substance (s ... Other

Adequacy of study
weight of evidence ...

Robust study summary
 Used for classification
 Used for SDS

Study period

Reliability
... Other

Rationale for reliability incl. deficiencies
... Other

Justification for type of information
A | X
<endpoint-specific justification>

Cross-reference

Reason / purpose	Related information
read-across source	OECD / Boiling point / Boiling point.002 / Test s

Data reporting in IUCLID 6



Target data: read-across record

Reporting of read-across information (9b)

Checklist for analogue approach:

- The target record
 - Leave empty the fields that relate to the experimental setup of the source study (provided in source data)
 - Identify the read-across target material in the field 'Test material information'
 - Fill in the result for the read-across target material
 - Under 'Applicant's summary and conclusion', indicate (if applicable) how estimated effects relate to C&L criteria for target substance, and how results impact distribution of target material.
 - Briefly summarise read-across approach and applicability of results in the Executive summary (optional).

The screenshot shows the IUCLID 6 data entry interface for a read-across record. The form is divided into several sections:

- Data source** (dropdown menu)
- Materials and methods** (expandable section)
 - Test guideline**: A table with columns 'Qualifier' and 'Guideline'.
 - Principles of method if other than guideline**: A text field with a search icon and a close icon.
 - GLP compliance**: A text field with a dropdown menu and a 'Remarks' label.
 - Other quality assurance**: A text field with a dropdown menu and an 'Other' label.
 - Type of method**: A text field with a dropdown menu and an 'Other' label.
- Test material** (expandable section)
 - Test material information**: A text field containing 'testene', highlighted with a red box.
- Results and discussion** (expandable section)
 - Boiling point**: A table with columns 'Key result', 'Boiling pt.', and 'Atm. press.'. The row containing a checked box, '100.0 °C', and '1.0 atm' is highlighted with a red box.
- Overall remarks, attachments** (dropdown menu)
- Applicant's summary and conclusion** (dropdown menu)

Reporting of read-across information (10)


Analogue approach, source and target records are not identical:

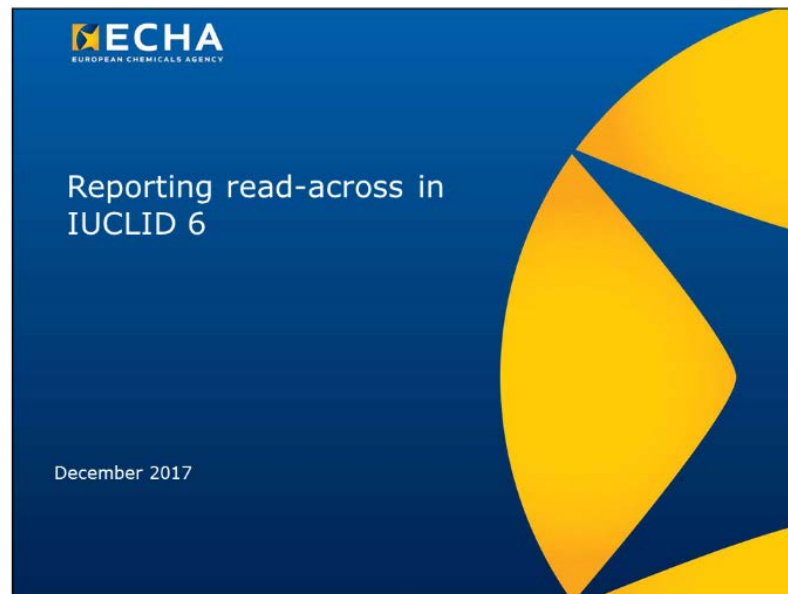
	Chapter/ / field	Source record	Target record
i	Administrative data		
	Endpoint	same	same
	Type of information	experimental study	read-across...
	Adequacy of study	key study	key study or weight of evidence (if used to fulfil information requirement)
	Reliability	X	
	Rationale for reliability incl. deficiencies	X	
	Justification for type of information		endpoint-specific justification for read-across
	Attached justification		X
	Cross-reference		link to source record
	ii	Data source	X
iii	Materials and methods	X	
iv	Test materials	tested material	read-across target material (main constituent of registered substance, component of more complex substance, etc.)
			Result for target material, including any corrections for MW etc.
v	Result and discussion	experimental result	Result for target material, including any corrections for MW etc.
vii	Applicant's summary and conclusion	GHS criteria and implications for distribution of substance for source material. Executive summary of experimental study.	GHS criteria and implications for distribution of substance for target material. Executive summary of read-across approach.

- More information in a presentation available on the IUCLID website

<https://iuclid6.echa.europa.eu/training-material>

How to report read-across in IUCLID

- [Presentation \[EN\]](#) ( PDF, 13 MB)



Reporting data in IUCLID

Data waivers



Tips based on experience – Data waivers



- Do not report study results as data waivers

OECD / Flammability / FlammabilityDW.001 / Complete_fullITB1 / myrtecaine / 2-[2-(6,6-dimethylbicyclo[3.1.1]hept-2-en-2-yl)ethoxy]-N,N-diethylet... OECD

Administrative data ^

Endpoint
flammable solids ... Remarks

Type of information
... Other ... Remarks

Adequacy of study
...

Robust study summary
 Used for classification
 Used for SDS


Study period
...

Reliability
... Other

Rationale for reliability incl. deficiencies
... Other ... Remarks

Data waiving
study technically not feasible ...

Justification for data waiving
other: The study does not need to be conducted... Further information under 'Justification for type of information' field

Justification for type of information
According to the study... 

Tips based on experience – Data waivers



- In case an information requirement has **not** been provided a justification must exist

A screenshot of the IUCLID 6 administrative data form. The browser address bar shows the URL: OECD / Flammability / FlammabilityDW.001 / Complete_fulITB1 / myrtecaine / 2-[2-(6,8-dimethylbicyclo[3.1.1]hept-2-en-2-yl)ethoxy]-N,N-diethyl... OECD. The form is titled "Administrative data" and contains several sections: Endpoint (flamable solids), Type of information (Other), Adequacy of study, Robust study summary, Used for classification, Used for SDS, Study period, Reliability (Other), Rationale for reliability incl. deficiencies (Other), and Data waiving. The "Data waiving" section is highlighted with a red box and contains a dropdown menu, a "Justification for data waiving" field, and a "Justification for type of information" field with a text input and a close button (X).

Tips based on experience – Data waivers



- 'Data waiving' picklist

A screenshot of a software interface with a 'Data waiving' picklist dialog box open. The background interface has several sections: 'Study period' (empty text field), 'Reliability' (empty dropdown), 'Rationale for reliability incl. deficiencies' (empty dropdown), 'Data waiving' (dropdown menu with a red box around it), 'Justification for data waiving' (dropdown menu), and 'Justification for type of information' (text area with a red 'X' icon). The 'Data waiving' dropdown is open, showing a list of options: 'study technically not feasible', 'study scientifically not necessary / other information available', 'exposure considerations', 'study waived due to provisions of other regulation', and 'other justification'. The dialog box is titled 'Pick list' and has a close button (X) in the top right corner. It contains the text 'Select a value' and a search filter icon (funnel) above the list. At the bottom of the dialog are 'OK' and 'Cancel' buttons.

Study period

Reliability

Rationale for reliability incl. deficiencies

Data waiving

Justification for data waiving

Justification for type of information

A₂ | X

Pick list

Select a value

study technically not feasible

study scientifically not necessary / other information available

exposure considerations

study waived due to provisions of other regulation

other justification

OK Cancel

Tips based on experience – Data waivers



- Use the existing justifications if applicable

Administrative data ^

Endpoint
flammable solids ...

Type of information
...

Adequacy of study
...

Robust study summary
 Used for classification
 Used for SDS

Study period
...

Reliability
...

Rationale for reliability incl. deficiencies
...

Data waiving
...

Justification for data waiving
▼ the study does not need to be conducted for explosives

Justification for type of information
A | X

Attached justification

Remarks

Select picklist values

the study does not need to be conducted because the substance is a gas and the concentration of the flammable gas in a mixture with inert gases is so low that, when mixed with air, the concentration is all time below the lower limit. - [study scientifically not necessary / other information available]

Remarks ...

the study does not need to be conducted for explosives - [study technically not feasible]

Remarks ...

the study does not need to be conducted because the substance is pyrophoric - [study technically not feasible]

Remarks ...

the study does not need to be conducted for organic peroxides - [study technically not feasible]

Remarks ...

the study does not need to be conducted for self-reactive substances - [study technically not feasible]

Remarks ...

Deselect all Select all OK Cancel

Tips based on experience – Data waivers



- If not applicable select 'other:' and provide a short description of the justification in the field next to

The screenshot shows the 'Administrative data' section of the IUCLID 6 interface. The 'Endpoint' field is set to 'flammable solids'. The 'Data waiving' section is highlighted, and the 'Justification for data waiving' field contains the text 'other: The study does not need to be conducted because...'. A dialog box titled 'Select picklist values' is open, showing a list of options with checkboxes. The 'other:' option is selected and highlighted with a red box. The dialog box also contains several 'Remarks' fields with pre-filled text justifying the waiver.

Administrative data ^

Endpoint
flammable solids

Type of information

Adequacy of study

Robust study summary

Used for classification

Used for SDS

Study period

Reliability

Rationale for reliability incl. deficiencies

Data waiving

Justification for data waiving
▼ other: The study does not need to be conducted because...

Justification for type of information

Select picklist values

Remarks
 the study does not need to be conducted because the organic substance does not contain metals or metalloids and hence, the classification procedure does not need to be applied - [study scientifically not necessary / other information available]

Remarks
 the study does not need to be conducted because the experience in production or handling shows that the substance does not react with water, e.g. the substance is manufactured with water or washed with water - [study scientifically not necessary / other information available]

Remarks
 the study does not need to be conducted because the substance is known to be soluble in water to form a stable mixture - [study scientifically not necessary / other information available]

Remarks
 other: The study does not need to be conducted because...]

Deselect all Select all OK Cancel

Tips based on experience – Data waivers



- If needed a detailed justification in the highlighted textbox

Data waiving

study technically not feasible ... ▼

Justification for data waiving

▼ other: The study does not need to be conducted because...

Justification for type of information

A₂ | X

Detailed justification...|

Tips based on experience – Data waivers



- Avoid **only** referring to other Endpoint study records or different places in the dossier

A screenshot of a web form for data waiver justification. The form has two main sections. The first section is titled 'Justification for data waiving' and contains a dropdown menu with the selected option 'other: See later'. The second section is titled 'Justification for type of information' and contains a text input field with the text 'See in CSR'. A large red 'X' is overlaid on the text input field, indicating that this justification is incorrect. The text 'A | X' is visible above the input field.

- The justification should be in the right place!

Reporting data in IUCLID

PNEC calculator



What is it?

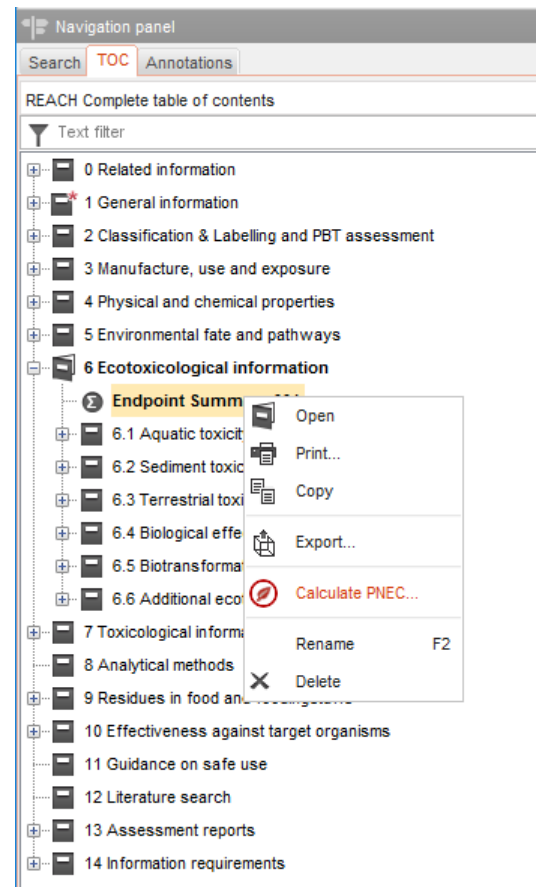
- The PNEC calculator offers you the possibility to calculate and report predicted no-effect concentrations (PNECs) in IUCLID according to ECHA Guidance on information requirements and chemical safety assessment, Chapter R.10.

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_{oral} 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, there is a sub-header 'PNEC calculator' and a refresh icon. The main content area is divided into two parts. The upper part is a table with two columns: 'Environmental compartment' and 'PNEC Scenario'. The lower part is a configuration panel for the 'Aqua' compartment, which is currently selected. This panel has four tabs: 'Aqua', 'Sediment', and 'Soil'. The 'Aqua' tab is active and shows four sections: 'Freshwater', 'Freshwater, intermittent', 'Marine', and 'Marine, intermittent'. Each section contains a 'Dose descriptor' dropdown menu, an 'Assessment factor' input field, and a 'Justification' dropdown menu. The 'Freshwater' section has an assessment factor of 10.0. The 'Freshwater, intermittent' section has an assessment factor of 100.0. The 'Marine' section has an assessment factor of 100.0. The 'Marine, intermittent' section has an assessment factor of 1000.0. At the bottom of the interface, there is a footer with a help icon, the text 'PNEC calculator', and four buttons: 'Edit', 'Print', 'Finish', and 'Cancel'.

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

Aqua | Sediment | Soil

Freshwater

Dose descriptor: (default) 6.1.2 Long-term toxicity to fish.001 - EC10, LC10 or NOEC for fres...
Assessment factor: 10.0
Justification: Default (PNEC calculator plug-in)

Freshwater, intermittent

Dose descriptor: (default) 6.1.1 Short-term toxicity to fish.001 - LC50 for freshwater fish - 1...
Assessment factor: 100.0
Justification: Default (PNEC calculator plug-in)

Marine

Dose descriptor: (default) 6.1.2 Long-term toxicity to fish.001 - EC10, LC10 or NOEC for mari...
Assessment factor: 100.0
Justification: Default (PNEC calculator plug-in)

Marine, intermittent

Dose descriptor: (default) 6.1.1 Short-term toxicity to fish.001 - LC50 for marine water fish -...
Assessment factor: 1000.0
Justification: Default (PNEC calculator plug-in)

?

PNEC calculator

Edit Print Finish 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.

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

Aqua | Sediment | Soil

Freshwater

Dose descriptor: (default) 6.1.2 Long-term toxicity to fish.001 - EC10, LC10 or NOEC for fres...
Assessment factor: 10.0
Justification: Default (PNEC calculator plug-in)

Freshwater, intermittent

Dose descriptor: (default) 6.1.1 Short-term toxicity to fish.001 - LC50 for freshwater fish - 1...
Assessment factor: 100.0
Justification: Default (PNEC calculator plug-in)

Marine

Dose descriptor: (default) 6.1.2 Long-term toxicity to fish.001 - EC10, LC10 or NOEC for mari...
Assessment factor: 100.0
Justification: Default (PNEC calculator plug-in)

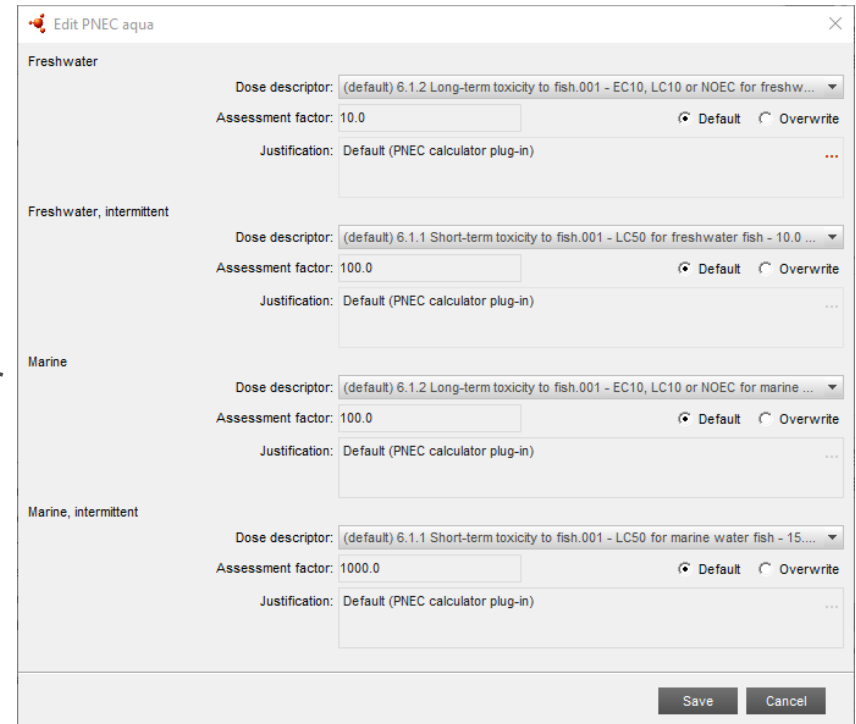
Marine, intermittent

Dose descriptor: (default) 6.1.1 Short-term toxicity to fish.001 - LC50 for marine water fish -...
Assessment factor: 1000.0
Justification: Default (PNEC calculator plug-in)

Buttons: Edit, Print, Finish, 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.



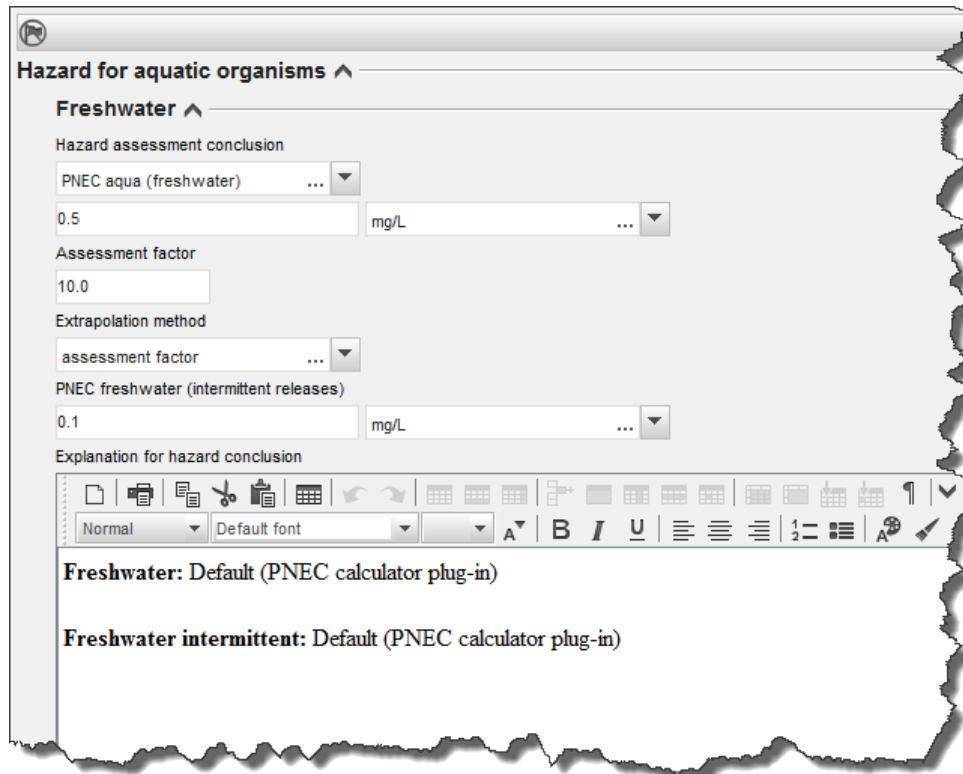
The screenshot shows the 'Edit PNEC aqua' window with the following configuration options:

Environment	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 rich text editor with a toolbar and two lines of text: "Freshwater: Default (PNEC calculator plug-in)" and "Freshwater intermittent: Default (PNEC calculator plug-in)".

Reporting data in IUCLID

DNEL calculator



What is it?

- The DNEL generator offers you the possibility to calculate and report derived non-effect levels (DNELs) in IUCLID according to ECHA Guidance on information requirements and chemical safety assessment, Chapter R.8.
- It has been developed in collaboration with the State Secretariat for Economic Affairs SECO from the Swiss Confederation.



Schweizerische Eidgenossenschaft
Confédération suisse
Confederazione Svizzera
Confederaziun svizra

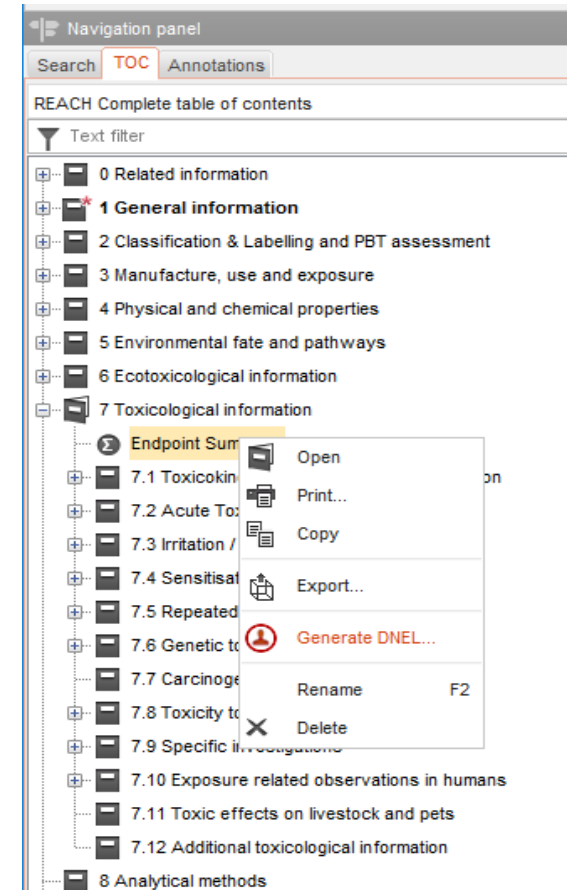
Eidgenössisches Departement für
Wirtschaft, Bildung und Forschung WBF
Staatssekretariat für Wirtschaft SECO

Purpose

- DNEL derivation is a key element for the risk characterisation of a chemical substance.
- The DNEL generator allows you to derive DNELs automatically from the data already available in the **endpoint summaries (sections 7.1, 7.5 and 7.8) of a substance dataset or template** and report them back in the corresponding endpoint summary under section '*7 Toxicological information*'.
- Currently, DNEL calculator only supports the **derivation of workers and general population DNELs for long-term systemic effects for oral, dermal and inhalation routes** according to the ECHA Guidance. Thus, the current version does not support the derivation of DNELs using human data, for acute toxicity, for local effects or for threshold carcinogens.

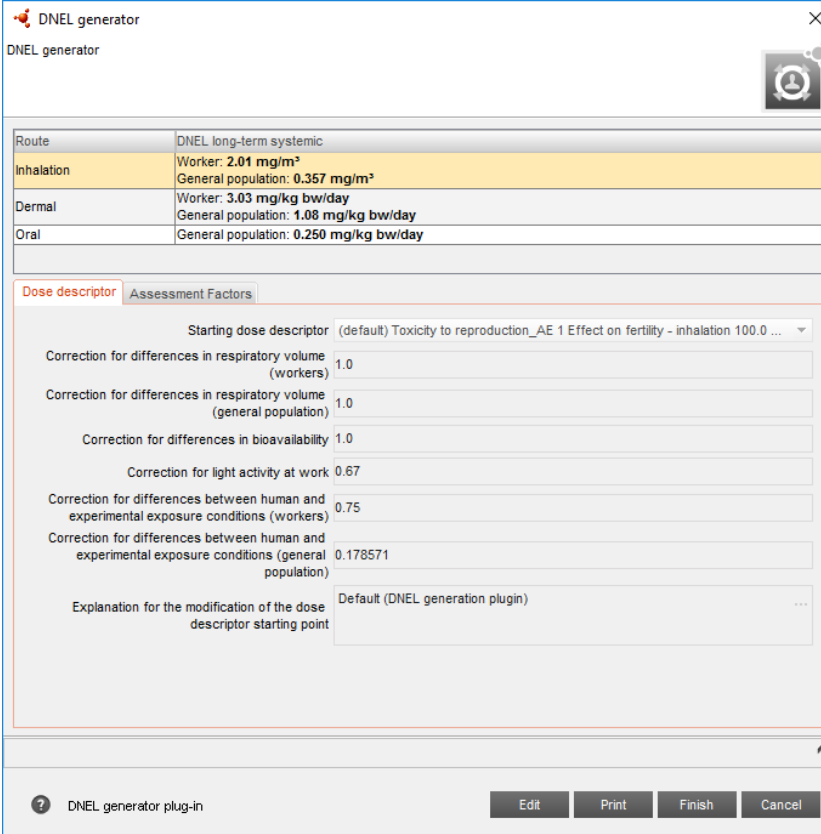
Overview – how it works?

- How to use it?
 - You can use the DNEL calculator by right-clicking the endpoint summary under section '7 Toxicological information' and selecting 'Generate DNEL' from the displayed menu.



Overview – how it works?

- Outcome
 - The results (DNELs calculated according to the Guidance R8) are displayed in a tabular format by route.
 - The dose descriptor used as starting point for the selected route and the parameters used to correct it are set by the tool and displayed in the tab called '*Dose descriptor*' as read-only.
 - The ECHA default assessment factors used to address uncertainties in the extrapolation of experimental animal data to real human exposure situations are displayed in the tab called '*Assessment Factors*' as read-only.



The screenshot shows the 'DNEL generator' software window. It displays a table of results for different routes and a 'Dose descriptor' tab with various assessment factors.

Route	DNEL long-term systemic
Inhalation	Worker: 2.01 mg/m³ General population: 0.357 mg/m³
Dermal	Worker: 3.03 mg/kg bw/day General population: 1.08 mg/kg bw/day
Oral	General population: 0.250 mg/kg bw/day

Dose descriptor | Assessment Factors

Starting dose descriptor: (default) Toxicity to reproduction_AE 1 Effect on fertility - inhalation 100.0 ...

Correction for differences in respiratory volume (workers): 1.0

Correction for differences in respiratory volume (general population): 1.0

Correction for differences in bioavailability: 1.0

Correction for light activity at work: 0.67

Correction for differences between human and experimental exposure conditions (workers): 0.75

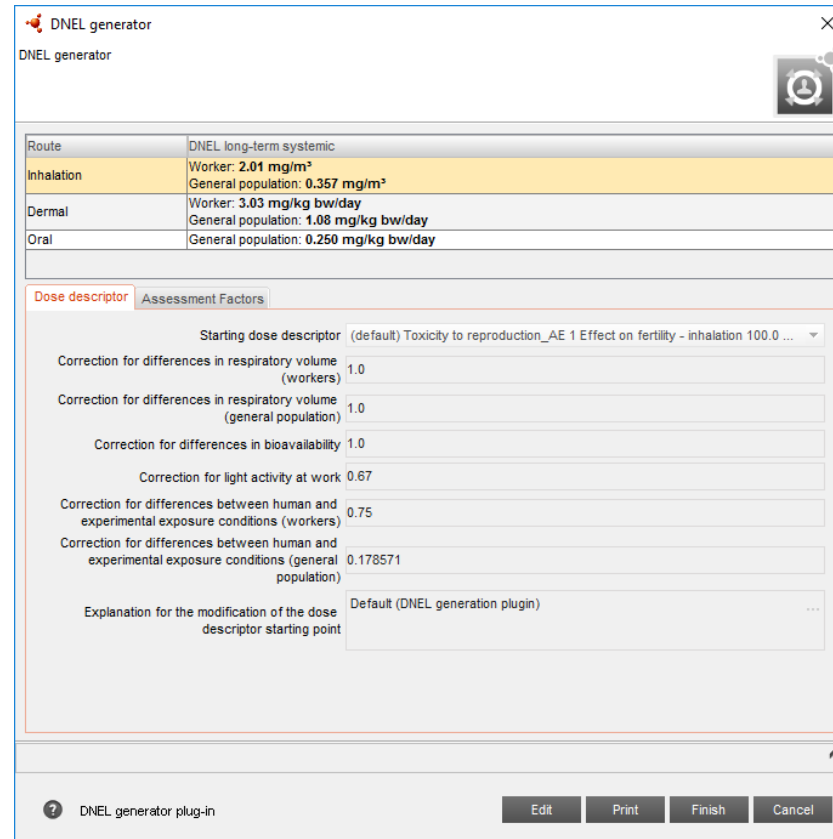
Correction for differences between human and experimental exposure conditions (general population): 0.178571

Explanation for the modification of the dose descriptor starting point: Default (DNEL generation plugin) ...

DNEL generator plug-in | Edit | Print | Finish | Cancel

Overview – how it works?

- Functionalities
 - **Edit button** enables to change the selection of the initial dose descriptor and some parameters used to derive the DNELs in a pop-up window.
 - **Print button** generates a report in a .rtf format containing the derived DNELs information as in section 5.11 of the CSR.
 - **Finish button** closes the calculator after saving the results in the corresponding endpoint summary under section '7 *Toxicological information*'.
 - **Cancel button** closes the calculator without any further action.



The screenshot shows the 'DNEL generator' application window. The main area displays a table of routes and their corresponding DNEL values for workers and the general population. Below the table, there are two tabs: 'Dose descriptor' (selected) and 'Assessment Factors'. The 'Dose descriptor' tab shows a list of correction factors for various parameters, each with a numerical value. At the bottom of the window, there is a status bar with a question mark icon and the text 'DNEL generator plug-in', and a row of four buttons: 'Edit', 'Print', 'Finish', and 'Cancel'.

Route	DNEL long-term systemic
Inhalation	Worker: 2.01 mg/m³ General population: 0.357 mg/m³
Dermal	Worker: 3.03 mg/kg bw/day General population: 1.08 mg/kg bw/day
Oral	General population: 0.250 mg/kg bw/day

Dose descriptor | Assessment Factors

Starting dose descriptor (default) Toxicity to reproduction_AE 1 Effect on fertility - inhalation 100.0 ...

Correction for differences in respiratory volume (workers) 1.0

Correction for differences in respiratory volume (general population) 1.0

Correction for differences in bioavailability 1.0

Correction for light activity at work 0.67

Correction for differences between human and experimental exposure conditions (workers) 0.75

Correction for differences between human and experimental exposure conditions (general population) 0.178571

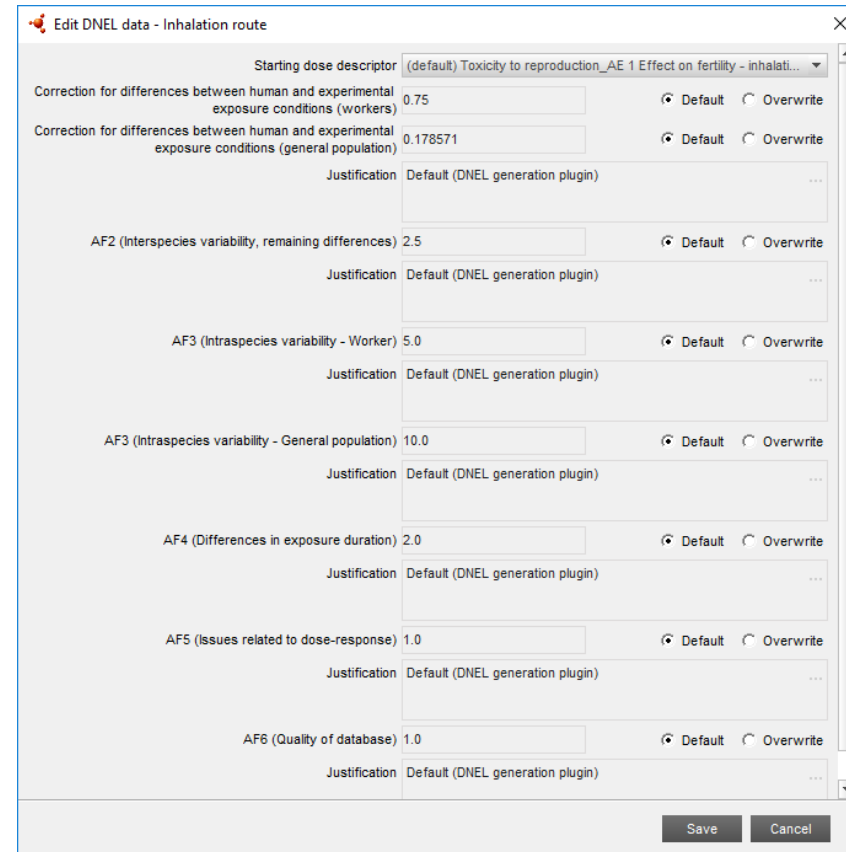
Explanation for the modification of the dose descriptor starting point Default (DNEL generation plugin) ...

DNEL generator plug-in

Edit Print Finish Cancel

Overview – how it works?

- Edit mode
 - Allows the user to:
 - select a different dose descriptor as starting point,
 - use non-default correction factors for differences between human and experimental exposure conditions,
 - use non-default assessment factors.
 - Any modification from default requires the user to provide a justification.



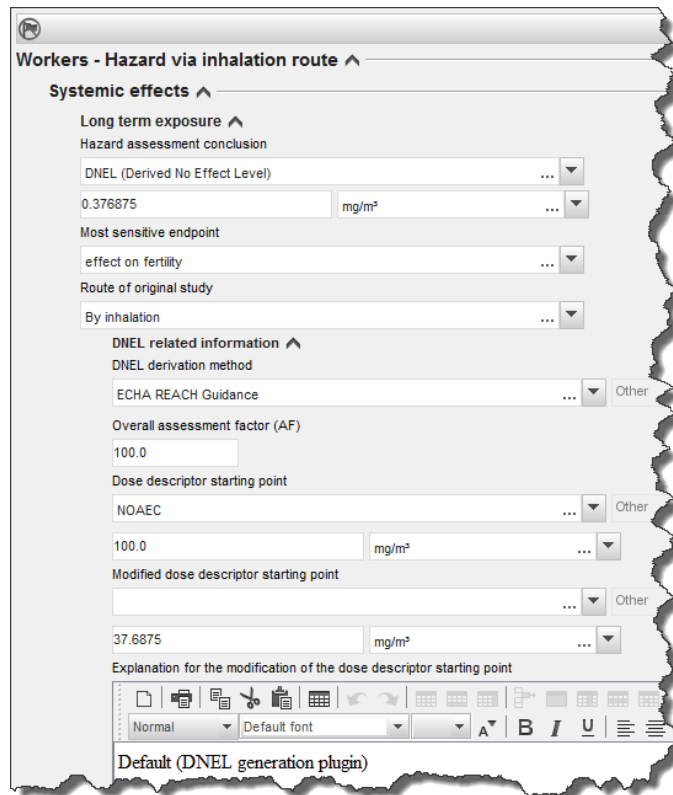
Starting dose descriptor: (default) Toxicity to reproduction_AE 1 Effect on fertility - inhalati...

Parameter	Value	Default	Overwrite	Justification
Correction for differences between human and experimental exposure conditions (workers)	0.75	<input checked="" type="radio"/>	<input type="radio"/>	
Correction for differences between human and experimental exposure conditions (general population)	0.178571	<input checked="" type="radio"/>	<input type="radio"/>	
AF2 (Interspecies variability, remaining differences)	2.5	<input checked="" type="radio"/>	<input type="radio"/>	Default (DNEL generation plugin)
AF3 (Intraspecies variability - Worker)	5.0	<input checked="" type="radio"/>	<input type="radio"/>	Default (DNEL generation plugin)
AF3 (Intraspecies variability - General population)	10.0	<input checked="" type="radio"/>	<input type="radio"/>	Default (DNEL generation plugin)
AF4 (Differences in exposure duration)	2.0	<input checked="" type="radio"/>	<input type="radio"/>	Default (DNEL generation plugin)
AF5 (Issues related to dose-response)	1.0	<input checked="" type="radio"/>	<input type="radio"/>	Default (DNEL generation plugin)
AF6 (Quality of database)	1.0	<input checked="" type="radio"/>	<input type="radio"/>	Default (DNEL generation plugin)

Buttons: Save, Cancel

Overview – how it works?

- Reporting in IUCLID
 - It is done in the corresponding endpoint summary under section ‘7 Toxicological information’ from which the DNEL calculator was started.



Workers - Hazard via inhalation route ^

Systemic effects ^

Long term exposure ^

Hazard assessment conclusion

DNEL (Derived No Effect Level) ...

0.376875 mg/m³ ...

Most sensitive endpoint

effect on fertility ...

Route of original study

By inhalation ...

DNEL related information ^

DNEL derivation method

ECHA REACH Guidance ... Other

Overall assessment factor (AF)

100.0

Dose descriptor starting point

NOAEC ... Other

100.0 mg/m³ ...

Modified dose descriptor starting point

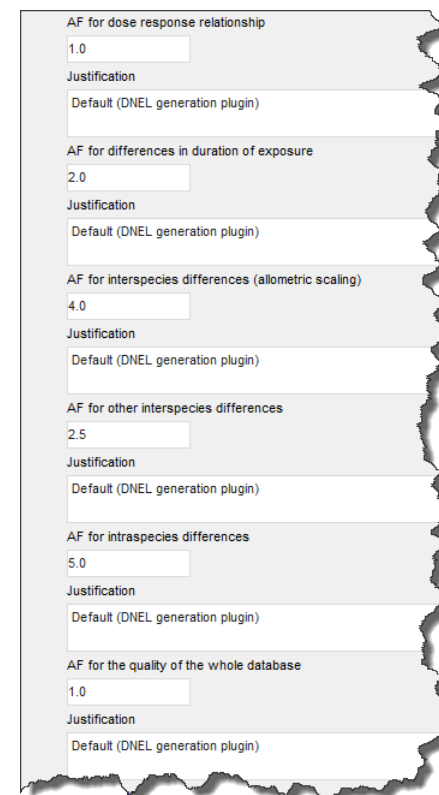
... Other

37.6875 mg/m³ ...

Explanation for the modification of the dose descriptor starting point

Normal Default font A^v B I U

Default (DNEL generation plugin)



AF for dose response relationship

1.0

Justification

Default (DNEL generation plugin)

AF for differences in duration of exposure

2.0

Justification

Default (DNEL generation plugin)

AF for interspecies differences (allometric scaling)

4.0

Justification

Default (DNEL generation plugin)

AF for other interspecies differences

2.5

Justification

Default (DNEL generation plugin)

AF for intraspecies differences

5.0

Justification

Default (DNEL generation plugin)

AF for the quality of the whole database

1.0

Justification

Default (DNEL generation plugin)

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:

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

Reporting data in IUCLID

Opt-out under REACH



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



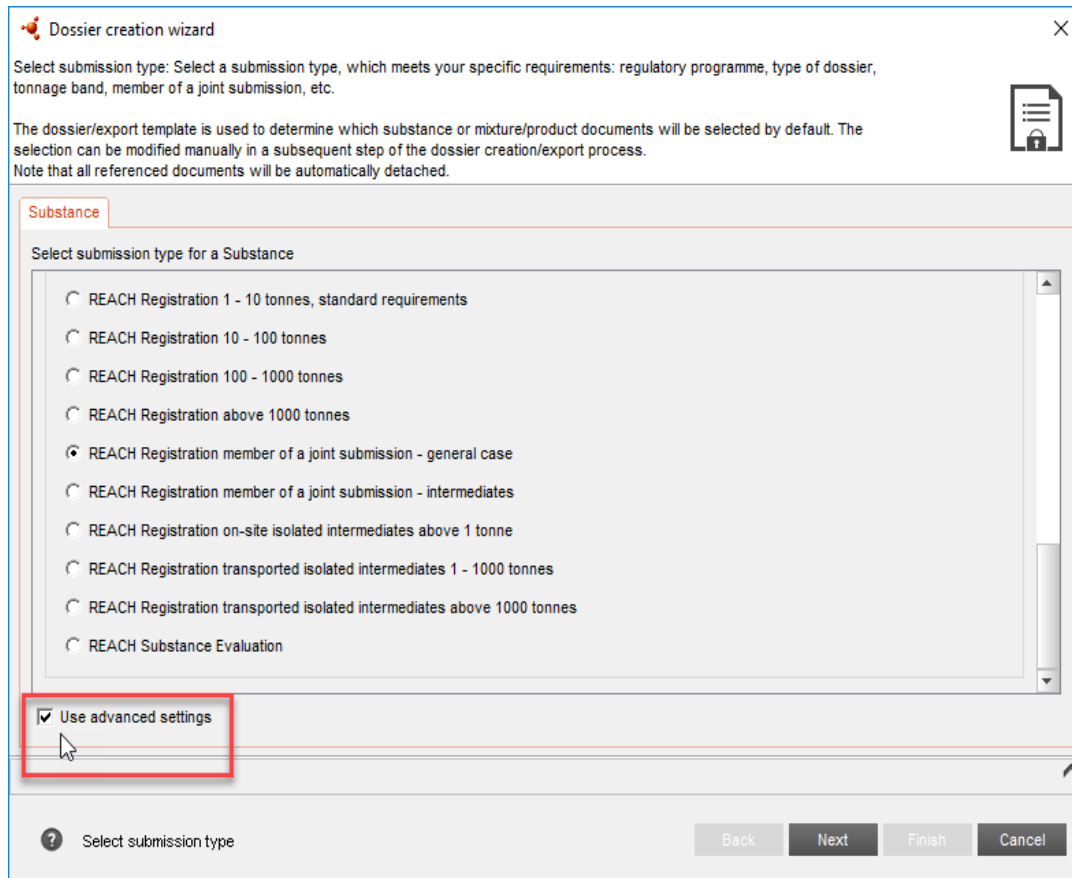
REACH opt-outs

- 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. Section 14, 'Information requirements', is expanded to show 'Opt-out information for REACH registration', which is highlighted with a red box. A yellow box highlights the 'Opt-out information for REACH registration' option. The right panel, titled 'EU_REACH / Opt-out information', shows the 'Data selected for opt-out' section. Under 'Documents', 'OECD / Bioaccumulation: aquatic' is selected and highlighted with a red box. Under 'Justification', 'Justification for the opt-out' is entered and highlighted with a red box. The bottom right panel, 'Information panel', shows the 'Type' set to 'Fixed Record', the 'UUID' as '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

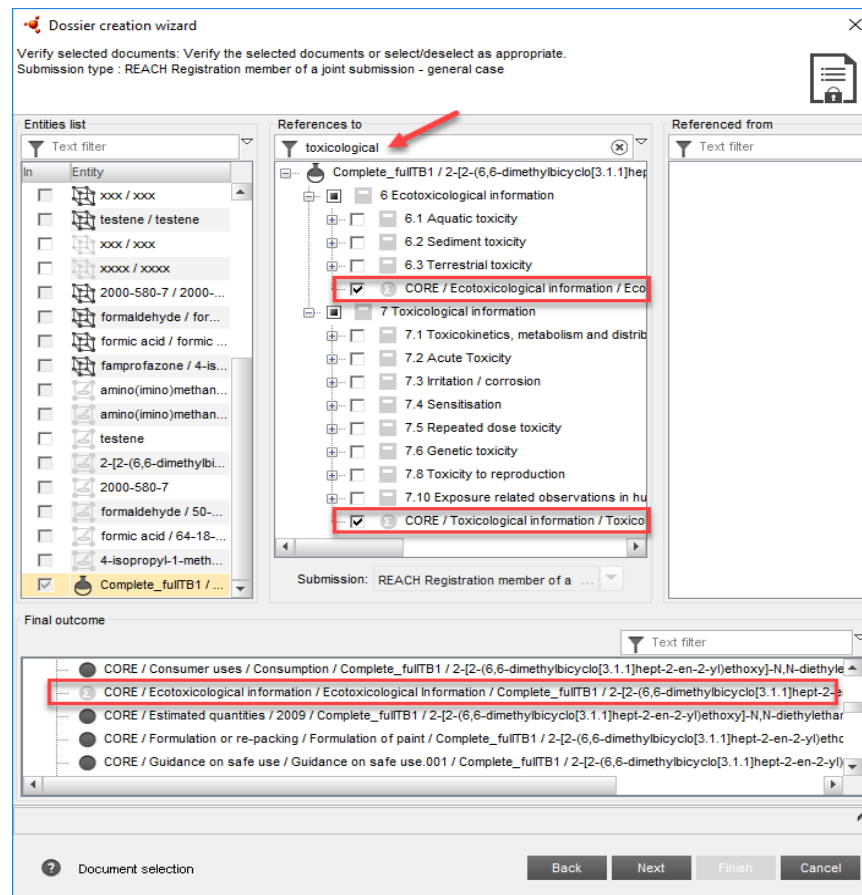
Use advanced settings

? 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. The 'References to' panel is active, showing 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 / Toxic...'. The 'Final outcome' panel at the bottom shows a list of selected documents, with one item highlighted in red: 'CORE / Ecotoxicological information / Ecotoxicological Information / Complete_fullTB1 / 2-[2-(6,6-dimethylbicyclo[3.1.1]hept-2-en-2-yl)ethoxy]-N,N-diethyl-'. The 'Entities list' on the left shows various chemical entities, and the 'Referenced from' panel on the right is currently empty.

Reporting data in IUCLID

Changes between IUCLID 5 and 6



Amendment to REACH Annexes VII and VIII (1)

- **What?**

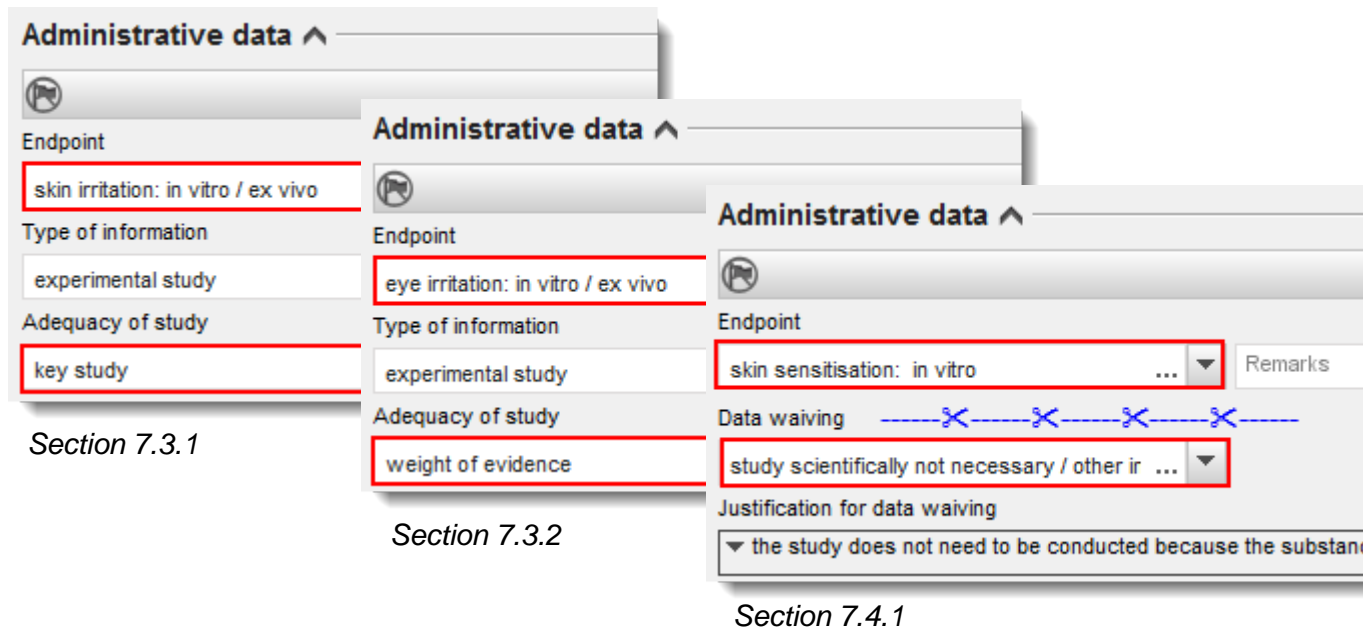
- Information requirements on skin corrosion/irritation and serious eye damage/eye irritation amended; entered into effect on **June 21, 2016**.
- Amendment makes the *in vitro* studies the standard information requirement at Annexes VII and VIII; *in vivo* studies to be considered only if *in vitro* studies are not applicable, or results are not adequate for classification and risk assessment.
- Amendment to the skin sensitisation requirement has been approved; prepared for publication in the Official Journal of the EU in the **coming month**.
- Amendment makes *in vitro* or *in chemico* studies the standard information requirement at Annex VII; *in vivo* studies to be considered only if *in vitro/in chemico test methods* are not applicable, or results are not adequate for classification and risk assessment. In such cases, the murine local lymph node assay (LLNA) to be used.

https://echa.europa.eu/view-article/-/journal_content/title/reach-annexes-amended-registrants-to-use-alternative-test-methods
<http://eur-lex.europa.eu/eli/reg/2016/863/oj>
<http://ec.europa.eu/transparency/regcomitology/index.cfm?do=search.documentdetail&XMmA1sY1+dPFA15wY23QjBDn7Qd++m5oh9aiDXqCyio=>

Amendment to REACH Annexes VII and VIII (2)

- **Consequence for reporting in IUCLID?**

- To be complete, registration dossiers with Annex VII requirements and above, must contain at least one endpoint study record addressing the *in vitro* (*in chemico*) requirement;
- Endpoint study record must be key study, weight of evidence, or data waiving.



The image displays three overlapping screenshots of the IUCLID 6 administrative data form, illustrating different reporting options for endpoint studies. Each screenshot is labeled with a section reference:

- Section 7.3.1:** Shows the form with the following fields highlighted in red:
 - Endpoint: skin irritation: in vitro / ex vivo
 - Type of information: experimental study
 - Adequacy of study: key study
- Section 7.3.2:** Shows the form with the following fields highlighted in red:
 - Endpoint: eye irritation: in vitro / ex vivo
 - Type of information: experimental study
 - Adequacy of study: weight of evidence
- Section 7.4.1:** Shows the form with the following fields highlighted in red:
 - Endpoint: skin sensitisation: in vitro
 - Data waiving: study scientifically not necessary / other ir ...
 - Justification for data waiving: the study does not need to be conducted because the substance

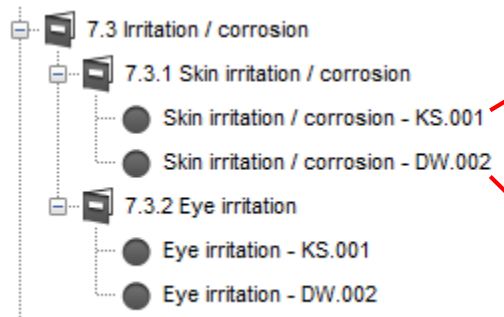
Amendment to REACH Annexes VII and VIII (3)

- **Consequence for reporting in IUCLID?**

- **If an *in vivo* study exists** that was carried out or initiated before the Annex amendment took effect, this should be reported as an endpoint study record with the appropriate ‘Adequacy of study’, and the ‘Endpoint’ selection “... in vivo”.
- **In addition**, you must include another endpoint study record in the same section, with the ‘Endpoint’ selection “... in vitro”, indicate it as a Data waiving with rationale “study scientifically not necessary / other information available”, and the following ‘Justification for data waiving’ picklist selection:
 - an in vitro skin irritation study does not need to be conducted because adequate data from an in vivo skin irritation study are available (section 7.3.1)
 - an in vitro eye irritation study does not need to be conducted because adequate data from an in vivo eye irritation study are available (section 7.3.2)
 - other: + free text: “an in vitro or in chemico skin sensitisation study does not need to be conducted because adequate data from an in vivo skin sensitisation study are available” (section 7.4.1)

Amendment to REACH Annexes VII and VIII (4)

- **Consequence for reporting in IUCLID?**
 - Example: section 7.3.1, information from existing *in vivo* study available



Administrative data ^

Endpoint
skin irritation: in vivo ... Remarks

Type of information
experimental study ... Other

Adequacy of study
key study ...

Administrative data ^

Endpoint
skin irritation: in vitro / ex vivo ... Remarks

Data waiving ----- ✂ ----- ✂ ----- ✂ ----- ✂ -----

study scientifically not necessary / other infor ...

Justification for data waiving
▼ an in vitro skin irritation study does not need to be conducted because adequate data from an in vivo skin irritation study are available - [study scientifically not necessary / other information available]

! Add a link in the 'Cross reference' table of DW record to the KS record, to show where the *in vivo* information is provided.

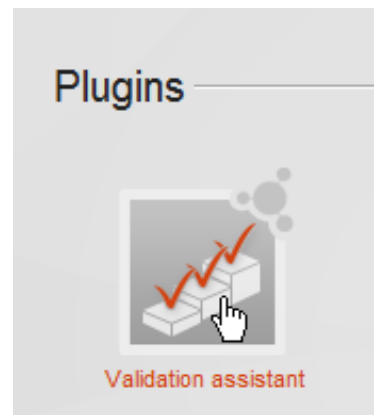
IUCLID features



Validation assistant

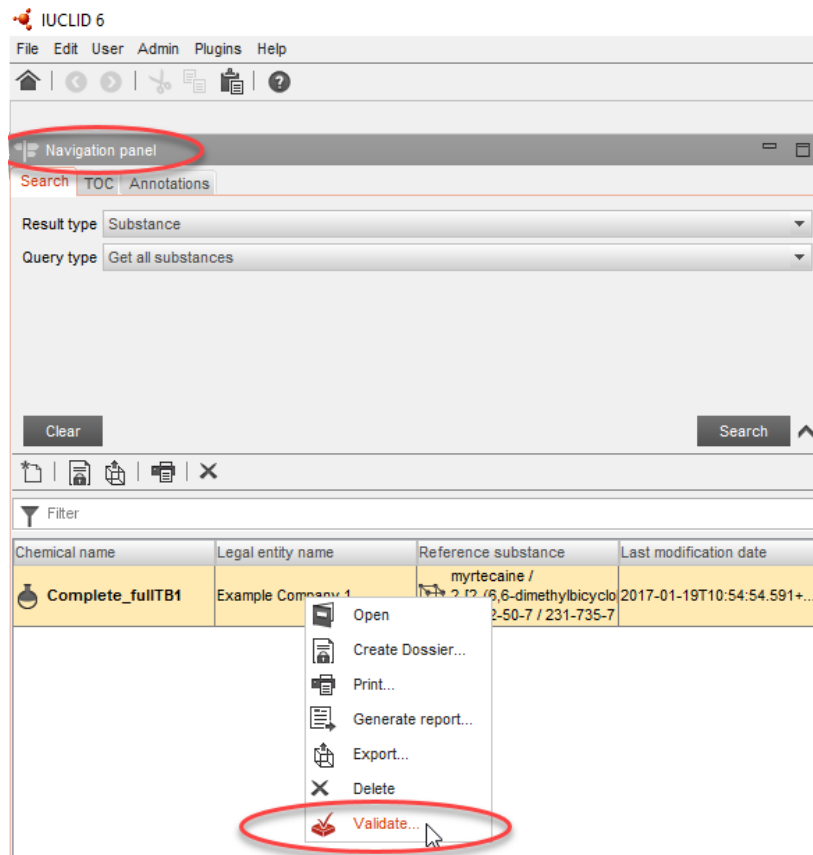


- Validation Assistant plug-in



Using the Validation Assistant

- Use the Validation Assistant on your substance dataset



The screenshot displays the IUCLID 6 software interface. At the top, the menu bar includes 'File', 'Edit', 'User', 'Admin', 'Plugins', and 'Help'. Below the menu bar is a navigation panel, which is circled in red. The main area contains search filters for 'Result type' (set to 'Substance') and 'Query type' (set to 'Get all substances'). A 'Clear' button and a 'Search' button are visible. Below the search area is a table with columns: 'Chemical name', 'Legal entity name', 'Reference substance', and 'Last modification date'. The first row of data is highlighted in yellow and contains the following information: 'Complete_fullTB1', 'Example Company 1', 'myrtecaine / 2,2,6,6-tetramethylbicyclo[2.2.1]heptane-2,5,7,7-tetramine', and '2017-01-19T10:54:54.591+'. A context menu is open over this row, listing actions: 'Open', 'Create Dossier...', 'Print...', 'Generate report...', 'Export...', 'Delete', and 'Validate...'. The 'Validate...' option is circled in red.

Chemical name	Legal entity name	Reference substance	Last modification date
Complete_fullTB1	Example Company 1	myrtecaine / 2,2,6,6-tetramethylbicyclo[2.2.1]heptane-2,5,7,7-tetramine	2017-01-19T10:54:54.591+...

Using the Validation Assistant



- Select the scenario that applies to your substance

The screenshot shows a window titled "Validation assistant wizard" with the subtitle "Validation assistant - Submission type specification". The main area is titled "Dossier type" and contains a "Select submission type" dropdown menu. A list of options is displayed, with "REACH Registration 1 - 10 tonnes, standard requirements" selected. To the left of the list is a checkbox labeled "Use advanced settings" which is currently unchecked. At the bottom of the window, there is a red error message: "Please select a submission type". Below the error message is a help icon and the text: "Provide the submission type information in order to determine the scenario of the validation." At the bottom right, there are four buttons: "Back", "Next", "Finish", and "Cancel".

Validation assistant wizard

Validation assistant - Submission type specification

Dossier type

Select submission type

Use advanced settings

- 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

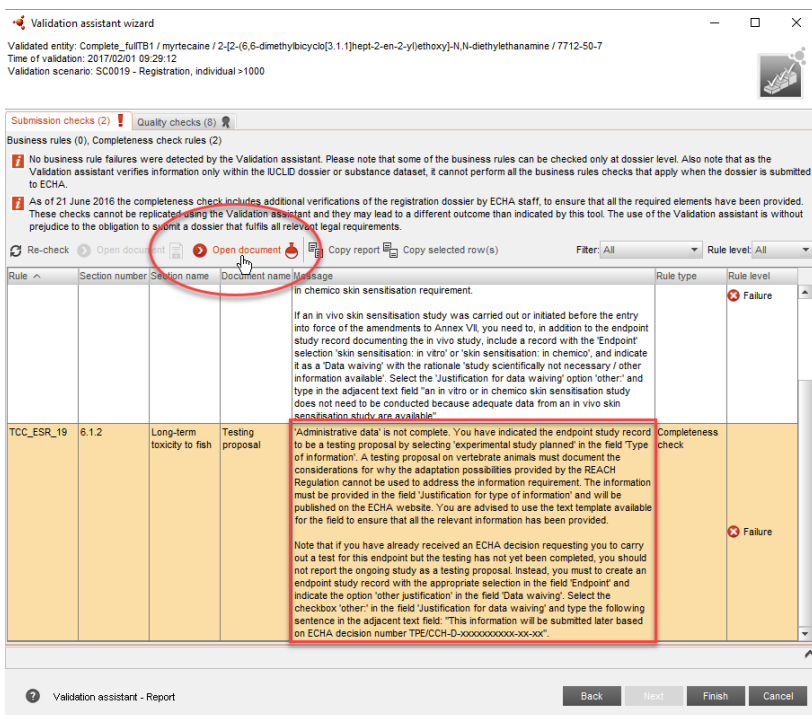
Please select a submission type

Provide the submission type information in order to determine the scenario of the validation.

Back Next Finish Cancel

Click on the failure

- Open document in substance dataset



Validation assistant wizard

Validated entity: Complete_fuitB1 / myrtecaine / 2-[2-(6,6-dimethylbicyclo[3.1.1]hept-2-en-2-yl)ethoxy]-N,N-diethylethanamine / 7712-50-7
Time of validation: 2017/02/01 09:29:12
Validation scenario: SC0019 - Registration, individual >1000

Submission checks (2) Quality checks (6)

Business rules (0), Completeness check rules (2)

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

As of 21 June 2016 the completeness check includes additional verifications of the registration dossier by ECHA staff, to ensure that all the required elements have been provided. These checks cannot be replicated using the Validation assistant and they may lead to a different outcome than indicated by this tool. The use of the Validation assistant is without prejudice to the obligation to submit a dossier that fulfils all relevant legal requirements.

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

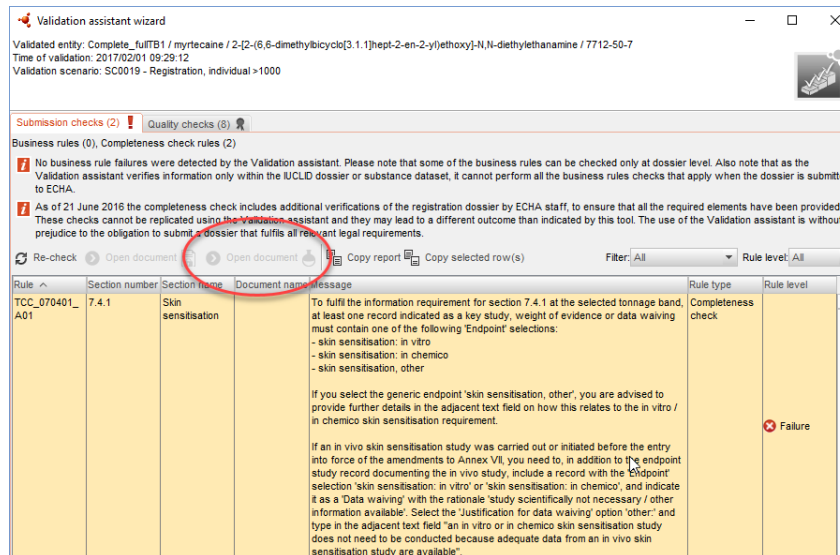
Rule	Section number	Section name	Document name	Message	Rule type	Rule level
				In chemico skin sensitisation requirement. If an in vivo skin sensitisation study was carried out or initiated before the entry into force of the amendments to Annex VII, you need to, in addition to the endpoint study record documenting the in vivo study, include a record with the 'Endpoint selection' 'skin sensitisation: in vitro' or 'skin sensitisation: in chemico', and indicate it as a 'Data waiving' with the rationale 'study scientifically not necessary / other information available'. Select the 'Justification for data waiving' option 'other' and type in the adjacent text field 'an in vitro or in chemico skin sensitisation study does not need to be conducted because adequate data from an in vivo skin sensitisation study are available'.	Completeness check	Failure
TCC_ESR_19	6.1.2	Long-term toxicity to fish	Testing proposal	'Administrative data' is not complete. You have indicated the endpoint study record to be a testing proposal by selecting 'experimental study planned' in the field 'Type of information'. A testing proposal on vertebrate animals must document the considerations for why the adaptation possibilities provided by the REACH Regulation cannot be used to address the information requirement. The information must be provided in the field 'Justification for type of information' and will be published on the ECHA website. You are advised to use the text template available for the field to ensure that all the relevant information has been provided. Note that if you have already received an ECHA decision requesting you to carry out a test for this endpoint but the testing has not yet been completed, you should not report the ongoing study as a testing proposal. Instead, you must to create an endpoint study record with the appropriate selection in the field 'Endpoint' and indicate the option 'other justification' in the field 'Data waiving'. Select the checkbox 'other' in the field 'Justification for data waiving' and type the following sentence in the adjacent text field: "This information will be submitted later based on ECHA decision number TPE/CCH-D-xxxxxx-xx-xx".	Completeness check	Failure

Validation assistant - Report

Back Next Finish Cancel

Click on the failure

- Open document in substance dataset is unavailable



Validation assistant wizard

Validated entity: Complete_fuitB1 / myrtecaine / 2-[2-(6,6-dimethylbicyclo[3.1.1]hept-2-en-2-yl)ethoxy]-N,N-diethylethanamine / 7712-50-7
Time of validation: 2017/02/01 09:29:12
Validation scenario: SC0019 - Registration, individual >1000

Submission checks (2) Quality checks (6)

Business rules (0), Completeness check rules (2)

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

As of 21 June 2016 the completeness check includes additional verifications of the registration dossier by ECHA staff, to ensure that all the required elements have been provided. These checks cannot be replicated using the Validation assistant and they may lead to a different outcome than indicated by this tool. The use of the Validation assistant is without prejudice to the obligation to submit a dossier that fulfils all relevant legal requirements.

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

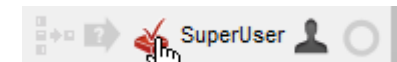
Rule	Section number	Section name	Document name	Message	Rule type	Rule level
TCC_070401_A01	7.4.1	Skin sensitisation		To fulfil the information requirement for section 7.4.1 at the selected tonnage band, at least one record indicated as a key study, weight of evidence or data waiving must contain one of the following 'Endpoint' selections: - skin sensitisation: in vitro - skin sensitisation: in chemico - skin sensitisation: other If you select the generic endpoint 'skin sensitisation, other', you are advised to provide further details in the adjacent text field on how this relates to the in vitro / in chemico skin sensitisation requirement. If an in vivo skin sensitisation study was carried out or initiated before the entry into force of the amendments to Annex VII, you need to, in addition to the endpoint study record documenting the in vivo study, include a record with the 'Endpoint' selection 'skin sensitisation: in vitro' or 'skin sensitisation: in chemico', and indicate it as a 'Data waiving' with the rationale 'study scientifically not necessary / other information available'. Select the 'Justification for data waiving' option 'other' and type in the adjacent text field 'an in vitro or in chemico skin sensitisation study does not need to be conducted because adequate data from an in vivo skin sensitisation study are available'.	Completeness check	Failure

Using the Validation Assistant



- Correct the failure in the substance dataset and unhide the VA report

The screenshot shows the IUCLID 6 Substance Information panel for a specific substance. The panel is titled "Complete_fullB1 / myrtecaine / 2-42-(6,6-dimethylbicyclo[3.1.1]hept-2-en-2-yl)ethoxy-N,N-diethylethanamine / 7712-50-7". The main content area is divided into several sections: "Substance name", "Public name", "Legal entity flags", "Legal entity", "Third party flags", "Third party", "Role in the supply chain", "Role flags", and "Identification of substance". The "Role flags" section includes checkboxes for "Manufacturer", "Importer", "Only representative", and "Downstream user". The "Identification of substance" section includes "Reference substance flags" and "Reference substance". The "Information panel" at the bottom right shows the "Information" tab selected, with fields for "Type" (Substance), "UID" (IUCS-167863c3-902e-49b8-aa95-827e560a380a), and "Dossier UID". A red arrow points to the "Information" tab in the bottom right corner of the panel.



Using the Validation Assistant



- Re-check the substance dataset

Submission checks (20) ! Quality checks (11) 👤

Business rules (0), Completeness check rules (20)

f No business rule failures were detected by the Validation assistant. Please note that some of the business rules can

f As of 21 June 2016 the completeness check includes additional verifications of the registration dossier by ECHA staff submit a dossier that fulfils all relevant legal requirements.

Re-check Open document Open document Copy report Copy selected row(s)

- Create the registration dossier and run the Validation Assistant on it too!

IUCLID 6

File Edit User Admin Plugins Help

Navigation panel

Search

Result type Dossier

Query type Get all dossiers

Clear Search

Filter

Dossier Name	Subject Name	Creation date
R_ABOVE_1000 / SUBSTANCE: C bryrtcaine / 2-[2-(6,6-dimethylbicyclo[3.1.1]hept-3-ylidene)ethyl]pyrrolidine 2017-01-19 / 1.2.0_n	Complete: fullTB1	2017-01-19T11:37:32.123+02:00

Open
Print...
Generate report...
Export...
Delete
Validate
Dissemination preview...
Compare...

Using the Validation Assistant



- Note the disclaimers!
They tell what the results mean
- Business rules
- Completeness checks

Validation assistant wizard

Validated entity: Complete_fullTB1 / myrtecaine / 2-[2-(6,6-dimethylbicyclo[3.1.1]hept-2-en-2-yl)ethoxy]-N,N-diethylethanamine / 7712-50-7
Time of validation: 2017/02/01 09:37:41
Validation scenario: SC0019 - Registration, individual >1000

Submission checks (0) ! Quality checks (8)

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

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

! No completeness check failures were detected by the Validation assistant. However, as of 21 June 2016 the completeness check includes additional verifications of the registration dossier by ECHA staff, to ensure that all the required elements have been provided. These checks cannot be replicated using the Validation assistant and they may lead to a different outcome than indicated by this tool. The use of the Validation assistant is without prejudice to the obligation to submit a dossier that fulfils all relevant legal requirements.

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

Rule	Section number	Section name	Document name	Message	Rule type	Rule level
------	----------------	--------------	---------------	---------	-----------	------------

Validation assistant - Report

Back Next Finish Cancel

- Completeness check
 - Checks if required elements provided
 - In case automatic rules cannot be used (i.e. deviations)
 - Does not check quality of the provided requirements
- Validation Assistant cannot predict manual checks performed by ECHA staff
- Certain areas of focus
 - Substance ID
 - Data waivers
 - CSR
 - Testing proposals

Useful links

Please note: We are not able to answer questions regarding the completeness of your dossier via Helpdesk or personal e-mails. Only able to perform the TCC in REACH-IT!

- Where can I know more about the manual checks at TCC?

https://echa.europa.eu/documents/10162/13652/manual_completeness_check_en.pdf

- ECHA Helpdesk

<http://echa.europa.eu/web/guest/contact>

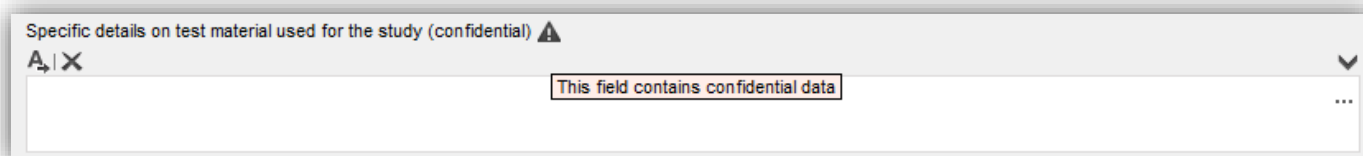
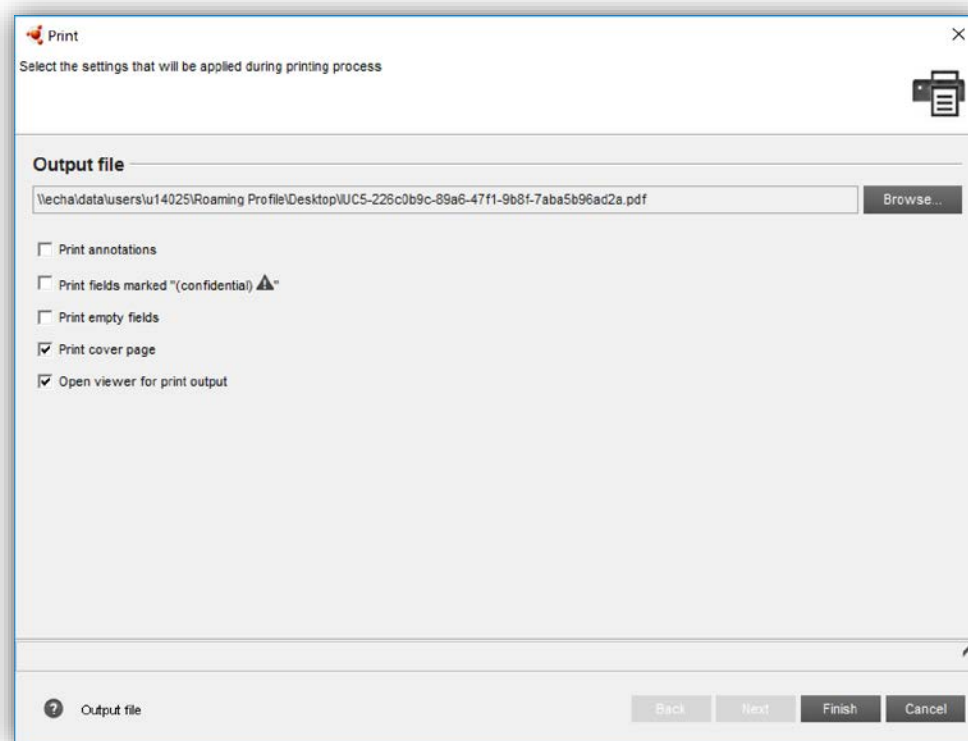


Print



Print option (confidential)

- New option added to allow users to decide if they wish to print a record or a dataset for the fields marked confidential in IUCLID
- This option also extends to the printing of entities in IUCLID for example
 - Reference substances
 - Literature references
 - Legal entities



Report generator



Report generator



Other reports available to run inside IUCLID 6.2

A number of other reports are also available in IUCLID 6.2

You will find these reports under 'Type of report' when you run The Report Generator wizard

Literature References generated from a Mixture/Product (including Literature References in any linked Substance); test_lit_refs

1. Literature References

Table 1.1. Literature References generated from a Mixture/Product (including Literature References in any linked Substance)

Type		Section information		Annex II/III requirement		UUID	
Biocidal product		Section No. 6.1 Section Name: Function and mode of control Name given to the Document: Function and mode of control.001		Effectiveness against target organisms		5bc334b8-3fc6-4b86-84b0-213dc0382888	
Reference type: study report	Title: title	Author: Author	Bibliographic source: source Year: 1222	Testing facility: No testing laboratory provided	Report no.: No report number provided	Study sponsor: No company owner provided	Report date: No report date provided
						Study number: No company study number provided	

Other reports available and compatible with IUCLID 6.2

- **Summary of Product Characteristics** report (for uploading into SPC Editor)
 - Can be generated from mixture/product datasets/dossiers as an XML
- Literature references report (RTF)
 - Can be generated from both substance and mixture/product datasets/dossiers
- Attachments report for BPR datasets and dossiers (RTF)
 - Can be generated from mixture/product datasets/dossiers
- Attachments report for substances (RTF)
 - Can be generated from substance datasets/dossiers
- BPR Confidentiality report (Article 66), for BPR datasets and dossiers (RTF/PDF/CSV)
 - Can now be generated as a CSV file and opened in Excel

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
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	<i>Under testing</i>
List of literature references - 2 May 2017	<i>Under testing</i>
List of attachments	<i>Under development</i>
List of annotations	<i>Under development</i>

Manage reports – what is it used for?

The Manage reports feature allows you to:

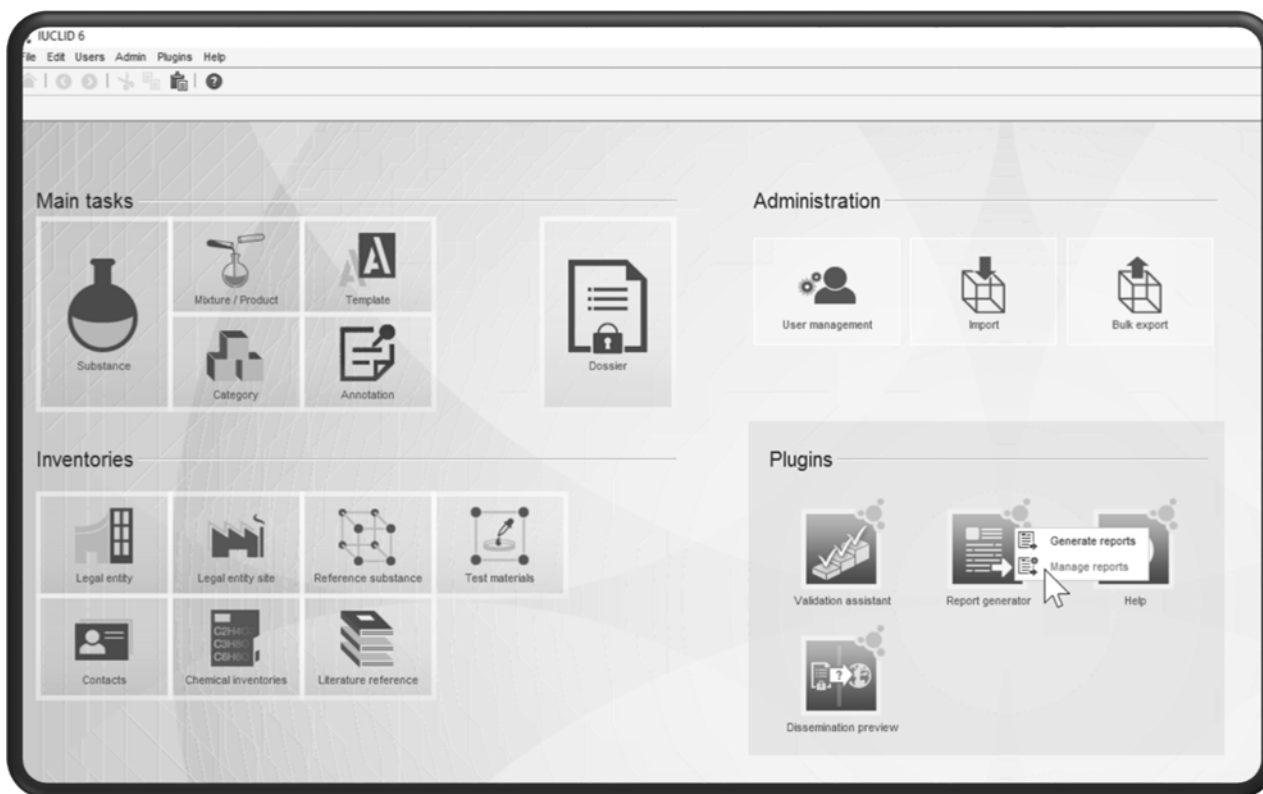
- **Upload and Store report templates in your own IUCLID installation and use these with the report generator**
- **Further customise your saved report:**
 - Select which outputs your report template supports, for example a TXT or DOC file,
 - Select the stylesheets you wish to have available to use 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

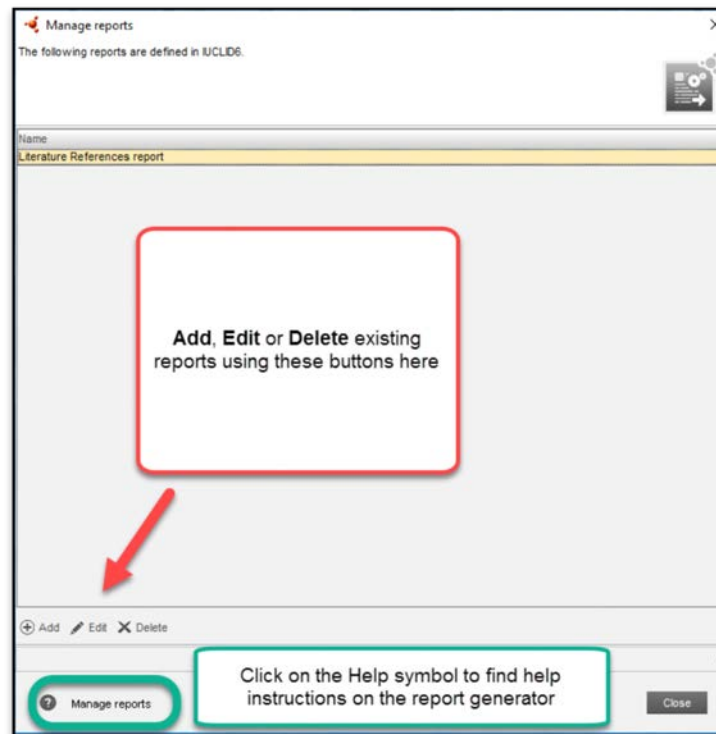
- Go to the IUCLID dashboard
- Left-click on the 'Report generator' icon
- Select 'Manage reports'



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

Edit report

Name: Literature References Report

Templates:

Main file	Template name	Description
⊕	literature_referen...	This is the main template for Literature References
⊖	literature_utilities.ftl	Lists all the relevant sections of a Mixture/Substance
⊖	macros_common.ftl	

⊕ Upload ⊖ Download ✕ Remove ✕ Remove all

Output:

Output type	Description
RTF	
XML	Output in TXT format

⊕ Add ✕ Remove ✕ Remove all

Stylesheets:

Stylesheet	Description
literature_references_...	Stylesheet with landscape formatting
BPR_reporting_custo...	

⊕ Upload ⊖ Download ✕ Remove ✕ Remove all

Applicable entities:

- Substances (including dossiers)
- Mixtures (including dossiers)

Submission types:

- Complete table of contents
- OECD SIDS
- OECD harmonised templates
- BPR Active substance information
- CLP alternative name request
- CLP notification
- CLP Regulation - CLH dossier
- REACH Complete table of contents
- REACH Annex XV - Restriction
- REACH Annex XV - SVHC
- REACH Application for authorisation
- REACH Downstream user report

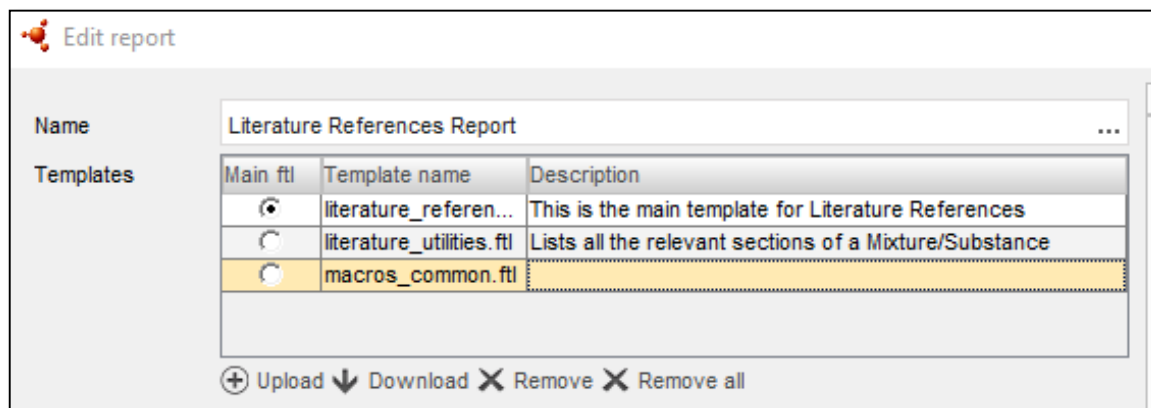
Save Close

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.

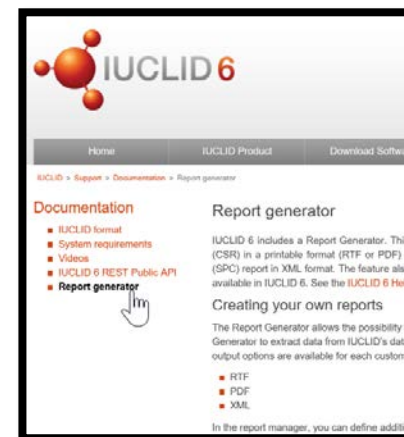
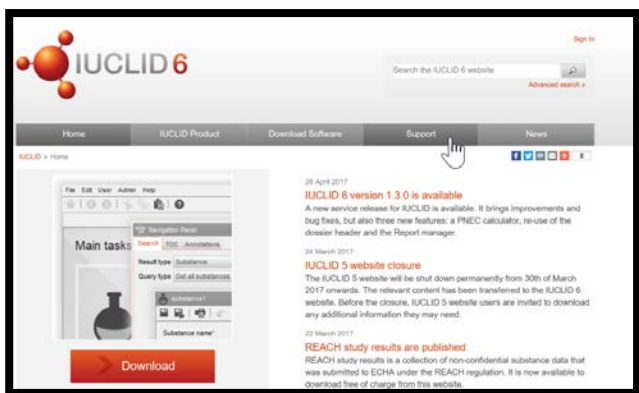
For example, a 'utilities' template in the example above lists all the relevant sections in a Substance and Mixture which I wish the Main template to include in the report.

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 templates

Available report templates

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



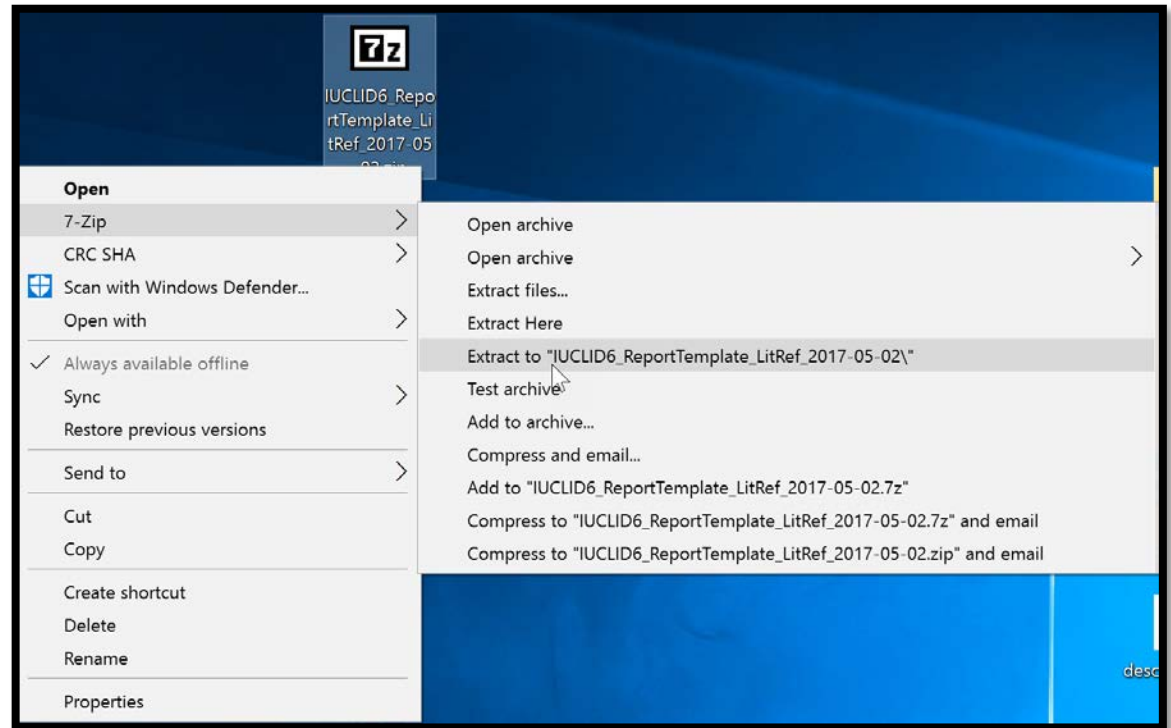
Downloading reports from the IUCLID 6 website

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:

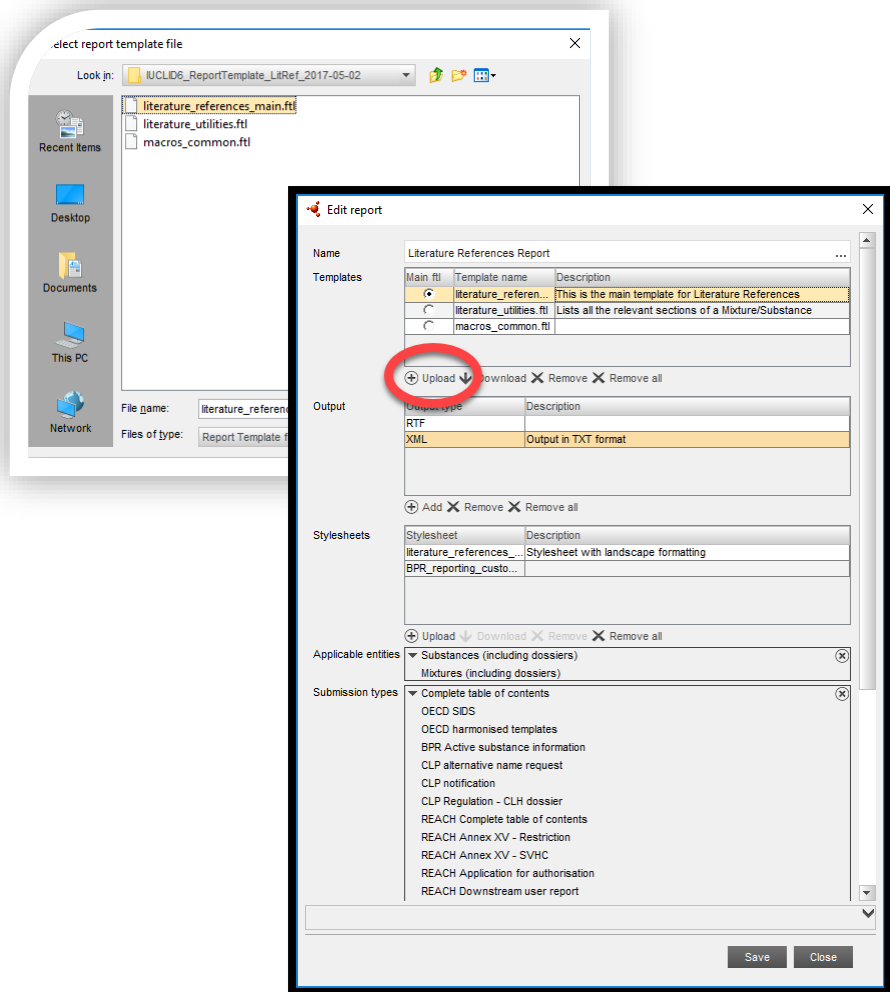
You then have a folder from which you can upload your report templates



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

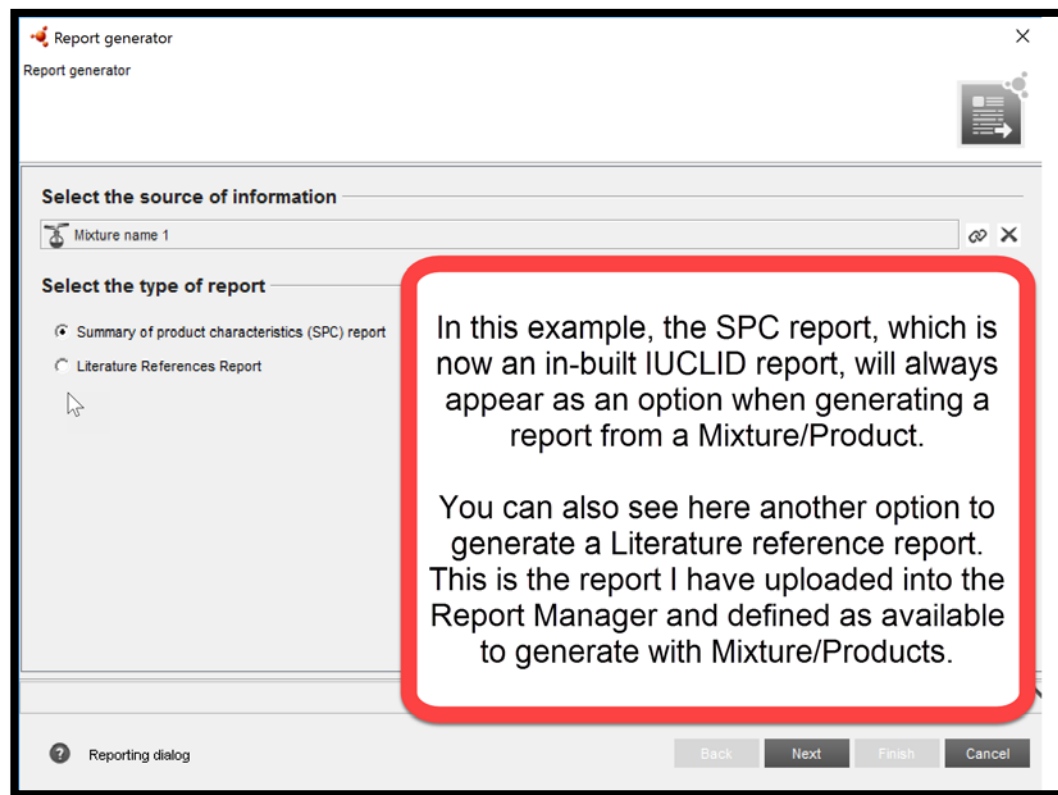
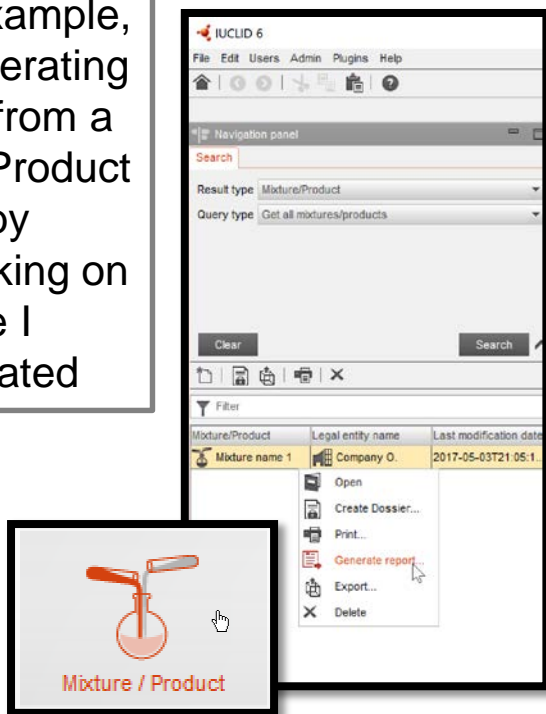
Report Generator



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



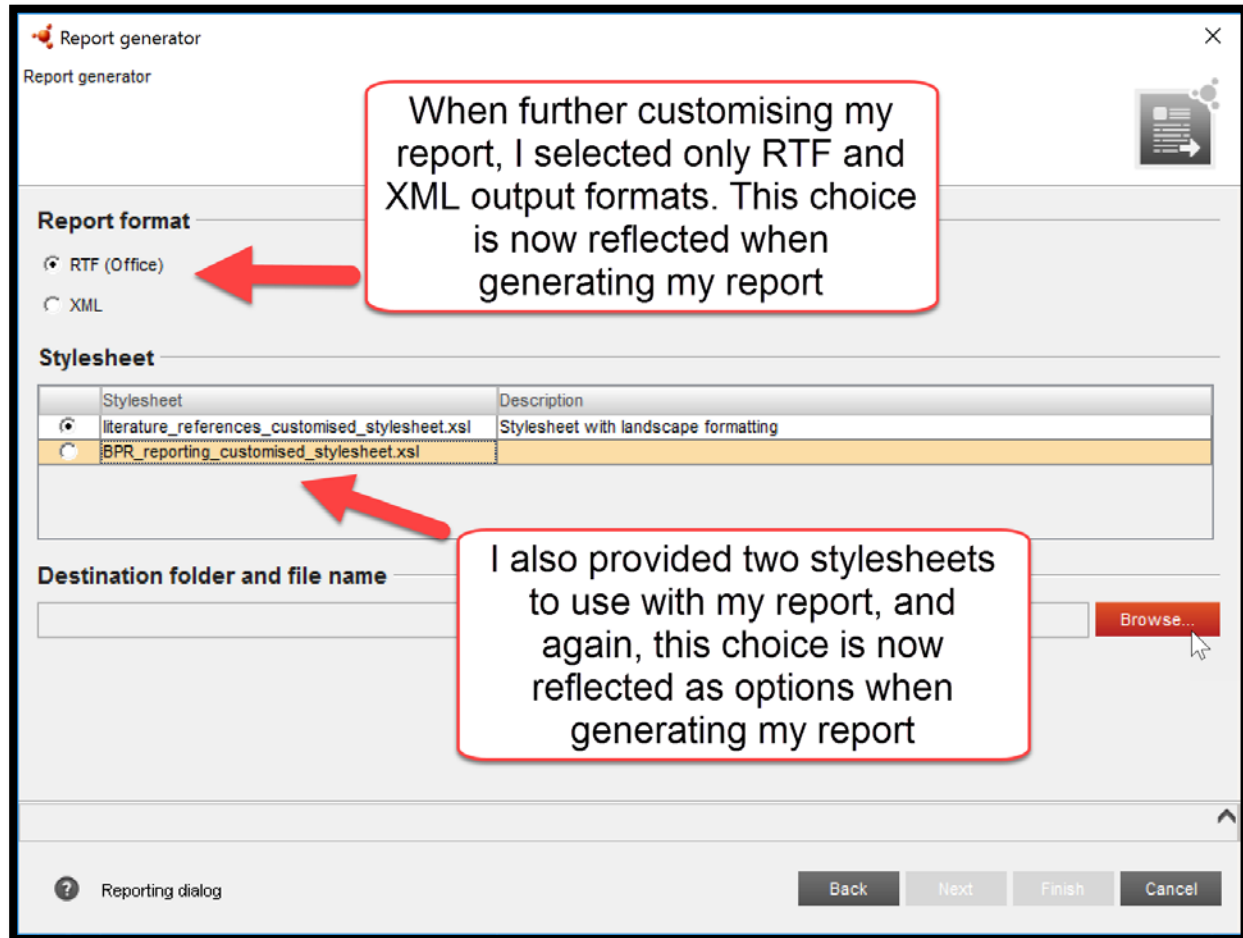
First step of the Report generator wizard

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

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



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>

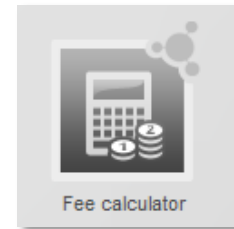
Fee calculator



Fee calculator



- The Fee Calculator allows registrants to estimate the fee to be paid for their REACH dossiers
- The fee calculation is based on the company size, tonnage band and confidentiality claims included in the IUCLID dossier
- Use the calculator before submitting the dossier in REACH-IT and make sure that you:
 - Register in the right tonnage band
 - You haven't claimed unwanted confidentiality claims

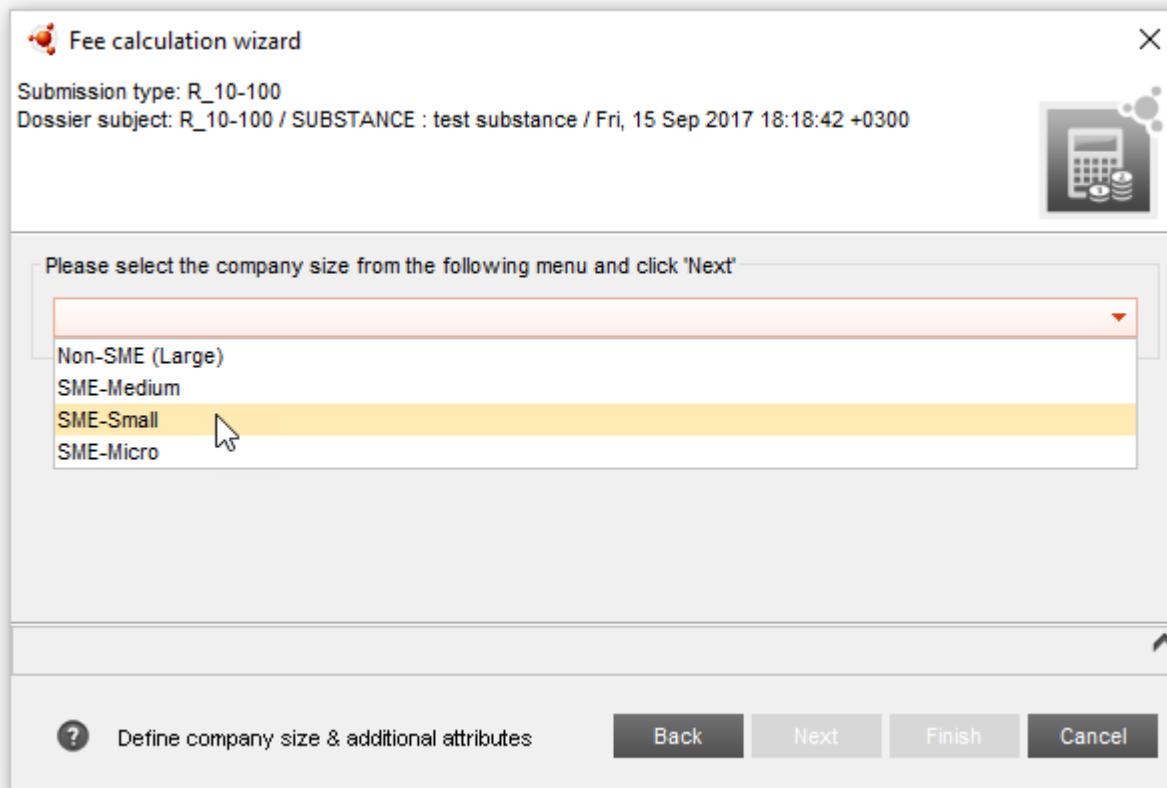


Dossier Name	Subject Name	Creation date
R_JS_MBER / SUBST, 2-[2-(6,6-dimethylbicy / Thu, 26 Oct 2017 15:4...	No Fail	Thu, 26 Oct 2017 15:40:...
R_JS_MBER / SUBST, 2-[2-(6,6-dimethylbicy / Thu, 26 Oct 2017 15:3...		Oct 2017 15:38:...
R_INT_JS_MBER / SU 2-[2-(6,6-dimethylbicy / Thu, 26 Oct 2017 15:3...		Oct 2017 15:33:...
R_JS_MBER / SUBST, 2-[2-(6,6-dimethylbicy / Thu, 26 Oct 2017 15:3...		Oct 2017 15:32:...
R_INT_TR_1-1000 / S 2-[2-(6,6-dimethylbicy / Thu, 26 Oct 2017 15:3...		Thu, 26 Oct 2017 15:31:...

- Open
- Print...
- Generate report...
- Export...
- Delete
- Validate...
- Dissemination preview...
- Calculate fee...
- Compare...

Selecting the company size

- Select the company size as indicated in REACH-IT
- When indicating your company size in REACH-IT make sure that you do it accordance with Commission Recommendation 2003/361/EC



Fee calculation wizard

Submission type: R_10-100
Dossier subject: R_10-100 / SUBSTANCE : test substance / Fri, 15 Sep 2017 18:18:42 +0300

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

- Non-SME (Large)
- SME-Medium
- SME-Small
- SME-Micro

Define company size & additional attributes

Back Next Finish Cancel

Indicators needed for the fee calculation

- Some indicators will appear when there are specific confidentiality claims in the dossier or when the fee waiver has been claimed
- When a confidentiality has been claimed for the IUPAC name and/or the Safety Data Sheet, you will need to indicate whether:
 - the substance is hazardous and if the substance is PBT or vPvB
 - 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 already included in the dossier
- 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

Indicators needed for the fee calculation

- 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

- 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

- Annex III criteria indicator

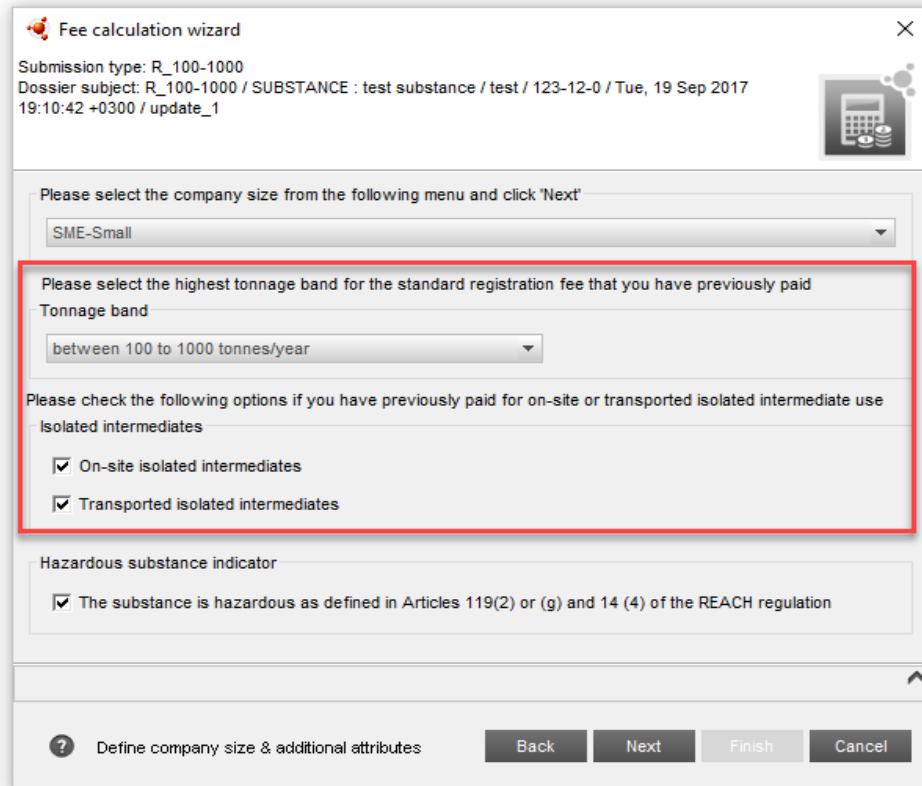
Check the following option if the Annex III criteria are not fulfilled

Annex III criteria indicator

- Not fulfilling Annex III criteria and voluntarily providing Annex VII. This means that:
 - there is no indication that the substance has CMR or PBT/vPvB properties, and
 - there is no indication that this is a substance with dispersive or diffuse uses, classified as hazardous for human health or as an environmental hazard under the CLP Regulation, and
 - the full Annex VIII is being provided

Calculate the fee of dossier updates

- If the dossier is an update, select the tonnage band of the previous paid submission
- Tick the appropriate box if the on-site or transported intermediate use has been previously paid



Fee calculation wizard

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

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

SME-Small

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

Tonnage band

between 100 to 1000 tonnes/year

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

Isolated intermediates

On-site isolated intermediates

Transported isolated intermediates

Hazardous substance indicator

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

Define company size & additional attributes

Back Next Finish Cancel

Fee calculator



Result window

- Fees calculated according to the information contained in the dossier and the information you provided in the indicators
- Table with the description and exact amount charged for each fee applied
- Section of the dossier where the confidentiality has been claimed
- At the bottom of the table: total amount of all the fees

Fee calculation wizard [Close]

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

Selected values

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

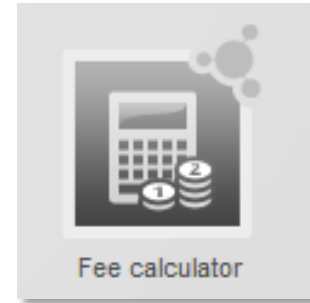
No ^	Fee description	Fee amount	Select
1	Fee for the update of registrations under article 22 from 10-100 tonnes range to over 1000 tonnes range	10159.0	<input checked="" type="checkbox"/>
2	Request of confidentiality for relevant tonnage band (dossier header)	571.0	<input checked="" type="checkbox"/>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

Total amount: € 14,154

Fee amounts [Back] [Next] [Finish] [Cancel]

Remember that...

- The fees calculated by the Fee calculator are only estimates
- The real invoice will be issued by REACH-IT after the submission of the dossier to ECHA

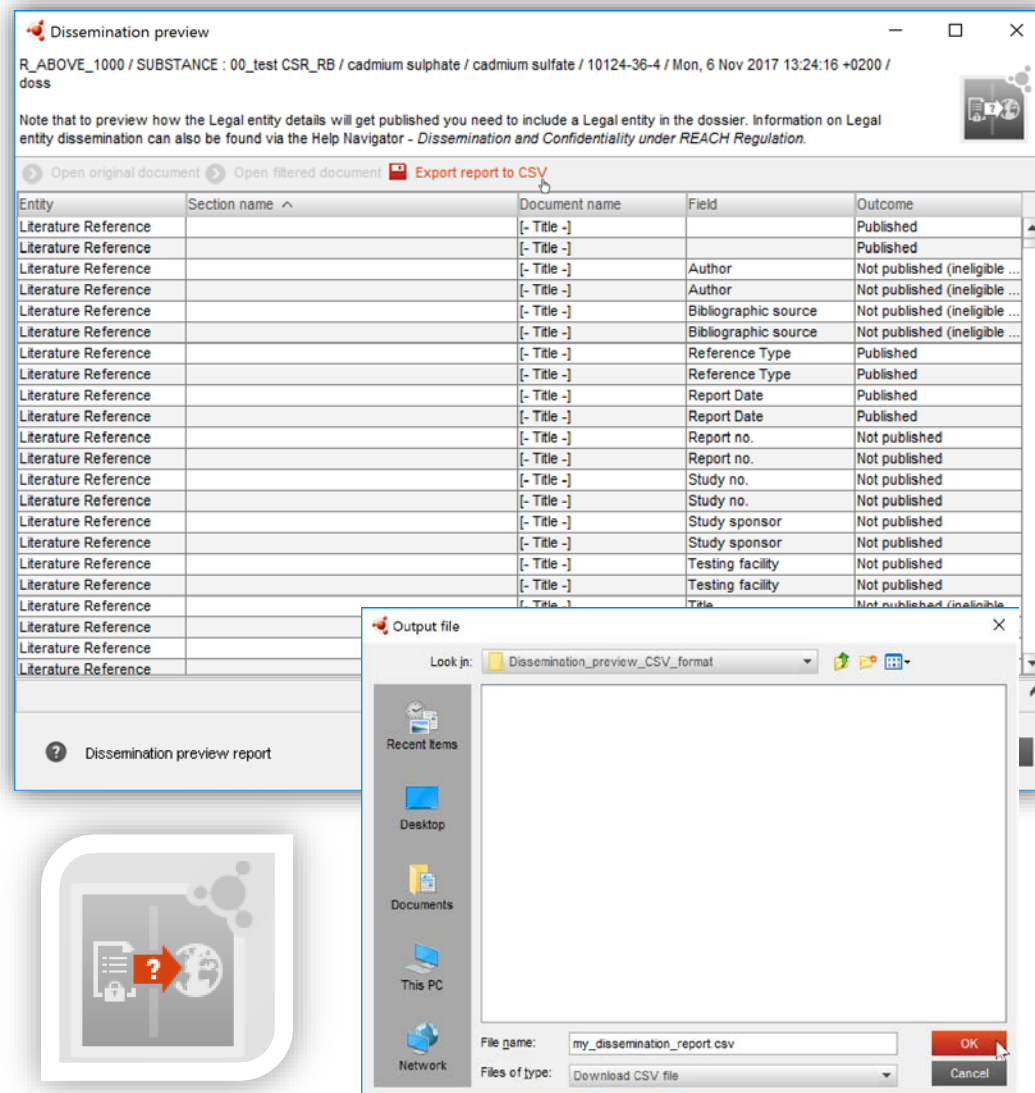


Dissemination preview



Dissemination preview

- Possibility to export and save the dissemination preview report as CSV file
- The report can then be opened in MS Excel
- In MS Excel, the report can then be further filtered and sorted, for example:
 - to only show the information which is published, or certain sections



The screenshot shows the 'Dissemination preview' window in IUCLID 6. The window title is 'Dissemination preview' and the URL is 'R_ABOVE_1000 / SUBSTANCE : 00_test_CSR_RB / cadmium sulphate / cadmium sulfate / 10124-36-4 / Mon, 6 Nov 2017 13:24:16 +0200 / doss'. A note states: 'Note that to preview how the Legal entity details will get published you need to include a Legal entity in the dossier. Information on Legal entity dissemination can also be found via the Help Navigator - Dissemination and Confidentiality under REACH Regulation.' Below the note are three buttons: 'Open original document', 'Open filtered document', and 'Export report to CSV'. The main area contains a table with the following columns: Entity, Section name, Document name, Field, and Outcome. The table lists various 'Literature Reference' entries with their respective fields and outcomes. An 'Output file' dialog box is open in the foreground, showing the file name 'Dissemination_preview_CSV_format' and the file type 'Download CSV file'. The 'File name' field contains 'my_dissemination_report.csv' and the 'Files of type' dropdown is set to 'Download CSV file'. The 'OK' button is highlighted.

Entity	Section name	Document name	Field	Outcome
Literature Reference		[- Title -]		Published
Literature Reference		[- Title -]		Published
Literature Reference		[- Title -]	Author	Not published (ineligible ...)
Literature Reference		[- Title -]	Author	Not published (ineligible ...)
Literature Reference		[- Title -]	Bibliographic source	Not published (ineligible ...)
Literature Reference		[- Title -]	Bibliographic source	Not published (ineligible ...)
Literature Reference		[- Title -]	Reference Type	Published
Literature Reference		[- Title -]	Reference Type	Published
Literature Reference		[- Title -]	Report Date	Published
Literature Reference		[- Title -]	Report Date	Published
Literature Reference		[- Title -]	Report no.	Not published
Literature Reference		[- Title -]	Report no.	Not published
Literature Reference		[- Title -]	Study no.	Not published
Literature Reference		[- Title -]	Study no.	Not published
Literature Reference		[- Title -]	Study sponsor	Not published
Literature Reference		[- Title -]	Study sponsor	Not published
Literature Reference		[- Title -]	Testing facility	Not published
Literature Reference		[- Title -]	Testing facility	Not published
Literature Reference		[- Title -]	Title	Not published (ineligible ...)



Comparison of dossiers



Purpose

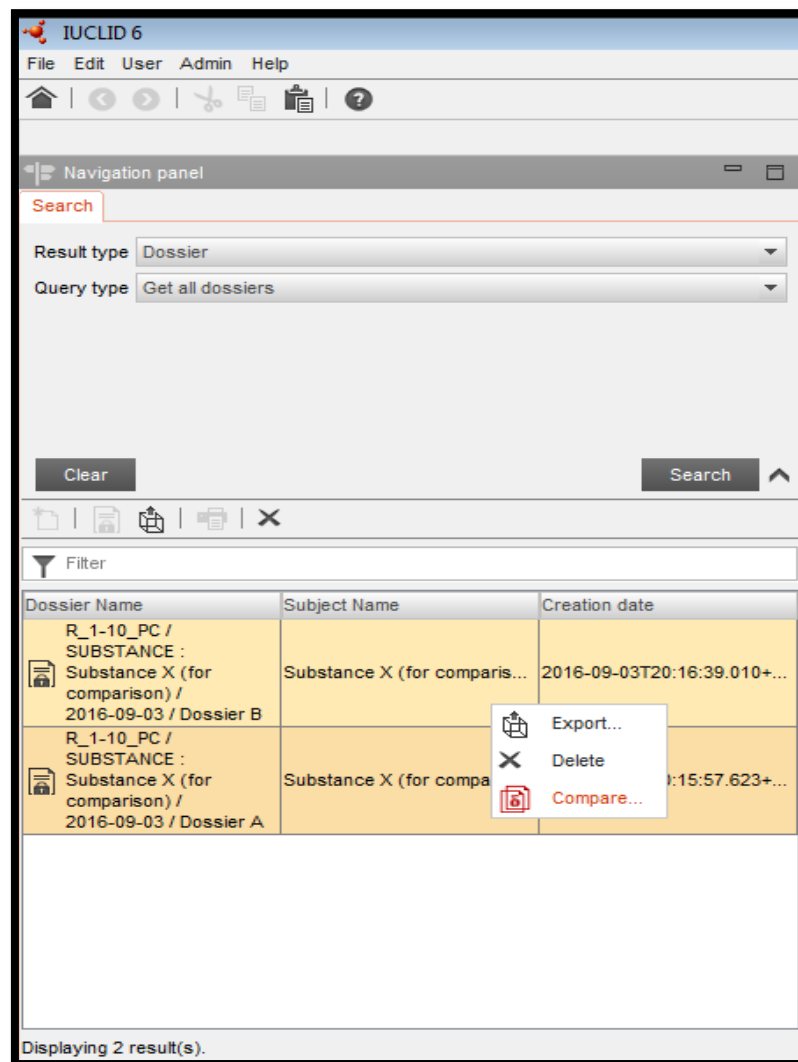
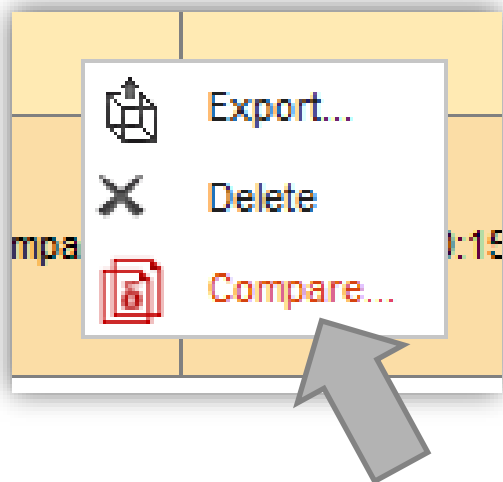
The Comparison tool has been updated and improved in IUCLID 6 to help you:

- To compare whether the same documents exist in two different dossiers, and also
- To compare the **content** of those documents, thereby allowing you to see in much greater detail the similarities and differences between two dossiers

Overview – how it works

- Two dossiers are compared and are considered identical when **ALL** documents within them have the same content of information.
- When the dossiers are found to have same UUIDs but different content, the comparison tool clearly highlights these for you so you can easily identify where the similarities and differences are to be found.

Comparison tool



IUCLID 6

File Edit User Admin Help

Navigation panel

Search

Result type Dossier

Query type Get all dossiers

Clear Search

Filter

Dossier Name	Subject Name	Creation date
R_1-10_PC / SUBSTANCE : Substance X (for comparison) / 2016-09-03 / Dossier B	Substance X (for comparis...	2016-09-03T20:16:39.010+...
R_1-10_PC / SUBSTANCE : Substance X (for comparison) / 2016-09-03 / Dossier A	Substance X (for compa...	2016-09-03T15:57.623+...

Export...
Delete
Compare...

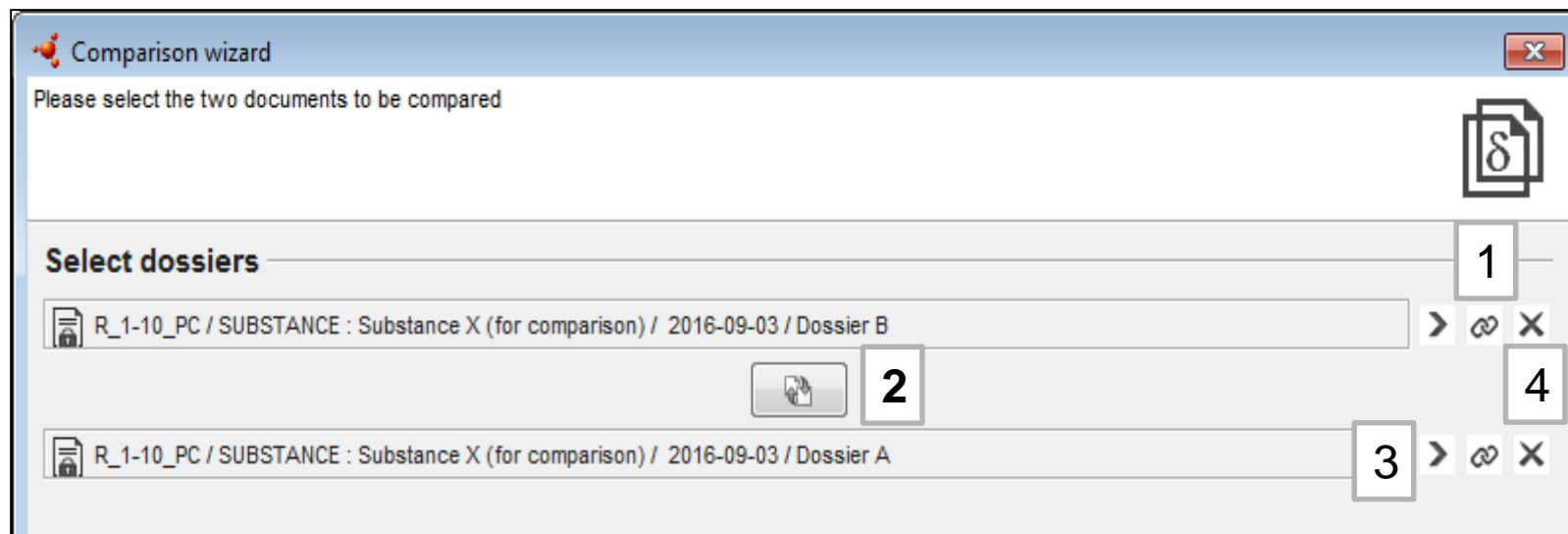
Displaying 2 result(s).

Comparison tool



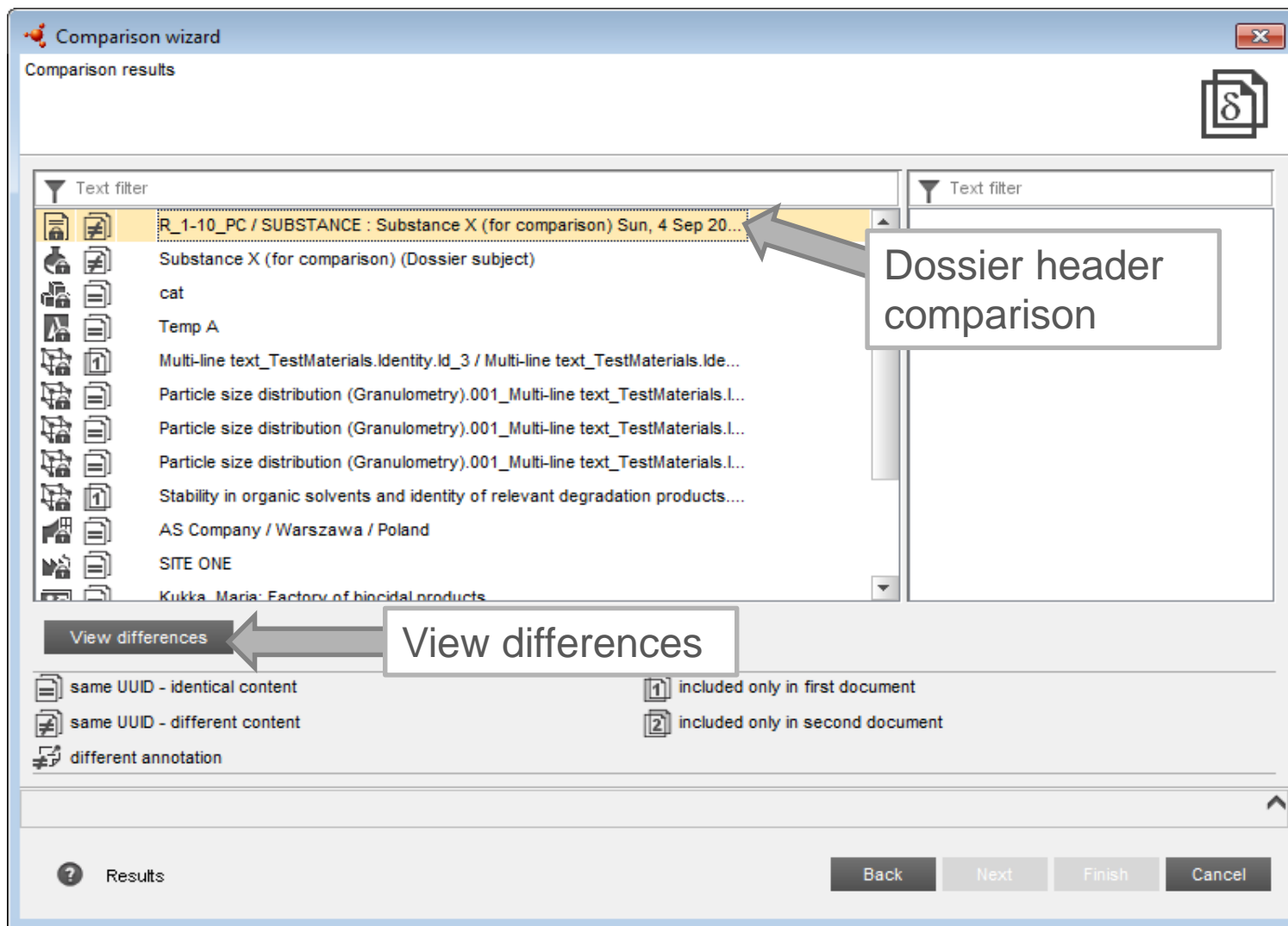
The first step of the Comparison wizard allows you to:

1. Choose a new or different dossier to compare
2. Select which dossier is to be considered as the first/second dossier in the comparison (see the Reference Key in the next wizard step)
3. Display a selected dossier in the data window of IUCLID
4. Remove the currently selected dossier



Comparison tool

Final Comparison step



Comparison wizard

Comparison results

Text filter

- R_1-10_PC / SUBSTANCE : Substance X (for comparison) Sun, 4 Sep 20...
- Substance X (for comparison) (Dossier subject)
- cat
- Temp A
- Multi-line text_TestMaterials.Identity.Id_3 / Multi-line text_TestMaterials.Ide...
- Particle size distribution (Granulometry).001_Multi-line text_TestMaterials.L...
- Particle size distribution (Granulometry).001_Multi-line text_TestMaterials.L...
- Particle size distribution (Granulometry).001_Multi-line text_TestMaterials.L...
- Stability in organic solvents and identity of relevant degradation products....
- AS Company / Warszawa / Poland
- SITE ONE
- Kukka_Maria: Factory of biocidal products

View differences

View differences

same UUID - identical content

same UUID - different content

different annotation

1 included only in first document

2 included only in second document

Results

Back Next Finish Cancel

Comparison tool

View Differences results table

Detailed comparison differences

Selected document > R_1-10_PC / SUBSTANCE : Substance X (for comparison) Sun, 4 Sep 2016 20:52:48 +0300 / Dossier J

Filter

show all show only different show only identical

Field	Value in 1st Document		
DOSSIER.R_1-10_PC	Dossier J		Dossier R
● DOSSIER.R_1-10_PC	Dossier J		Dossier R
SubmissionType			
● JointSubmission	false		false
InformationProvidedByLead			
● ChemicalSafetyReport	false		false
● GuidanceOnSafetyReport	false		false
● ReviewedByAssessor	false		false
TonnageBandsOfRegistrant			
● TonnageBand			
● OnSitelisolated			
● Transportedisolated			
SpecificSubmissions			
● SubmissionIsAnUpdate	false		false
● LastSubmissionType			
ReasonForUpdating			
● RequestDecisionRegulatoryBody	false		false
● SpontaneousUpdate	false		false
DossierSpecificInformation			
● PhaseIn	phase-in		phase-in

Filter

show all show only different show only identical

Comparison tool



Comparison wizard
Comparison results

Text filter

- R_1-10_PC / SUBSTANCE : Substance X (for comp...
- Substance X (for comparison) (Dossier subject)**
- cat
- Temp A
- Template R
- Multi-line text_TestMaterials.Identity.Id_3 / Multi-line t...
- Particle size distribution (Granulometry).001_Multi-lin...
- Particle size distribution (Granulometry).001_Multi-lin...
- Particle size distribution (Granulometry).001_Multi-lin...
- Stability in organic solvents and identity of relevant ...
- AS Company / Warszawa / Poland
- Mark r
- SITE ONE
- Erkens, Kyle; Organisation a
- Kukka, Maria; Factory of biocidal products
- Particle size distribution (Granulometry).001_Multi-lin...
- ANNO 1
- ANNO 1 (FOR COMP
- Annotation1

Text filter

- REACH Registration 1 - 10 tonnes, physicochemical requirements
 - 0 Related information
 - 0.1 Templates
 - Temp A
 - Template R
 - 0.4 Assessment entities
 - Assessment entities
 - CORE / Registered substance as such / Registered substance as such.001 / Substance X (for comparison)
 - 1 General information
 - 1.1 Identification
 - Identification
 - Substance X (for comparison)**
 - 1.2 Composition
 - CORE / Composition / Composition.001 / Substance X (for comparison)
 - CORE / Composition / CM CMC CMC CM 1 / Temp A
 - 1.5 Joint submission
 - CORE / Joint submission / Joint submission.001 / Substance X (for comparison)
 - 2 Classification & Labelling and PBT assessment
 - 2.1 GHS
 - CORE / GHS / GHS.001 / Substance X (for comparison)
 - CORE / GHS / GHS.001 / Substance X (for comparison)
 - 2.2 DSD - DPD
 - CORE / DSD - DPD / DSD - DPD.001 / Substance X (for comparison)
 - 3 Manufacture, use and exposure

View differences

Legend:
same UUID - identical content
same UUID - different content
different annotation
included only in first document
included only in second document

Results

Back Next Finish Cancel

Comparison tool

Detailed comparison differences

Selected document > CORE / GHS / GHS.001 / Substance B

Filter

show all show only different show only identical

Field	Value in 1st Document	Compare state	Value in 2nd Document
Classes			
Statements			
Labelling			
SignalWord			
HazardPictogramBlock			
HazardPictogram			
HazardPictogram[1]			
Code	GHS02: flame		
HazardStatementsBlock			
HazardStatements			
HazardStatements[1]			
HazardStatement	H200: Unstable explosives.		
AdditionalText	additional text field		
PrecautionaryStatementsBlock			
PrecautionaryStatements			
PrecautionaryStatements[1]			
PrecautionaryStatement	P210: Keep away from heat, hot s...		
AdditionalText			
LabelingRequirementsBlock			
LabelingRequirements			
LabelingRequirements[1]			
SupplHazardStatement	EUH006: Explosive with or without...		
AdditionalText			
AdditionalLabelling			

Hazard pictogram code is only in dossier 1

Precautionary statement is in both dossiers but has different content

Inventory management



Purpose

- To help users better manage their Inventory Entities:
 - Test materials
 - Legal entity
 - Legal Entity site
 - Reference Substance
 - Contact
 - Literature reference

Note: This does not include your ‘Chemical Inventories’

Overview – how it works:

- A user can replace one or more existing entities with a **single inventory entity** of the same type
- When a user replaces an entity, that entity will be replaced in every dataset where it is used: Substance / Mixture-Product / Template / Category (the entities in a dossier are not affected)
 - Note that Contact, Reference Substance and Legal Entity are used in other entities and will **also** be replaced.
- Any entity which is replaced is deleted from the IUCLID database
 - Before using the feature, you can save the contents of your current database using the Backup/Restore tool.

Using the Inventory Management to replace **Legal Entity 1** and **Legal Entity 2** with **Legal Entity 3**

Legal Entity 1

- Substance
 - Section 1.5
Lead registrant in a joint submission
- Category
- Legal Entity Site

Legal Entity 2

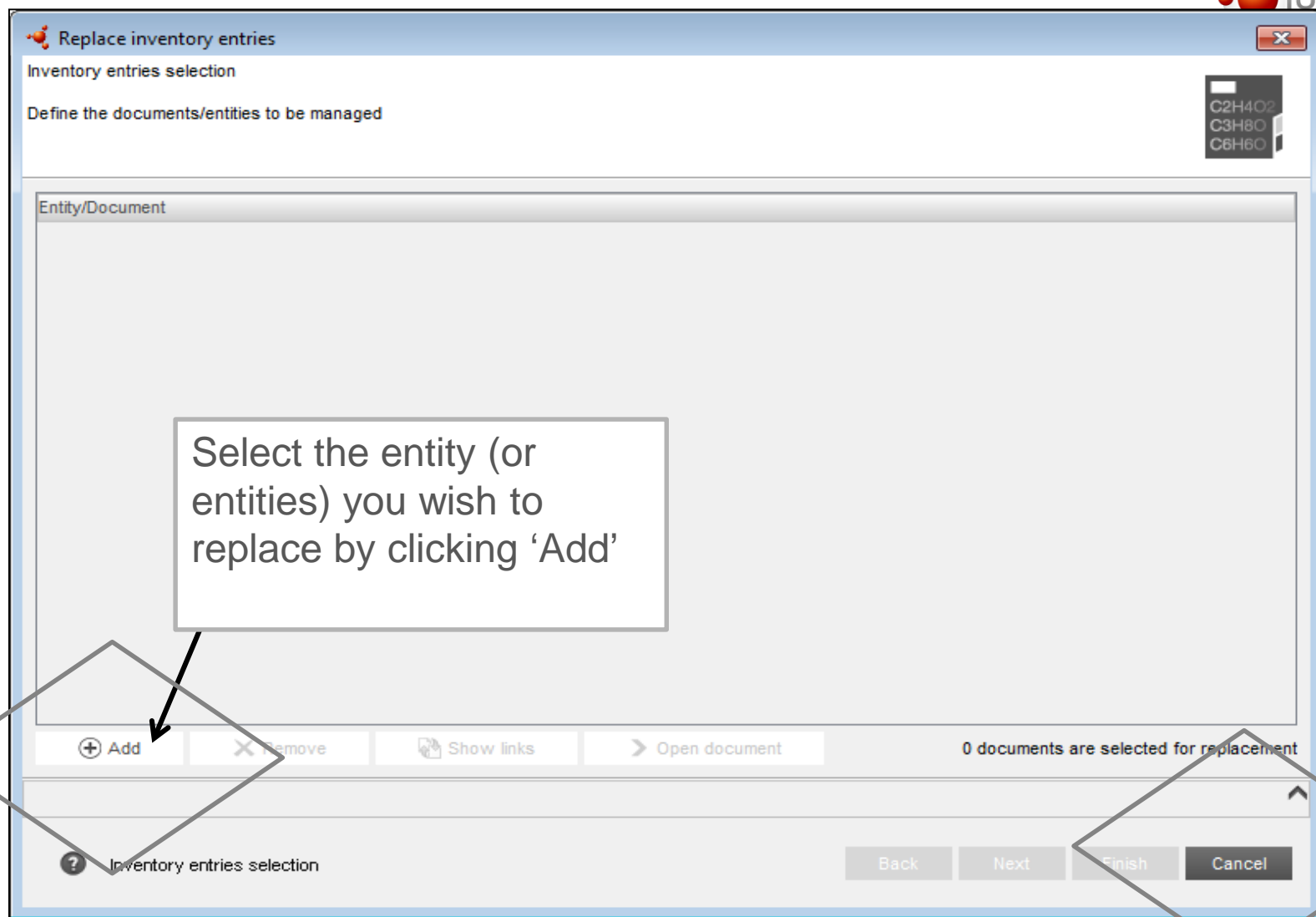
- Substance
 - Section 1.7
 - Section 1.8
- Template
- Mixture-Product
 - Section 1.3

Legal Entity 3

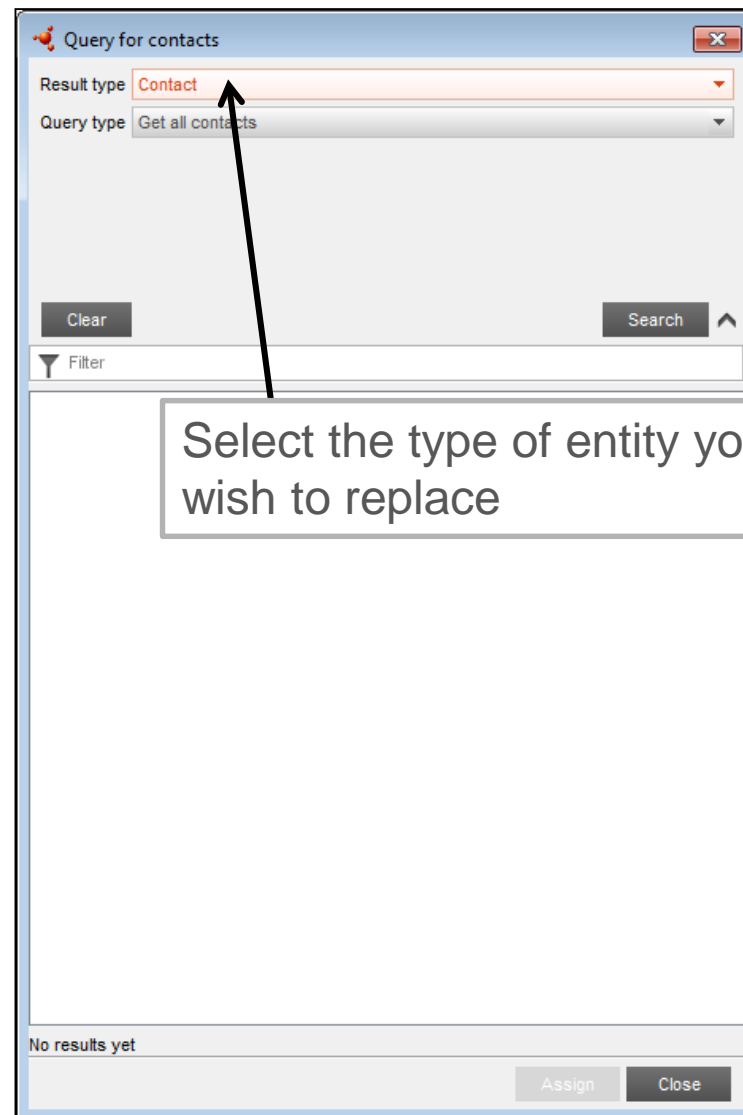
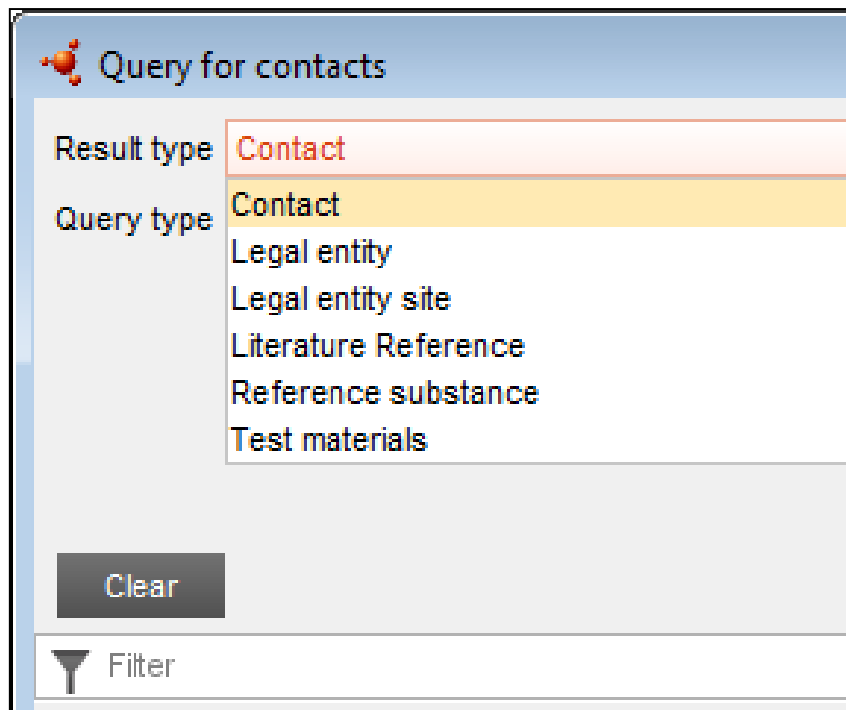
- Substance
 - Section 1.5
 - Section 1.7
 - Section 1.8
- Template
- Mixture-Product
 - Section 1.3
- Category
- Legal Entity Site

- Legal Entity 1 and 2, are also removed from the list of Legal Entities
- When replacing an entity in an Inherited Template, that entity will be replaced in All datasets where that template is used

Inventory Management



Inventory Management



Refine your search using the 'Query Type'

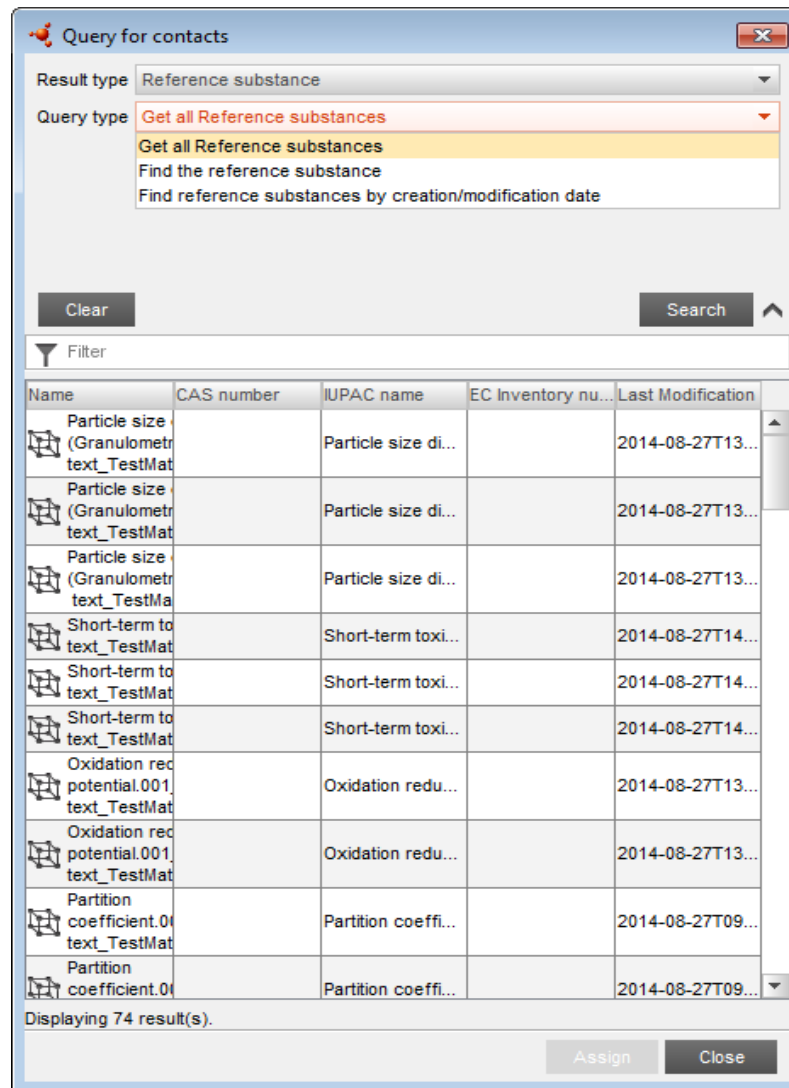
Get all

- Contacts, Legal Entities, Test Materials

Find an entity

- Search using the key information about the entity
- Search through a wildcard asterisk * if not sure as to the whole name

Search by creation/modification date



Query for contacts

Result type: Reference substance

Query type: Get all Reference substances

- Get all Reference substances
- Find the reference substance
- Find reference substances by creation/modification date

Clear Search

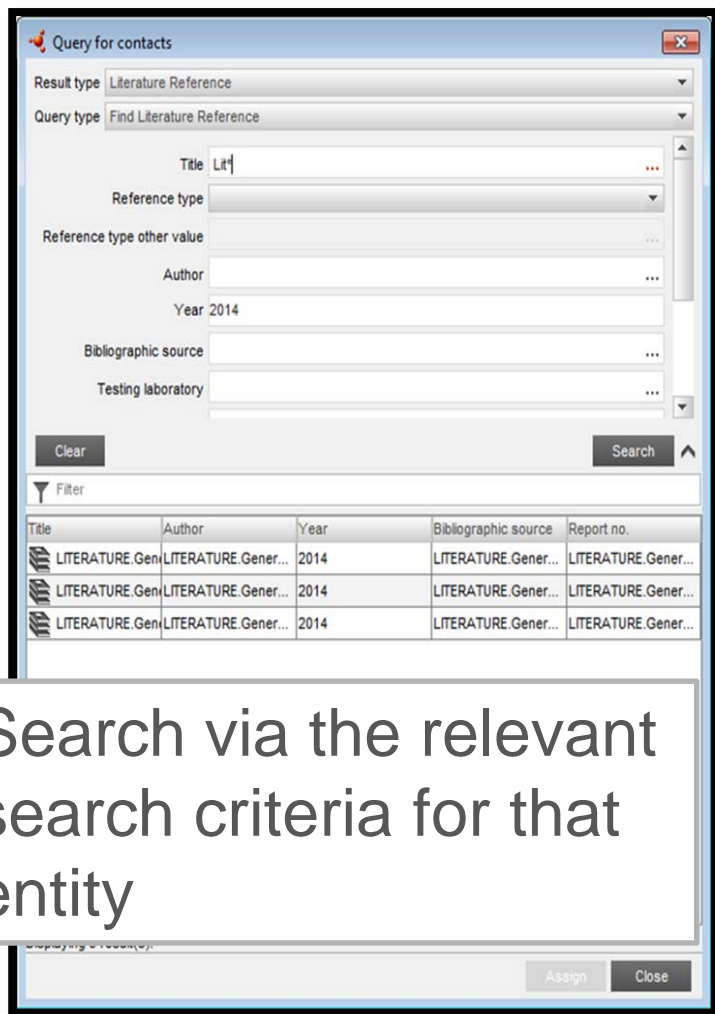
Filter

Name	CAS number	IUPAC name	EC Inventory nu...	Last Modification
Particle size (Granulometr text_TestMat		Particle size di...		2014-08-27T13...
Particle size (Granulometr text_TestMat		Particle size di...		2014-08-27T13...
Particle size (Granulometr text_TestMa		Particle size di...		2014-08-27T13...
Short-term to text_TestMat		Short-term toxi...		2014-08-27T14...
Short-term to text_TestMat		Short-term toxi...		2014-08-27T14...
Short-term to text_TestMat		Short-term toxi...		2014-08-27T14...
Oxidation rec potential.001, text_TestMat		Oxidation redu...		2014-08-27T13...
Oxidation rec potential.001, text_TestMat		Oxidation redu...		2014-08-27T13...
Partition coefficient.0 text_TestMat		Partition coeffi...		2014-08-27T09...
Partition coefficient.0 text_TestMat		Partition coeffi...		2014-08-27T09...

Displaying 74 result(s).

Assign Close

Inventory Management



Query for contacts

Result type: Literature Reference

Query type: Find Literature Reference

Title: Lit

Reference type: [dropdown]

Reference type other value: [dropdown]

Author: [dropdown]

Year: 2014

Bibliographic source: [dropdown]

Testing laboratory: [dropdown]

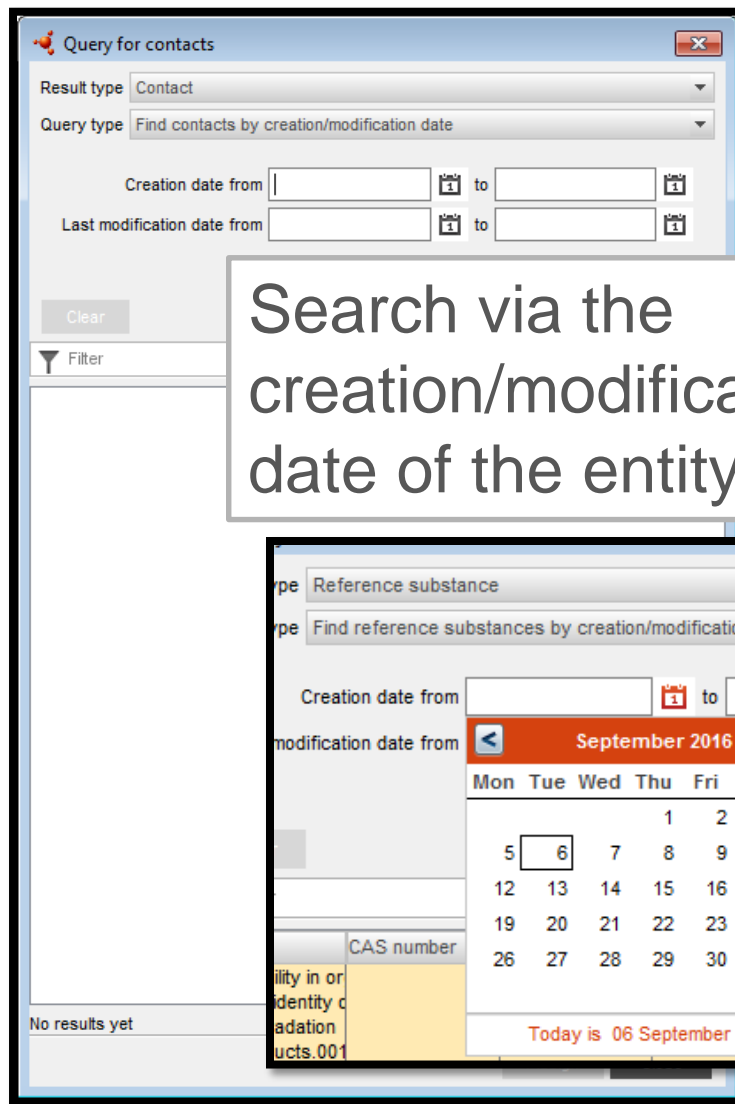
Clear Search

Filter

Title	Author	Year	Bibliographic source	Report no.
LITERATURE.Gen...	LITERATURE.Gener...	2014	LITERATURE.Gener...	LITERATURE.Gener...
LITERATURE.Gen...	LITERATURE.Gener...	2014	LITERATURE.Gener...	LITERATURE.Gener...
LITERATURE.Gen...	LITERATURE.Gener...	2014	LITERATURE.Gener...	LITERATURE.Gener...

Assign Close

Search via the relevant search criteria for that entity



Query for contacts

Result type: Contact

Query type: Find contacts by creation/modification date

Creation date from: [calendar] to: [calendar]

Last modification date from: [calendar] to: [calendar]

Clear

Filter

No results yet

Reference substance

Find reference substances by creation/modification date

Creation date from: [calendar] to: [calendar]

modification date from: [calendar]

CAS number

Today is 06 September 2016

Search via the creation/modification date of the entity

Inventory Management



Query for contacts

Result type: Legal entity

Query type: Get all legal entities

Clear Search

Filter

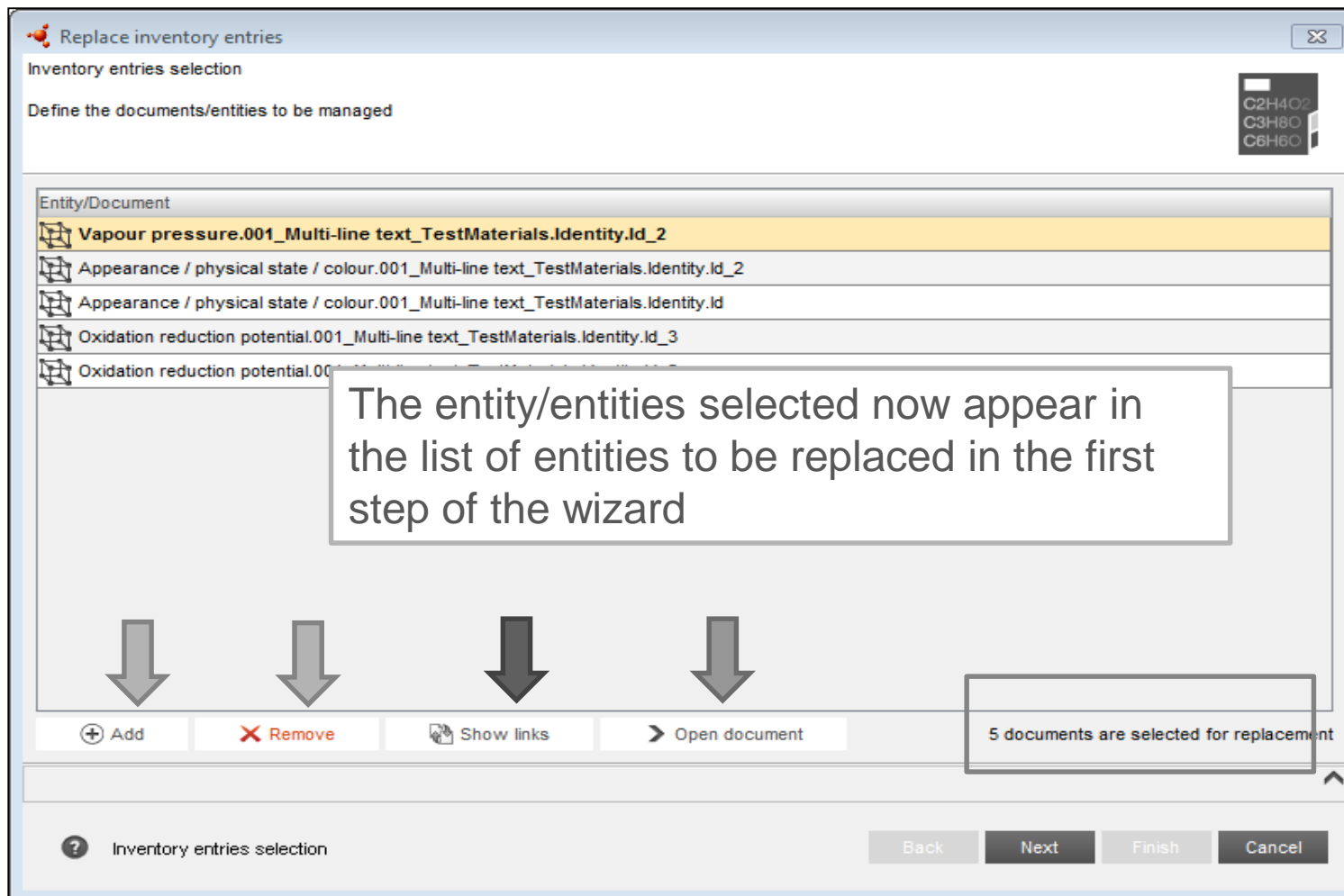
Legal entity name	Legal entity town	Legal entity country	Last modification date
AS Company	Warszawa	Poland	2016-09-02T09:43:4...
Mark r			2016-08-30T08:59:4...
New company	Helsinki	Finland	2016-02-03T16:35:5...
robi LE			2016-03-16T14:41:1...
BP manufacturer	Helsinki	Finland	2013-06-14T10:19:2...

Bulk selection of entities

Displaying 5 result(s).

Assign Close

Inventory Management



Replace inventory entries

Inventory entries selection

Define the documents/entities to be managed

Entity/Document

- Vapour pressure.001_Multi-line text_TestMaterials.Identity.Id_2**
- Appearance / physical state / colour.001_Multi-line text_TestMaterials.Identity.Id_2
- Appearance / physical state / colour.001_Multi-line text_TestMaterials.Identity.Id
- Oxidation reduction potential.001_Multi-line text_TestMaterials.Identity.Id_3
- Oxidation reduction potential.001_Multi-line text_TestMaterials.Identity.Id

The entity/entities selected now appear in the list of entities to be replaced in the first step of the wizard

↓ ↓ ↓ ↓

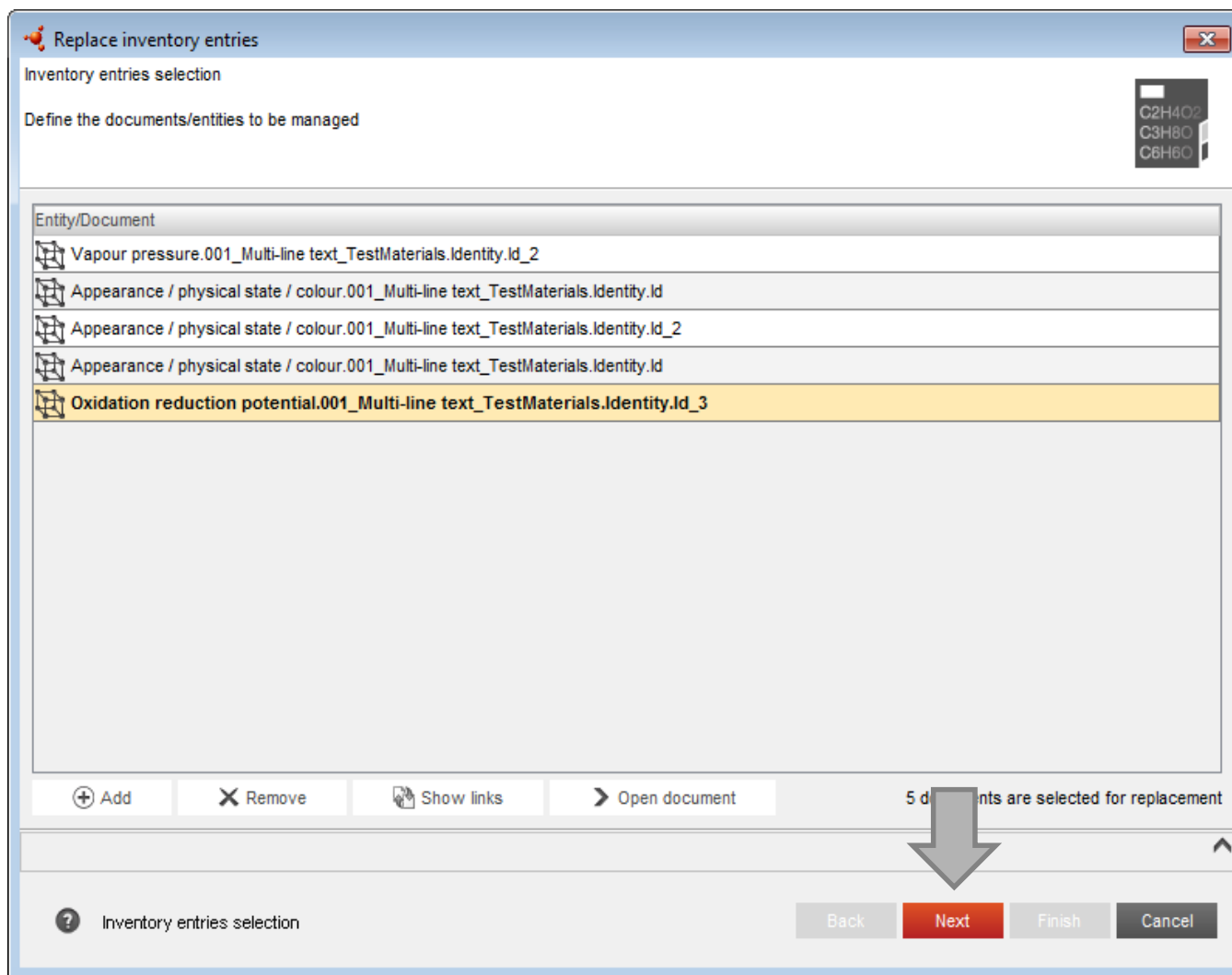
+ Add X Remove Show links > Open document

5 documents are selected for replacement

Inventory entries selection

Back Next Finish Cancel

Inventory Management



Replace inventory entries

Inventory entries selection

Define the documents/entities to be managed

Entity/Document

- Vapour pressure.001_Multi-line text_TestMaterials.Identity.Id_2
- Appearance / physical state / colour.001_Multi-line text_TestMaterials.Identity.Id
- Appearance / physical state / colour.001_Multi-line text_TestMaterials.Identity.Id_2
- Appearance / physical state / colour.001_Multi-line text_TestMaterials.Identity.Id
- Oxidation reduction potential.001_Multi-line text_TestMaterials.Identity.Id_3**

5 documents are selected for replacement

Inventory entries selection

Back Next Finish Cancel

Inventory Management



Replace inventory entries

Inventory entries selection

Define the document/entity to replace the selected ones

Select one document to replace the selected ones

Search box with icons: > ∞ X

Select the entity which will replace the previously selected entity/entities

Back Next Finish Cancel

Query for reference substances

Query type: **Find the reference substance**

Reference: **Find the reference substance**

Find reference substances by creation/modification date

CAS number (Inventory) ...

Inventory number ...

Inventory name ...

CAS number ...

CAS name ...

IUPAC name ...

Clear Search

Filter

Name	CAS number	IUPAC name	EC inventory nu...	Last Modification
Short-term to... text_TestMat		Short-term toxi...		2014-08-27T14...
Short-term to... text_TestMat		Short-term toxi...		2014-08-27T14...
				4-08-27T13...
				4-08-27T13...
				4-08-27T09...
Partition... coefficient.0... text_TestMat		Partition coeffi...		2014-08-27T09...
Partition... coefficient.0... text_TestMat		Partition coeffi...		2014-08-27T09...
Flash point.0...				

Displaying 68 result(s).

Assign Close

Use the Query Type to help define a specific entity

Inventory Management



Assign and move to the Next step

Query for reference substances

Query type: Get all Reference substances

Clear Search

Filter

Name	CAS number	IUPAC name	EC Inventory nu...	Last Modification
Oxidation red potential.001... text_TestMat		Oxidation redu...		2014-08-27T13...
Oxidation red potential.001... text_TestMat		Oxidation redu...		2014-08-27T13...
Short-term toxi text_TestMat		Short-term toxi...		2014-08-27T14...
Short-term toxi text_TestMat		Short-term toxi...		2014-08-27T14...
Short-term toxi text_TestMat		Short-term toxi...		2014-08-27T14...
Partition coefficient.01 text_TestMat		Partition coeffi...		2014-08-27T09...
Partition coefficient.01 text_TestMat		Partition coeffi...		2014-08-27T09...
Partition coefficient.01 text_TestMat		Partition coeffi...		2014-08-27T09...
Flash point.0 text_TestMat		Flash point.001...		2014-08-27T13...
Flash point.0 text_TestMat		Flash point.001...		2014-08-27T13...
Flash point.0 text_TestMat		Flash point.001...		2014-08-27T13...

Displaying 74 result(s).

Assign Close

Replace inventory entries

Inventory entries selection

Define the document/entity to replace the selected ones

Select one document to replace the selected ones

Oxidation reduction potential.001_Multi-line text_TestMaterials.Identity.Id_2 / Oxidation reduction potential.001_Multi-line text_TestMaterials.Identity.Id_2

Inventory entries selection

Back Next Finish Cancel






Replace inventory entries

Confirmation of inventory entries replacement



Confirm the documents/entities to be replaced

C2H4O2
C3H8O
C6H6O


Please confirm that the 5 selected entities

Entity/Document
 Appearance / physical state / colour.001_Multi-line text_TestMaterials.Identity.Id
 Oxidation reduction potential.001_Multi-line text_TestMaterials.Identity.Id_3
 Appearance / physical state / colour.001_Multi-line text_TestMaterials.Identity.Id_2
 Vapour pressure.001_Multi-line text_TestMaterials.Identity.Id_2
 Appearance / physical state / colour.001_Multi-line text_TestMaterials.Identity.Id

Entities which will be replaced

 Show links  Open document


will be replaced by the following entry

 Oxidation reduction potential.001_Multi-line text_TestMaterials.Identity.Id_2 / Oxidation reduction potential.001_Multi-line text_TestMaterials.Identity.Id_2

Entity which will be replacing all entities listed above

Once proceeding with this replacement :

- the 5 selected entries will be deleted
- all the references (inside raw datasets) to these 5 entries will

 Confirmation of inventory entries replacement

Back **Next** **Finish** **Cancel**

Inventory Management






Replace inventory entries


Confirmation of inventory entries replacement

Confirm the documents/entities to be replaced


C2H4O2
C3H8O
C6H6O

Please confirm that the 5 selected entities

Entity/Document
 Appearance / physical state / colour.001_Multi-line text_TestMaterials.Identity.Id
 Oxidation reduction potential.001_Multi-line text_TestMaterials.Identity.Id_3
 Appearance / physical state / colour.001_Multi-line text_TestMaterials.Identity.Id_2
 Vapour pressure.001_Multi-line text_TestMaterials.Identity.Id_2
 Appearance / physical state / colour.001_Multi-line text_TestMaterials.Identity.Id

 Show links > Open document

will be replaced by the following entry

 Oxidation reduction potential.001_Multi-line text_TestMaterials.Identity.Id_2 / Oxidation reduction potential.001_Multi-line text_TestMaterials.Identity.Id_2

Once proceeding with this replacement :

- the 5 selected entries will be deleted
- all the references (inside raw datasets) to these 5 entries will be replaced by references to the chosen inventory entry

Back Next **Finish** Cancel

Open the entity itself by clicking on 'Open Document'

Review what the entities are linked to by clicking on 'Show links'

Replace inventory entries

Replacement report

Report for the inventory entries replacements
Job ID: 6, execution date 02/09/2016 15:07:56

Replaced documents

Entity/Document	Document type	Document UUID
Appearance / physical state / colour.001_Multi-line text_TestMaterials.Identity.Id_2	Reference substance	a85141be-499f-37f2-9ad5-c24c786b0e23
Appearance / physical state / colour.001_Multi-line text_TestMaterials.Identity.Id	Reference substance	fe445b9b-b658-3dd6-b330-a77b7edc710e
Vapour pressure.001_Multi-line text_TestMaterials.Identity.Id_2	Reference substance	26ac2edb-e69a-3802-bad3-d0b940d6cb79
Oxidation reduction potential.001_Multi-line text_TestMaterials.Identity.Id_3	Reference substance	af304eb0118c
Appearance / physical state / colour.001_Multi-line text_TestMaterials.Identity.Id	Reference substance	901402b7bce

Replaced entity/entities

Document that replaced the above list

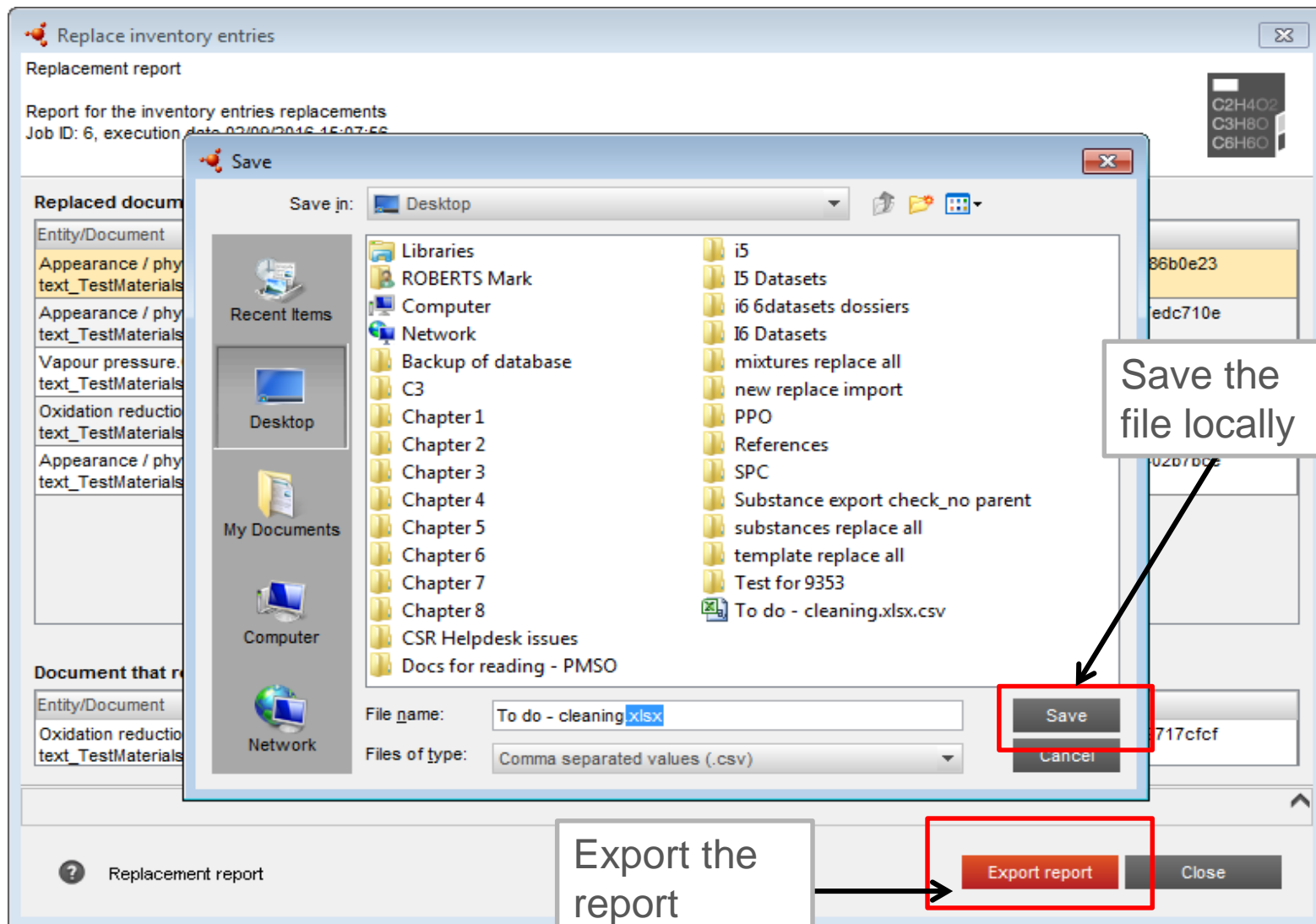
Entity/Document	Document type	Document UUID
Oxidation reduction potential.001_Multi-line text_TestMaterials.Identity.Id_2	Reference substance	1961dd75-0419-316c-9ce2-60a69717cfcf

The entity which has replaced the list above

Replacement report

Export report Close

Inventory Management



The screenshot displays the 'Replace inventory entries' dialog box in IUCLID 6. A 'Save' dialog box is overlaid on top, showing the file 'To do - cleaning.xlsx.csv' being saved to the Desktop. The 'Save' dialog box has a 'Save' button highlighted with a red box. A callout box with the text 'Save the file locally' and an arrow points to this button. Below the 'Save' dialog box, the 'Export report' button in the main dialog is also highlighted with a red box. A callout box with the text 'Export the report' and an arrow points to this button. The background shows a list of replaced documents and a 'Replacement report' section.

Compatibility between IUCLID versions



Note for REACH users

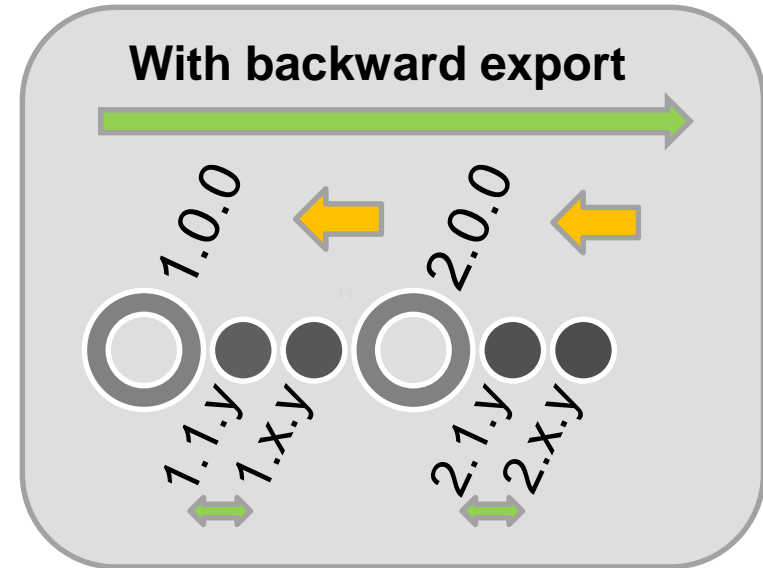
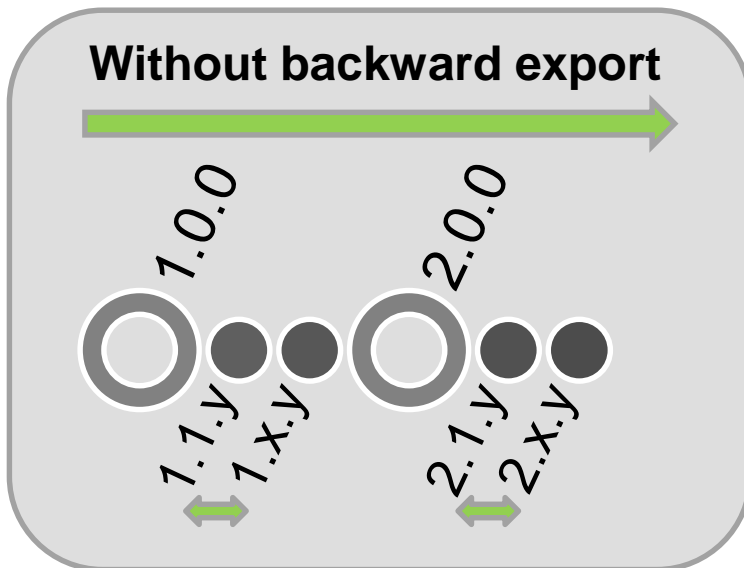
- IUCLID 6 is updated on 15 November. The new version (6.2) brings fixes and improvements.
- Although this update contains improvements, it is not mandatory for the users that need to prepare REACH registrations as ECHA IT systems will continue to be fully compatible with the version of IUCLID 6 published in April 2016 as well as this new version.
- In order to minimise the impact of this new version, ECHA has managed to provide a new export option that allows to exchange data generated with different versions of IUCLID 6.
- IUCLID users have the liberty to choose the most appropriate time for their IUCLID update (e.g. before or after the deadline) and still be able to submit dossiers to ECHA or exchange data between users, regardless of when they decide to update.
- The changes in this new version of IUCLID have no impact in the completeness check decisions by ECHA.

Validation assistant

- The Validation Assistant has been updated in order to work in the same way as before, i.e. no impact for REACH users, e.g.
 - Adapted all business rules and completeness check rules that check section 13 to the new IUCLID 6 v.2.0.0 format
- At the same time improvements have been made, for example
 - Implemented new quality rules (QLT) for hazard endpoints (sections 7.3.1, 7.3.2, 7.4.1, 7.6.1, 7.8.1, 7.8.2)
 - Improved completeness check rule TCC_0102_20 which checks that UVCB substances contain a composition or a justification for deviations
 - A new validation scenario for the new submission type 'Exchange of experimental data' (outside the REACH or CLP regulatory context)
- Full details are available in the release notes

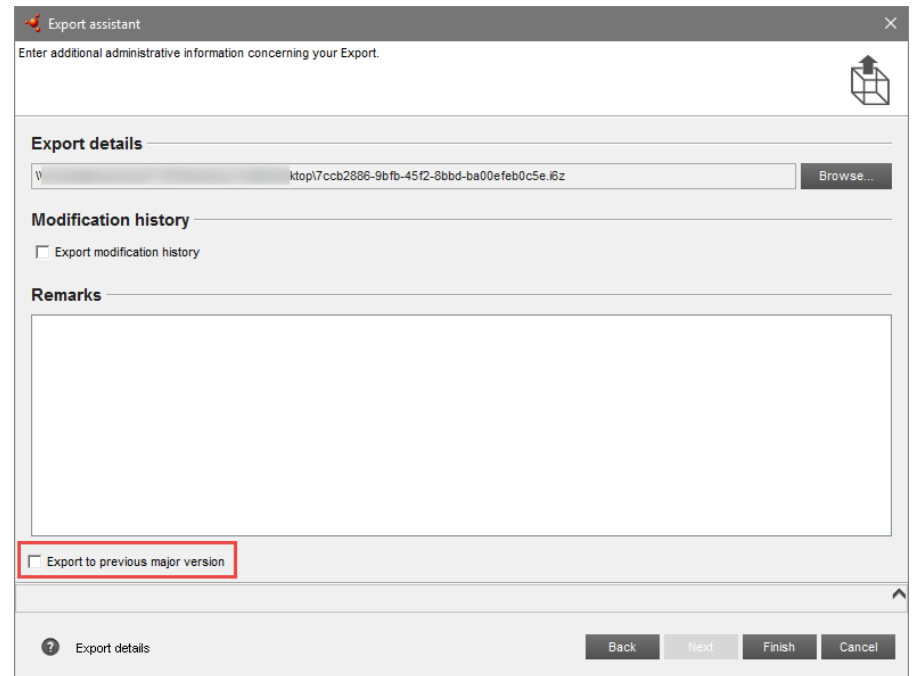
Extension of the compatibility between IUCLID versions

- Forward migration is still maintained (*i.e. the latest version of IUCLID 6 can accept all IUCLID 6, and IUCLID 5.6, files*)
- Aim: export of .i6z files from IUCLID 6 v2.0.0 that can be loaded in IUCLID6 v1.x.y
- Backward migration rules have been defined



Export in the previous version format

- Using the export function, there is an option to export to the previous IUCLID 6 format 'Export to previous major version'
- This option is available for datasets and dossiers
- Also available for bulk export
- You can use this option when you need to exchange information with a user who is still using IUCLID 6 version 1.x



The screenshot shows the 'Export assistant' dialog box in IUCLID 6. The title bar reads 'Export assistant'. Below the title bar, there is a subtitle: 'Enter additional administrative information concerning your Export.' The dialog is divided into several sections:

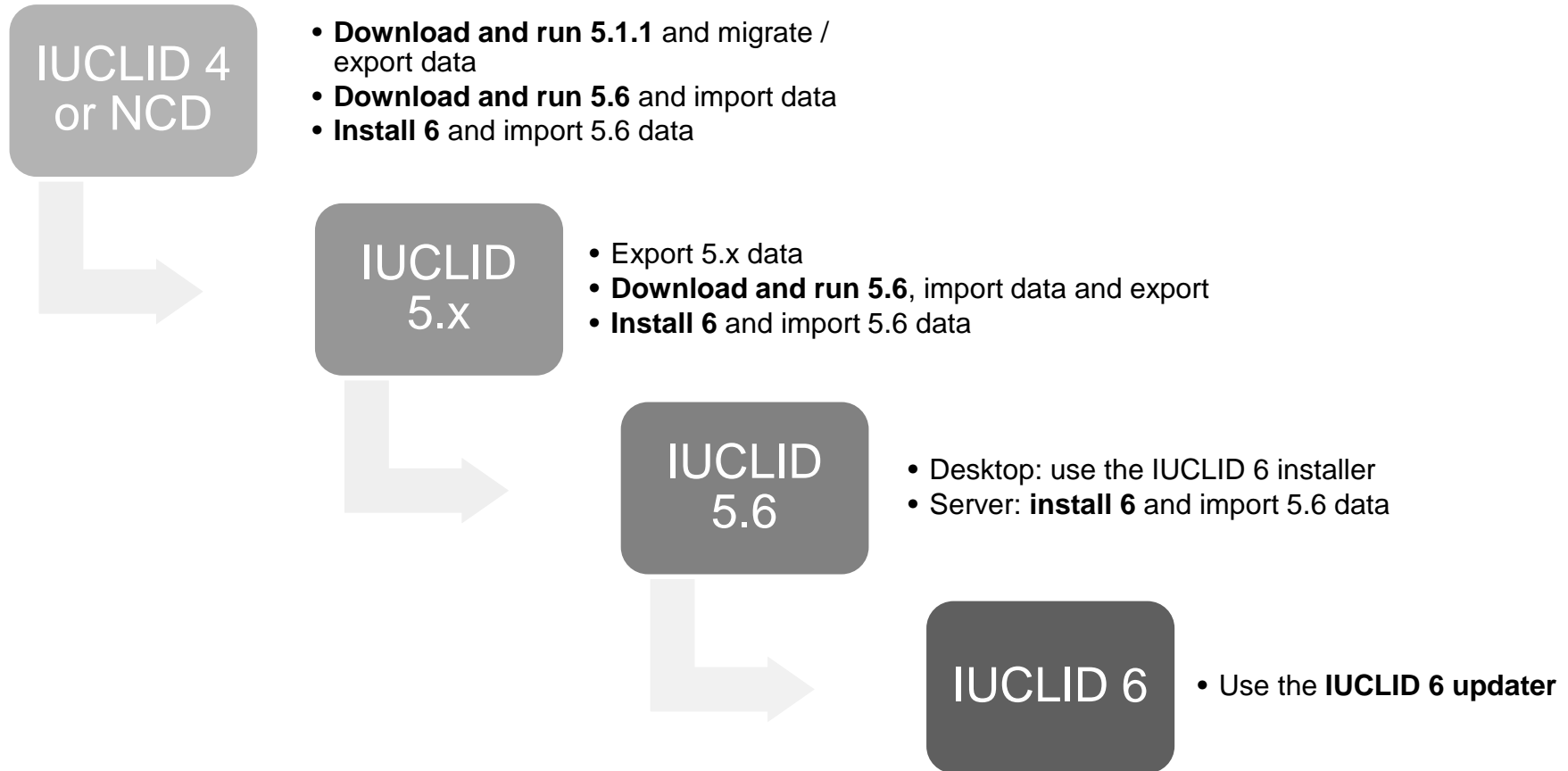
- Export details:** A text input field contains the value 'ktopl7ccb2886-9bfb-45f2-8bbd-ba00efeb0c5e.j6z'. To the right of the field is a 'Browse...' button.
- Modification history:** A checkbox labeled 'Export modification history' is currently unchecked.
- Remarks:** A large, empty text area for entering remarks.
- Export to previous major version:** A checkbox at the bottom of the dialog is checked and highlighted with a red rectangular box.

At the bottom of the dialog, there is a status bar with a question mark icon and the text 'Export details'. On the right side of the status bar, there are four buttons: 'Back', 'Next', 'Finish', and 'Cancel'.

What happens when exporting to the previous format?

- Backward migration rules are in place to transfer the information back to its previous location (reverse migration)
- When the backward migration is not possible, for example for new fields or new phrases in picklist, or new documents, the information is migrated to
 - The 'other:' field or a remark field if available (e.g. for picklists)
 - A generic text field (e.g. remarks or summary)
 - An attachment
- The data is kept during backward migration but the structure is lost in some cases
- When migrating back to the latest version of IUCLID 6, the standard migration rules are executed (i.e. the structure lost during the backward export is **not** recovered)

Different processes depending on your starting point

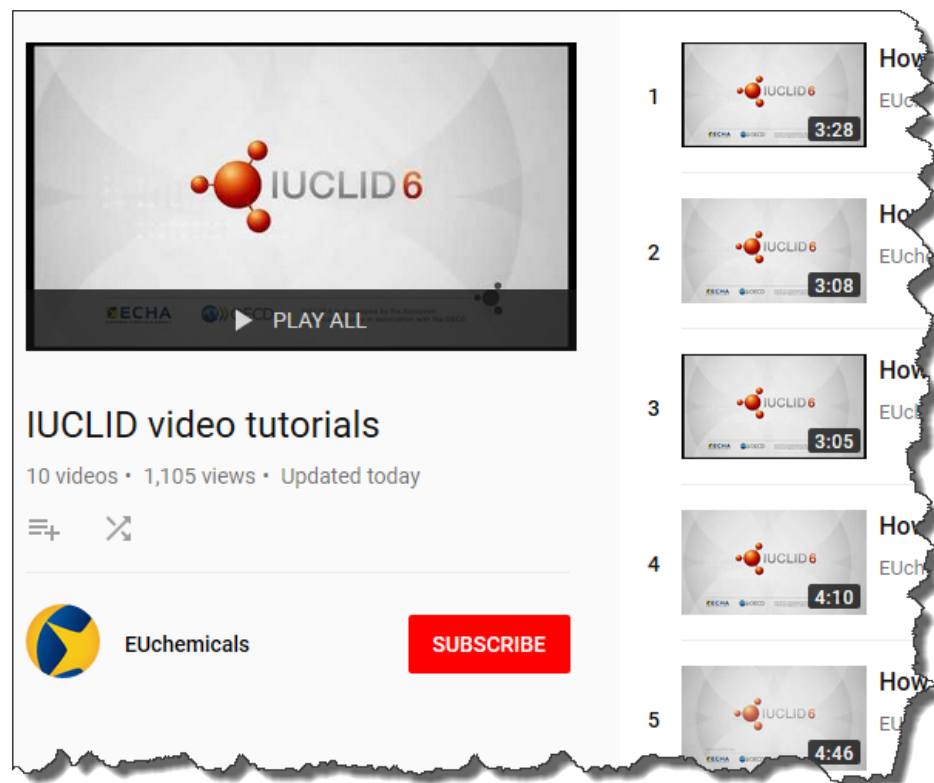


More information



Video tutorials

- Please check our video tutorials on the YouTube playlist
 - Install and update IUCLID 6
 - Run the Validation Assistant
 - Fee calculator
 - Exchange data between versions
 - IUCLID Cloud videos



IUCLID video tutorials

10 videos • 1,105 views • Updated today

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- 1 IUCLID 6 3:28
- 2 IUCLID 6 3:08
- 3 IUCLID 6 3:05
- 4 IUCLID 6 4:10
- 5 IUCLID 6 4:46

<https://www.youtube.com/playlist?list=PLOPGDACSD6qyDkdXwPua1Fjb5bJksY75k>

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





Thank you for your participation

echa.eu

iuclid6.echa.europa.eu

oecd.org/ehs/templates



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

