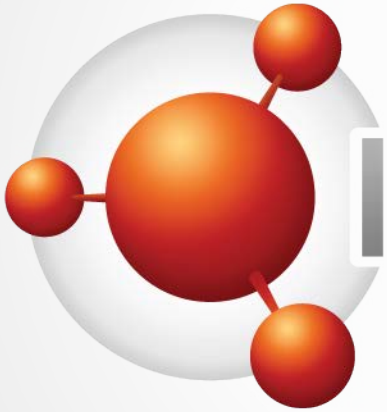


IUCLID 6

ECHA
EUROPEAN CHEMICALS AGENCY

OECD

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

REACH Stakeholder's IT Tools training

30 January 2018

ECHA EUROPEAN CHEMICALS AGENCY

OECD

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

Introduction to IUCLID

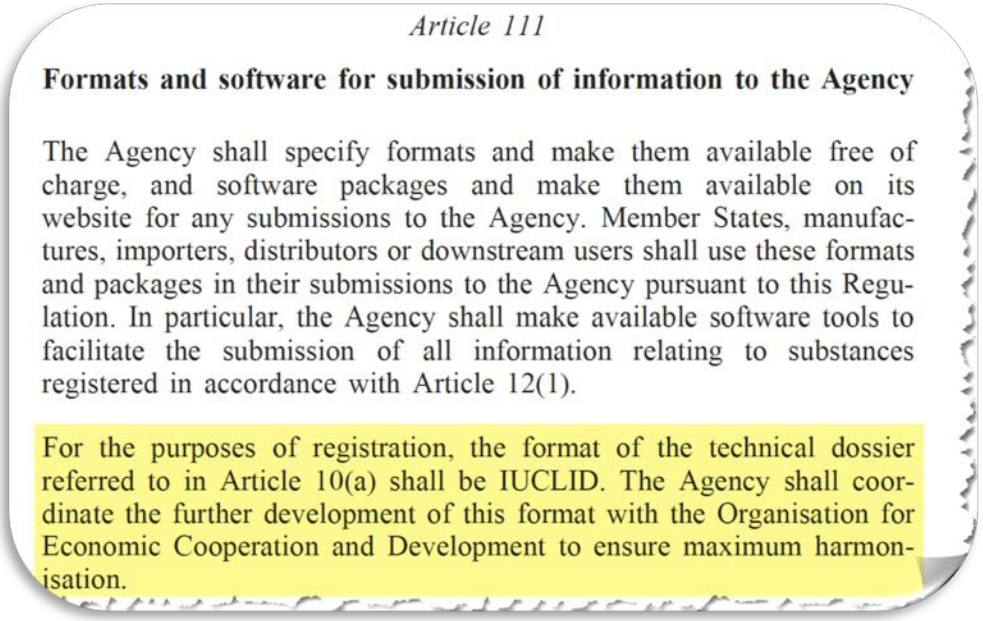
What is IUCLID? A multi-purpose tool

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



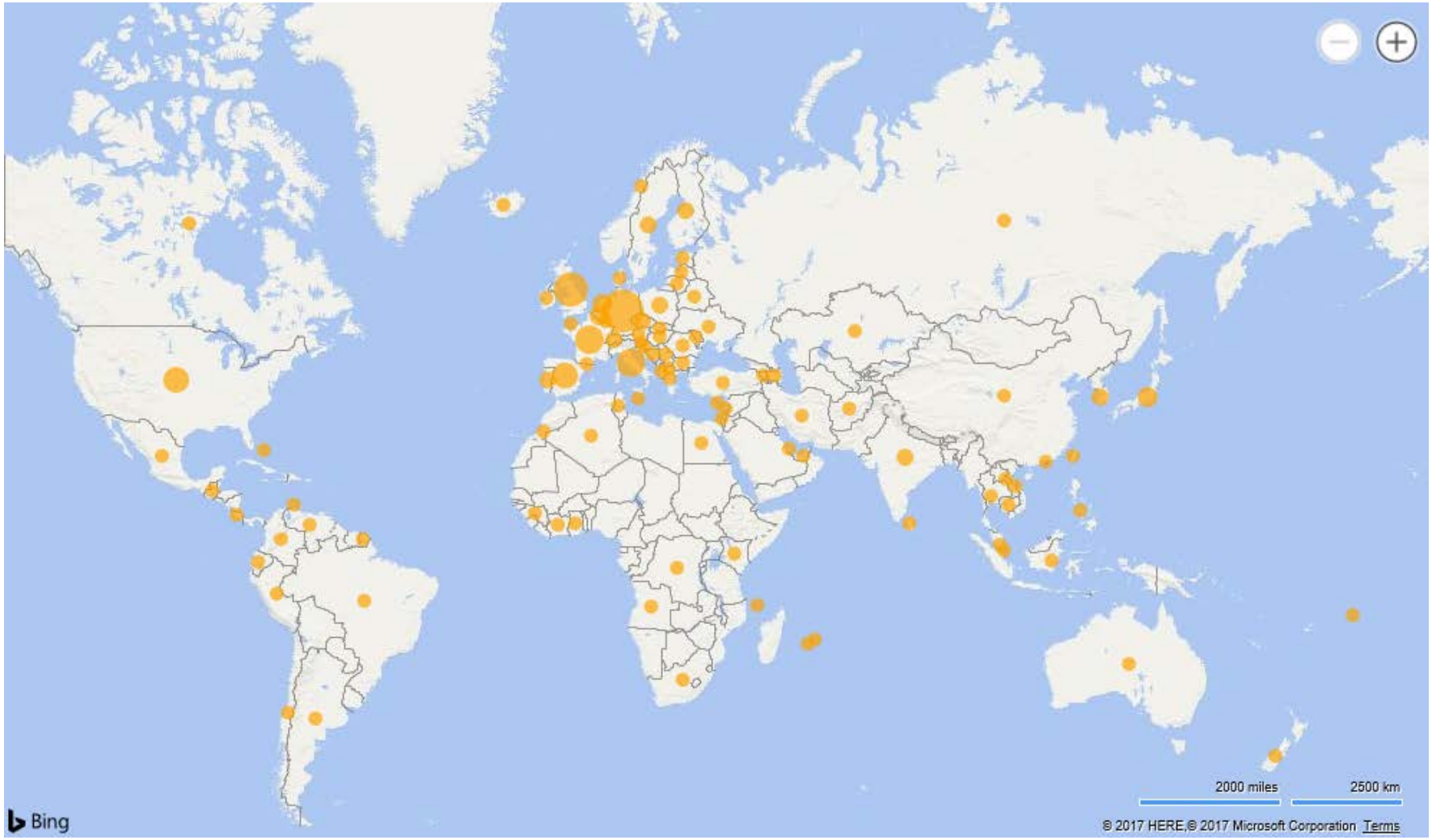
Article 111

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, manufactures, 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).

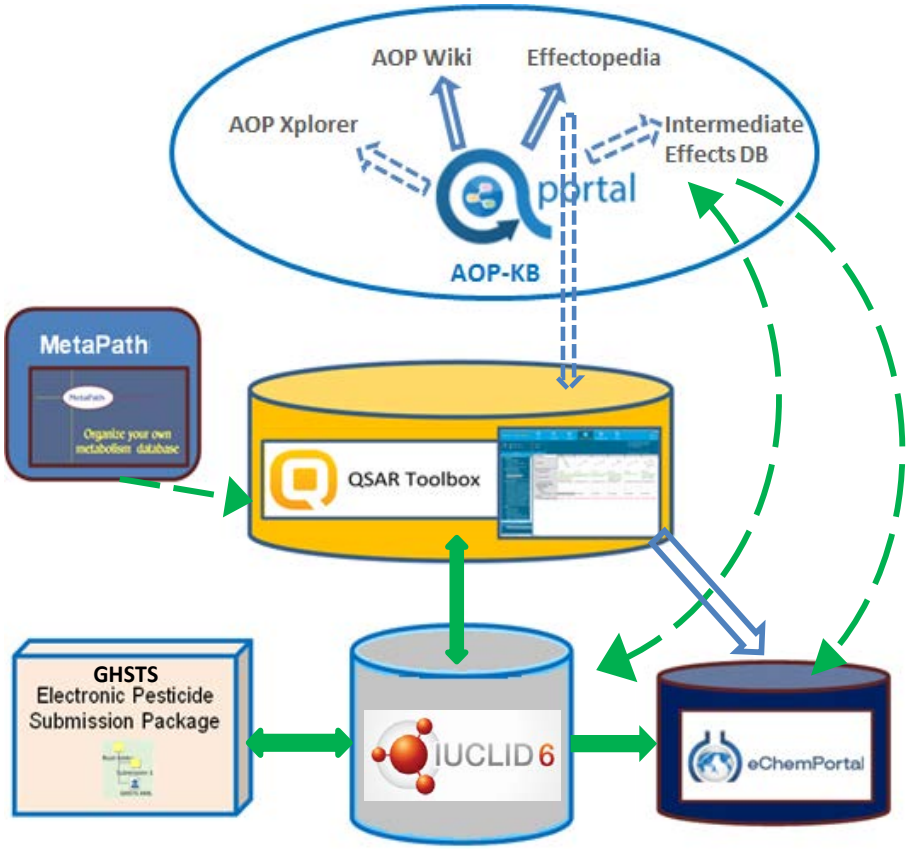
For the purposes of registration, the format of the technical dossier referred to in Article 10(a) shall be IUCLID. The Agency shall coordinate the further development of this format with the Organisation for Economic Cooperation and Development to ensure maximum harmonisation.

From where IUCLID 6 is downloaded?



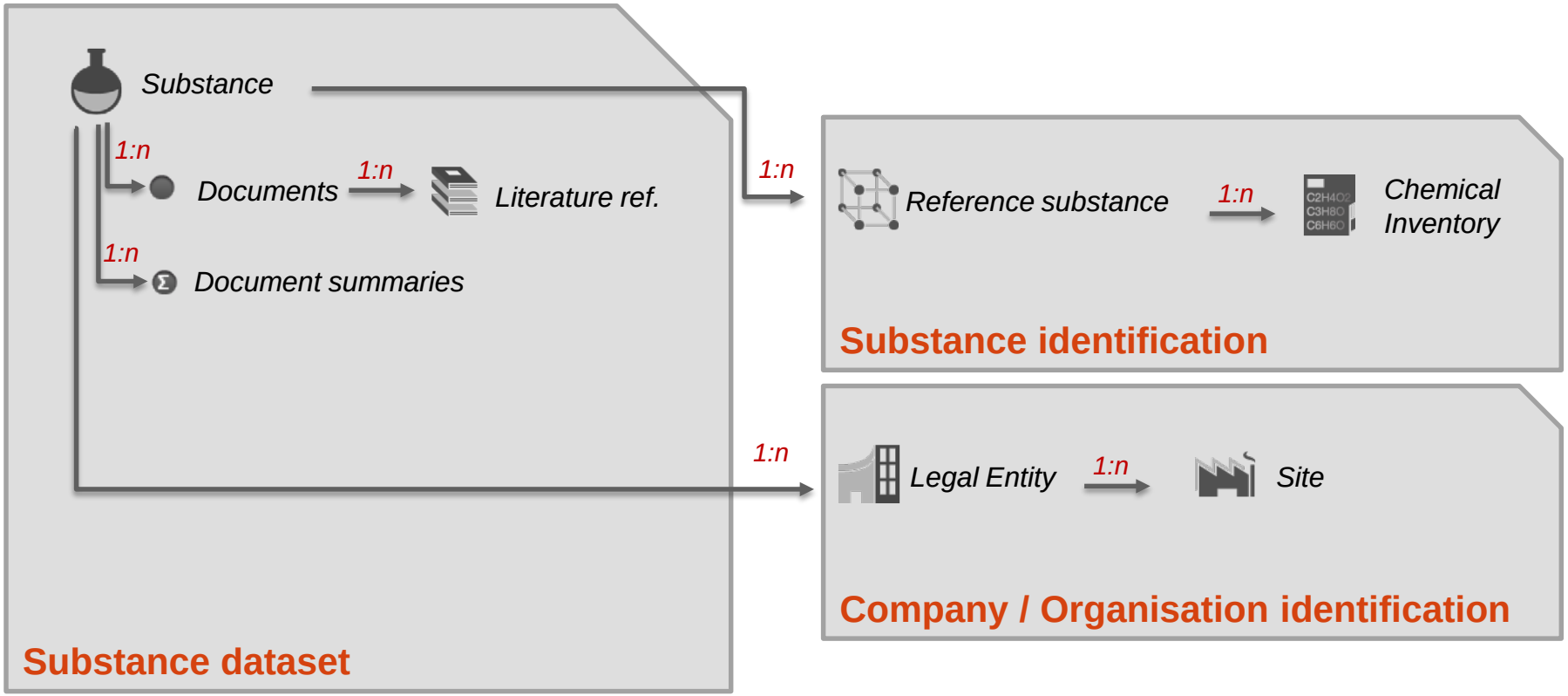
International cooperation

Organisation for Economic Co-operation and Development (OECD)



IUCLID entities (type of information)

Main entities and relationships (Substance)

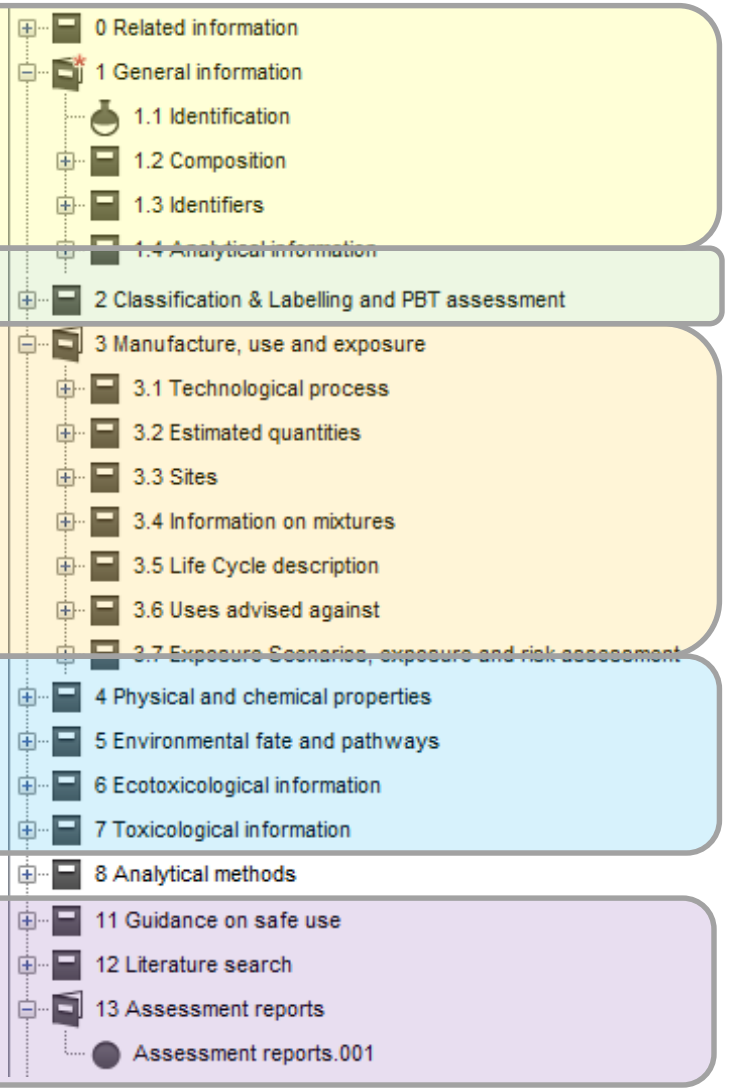


Attachments can be added to all entities and documents

Annotations can be linked to all entities and documents

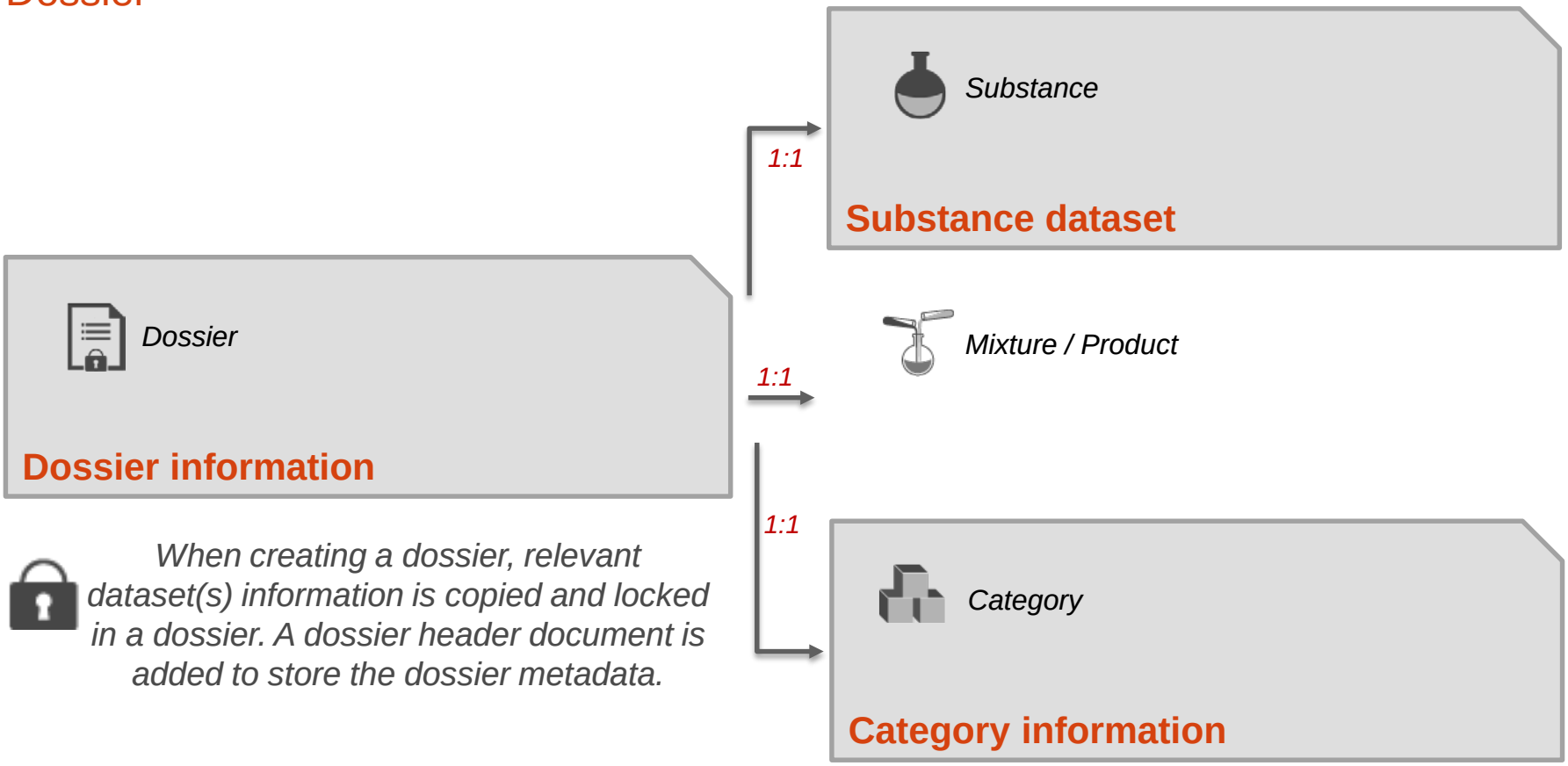
Information managed in IUCLID

- Substance identity
  - Substance identification
  - Composition(s)
- Classification and Labelling
- Use and exposure
- Study and endpoint summaries
- Assessment reports



IUCLID entities (type of information)

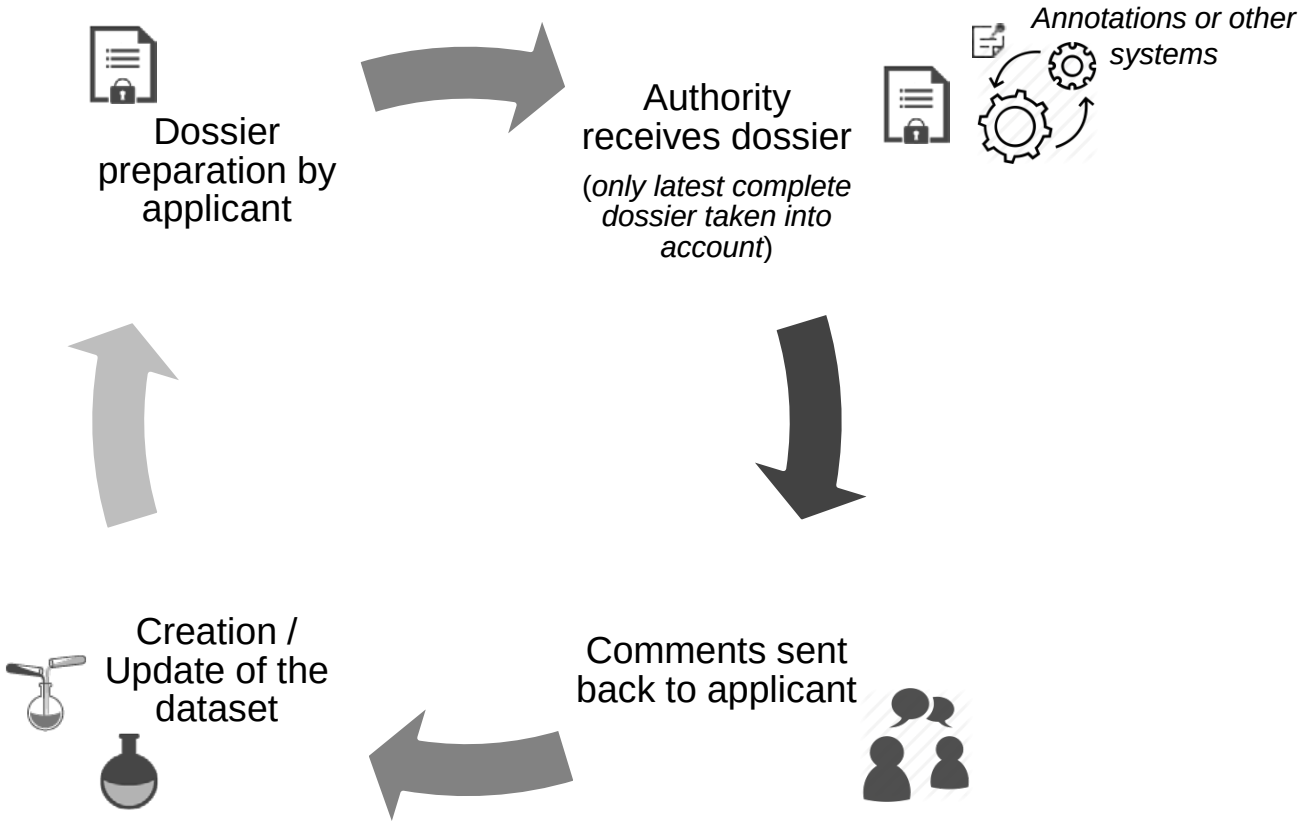
Dossier



When creating a dossier, relevant dataset(s) information is copied and locked in a dossier. A dossier header document is added to store the dossier metadata.

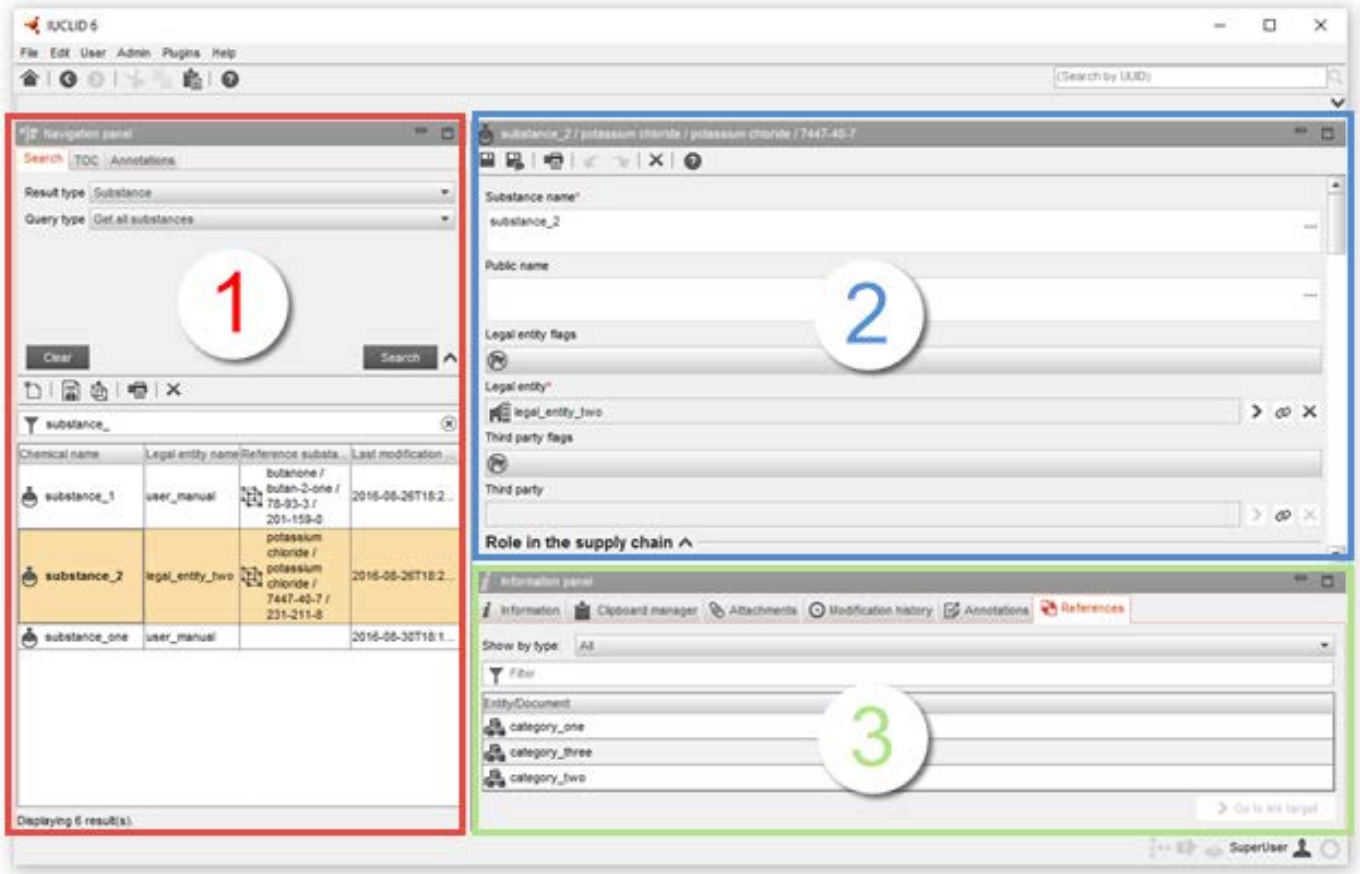
IUCLID and regulatory data submission

ECHA's approach



IUCLID 6 standard user interface

Main screen



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


?
Q
&
A
!

Questions and Answers

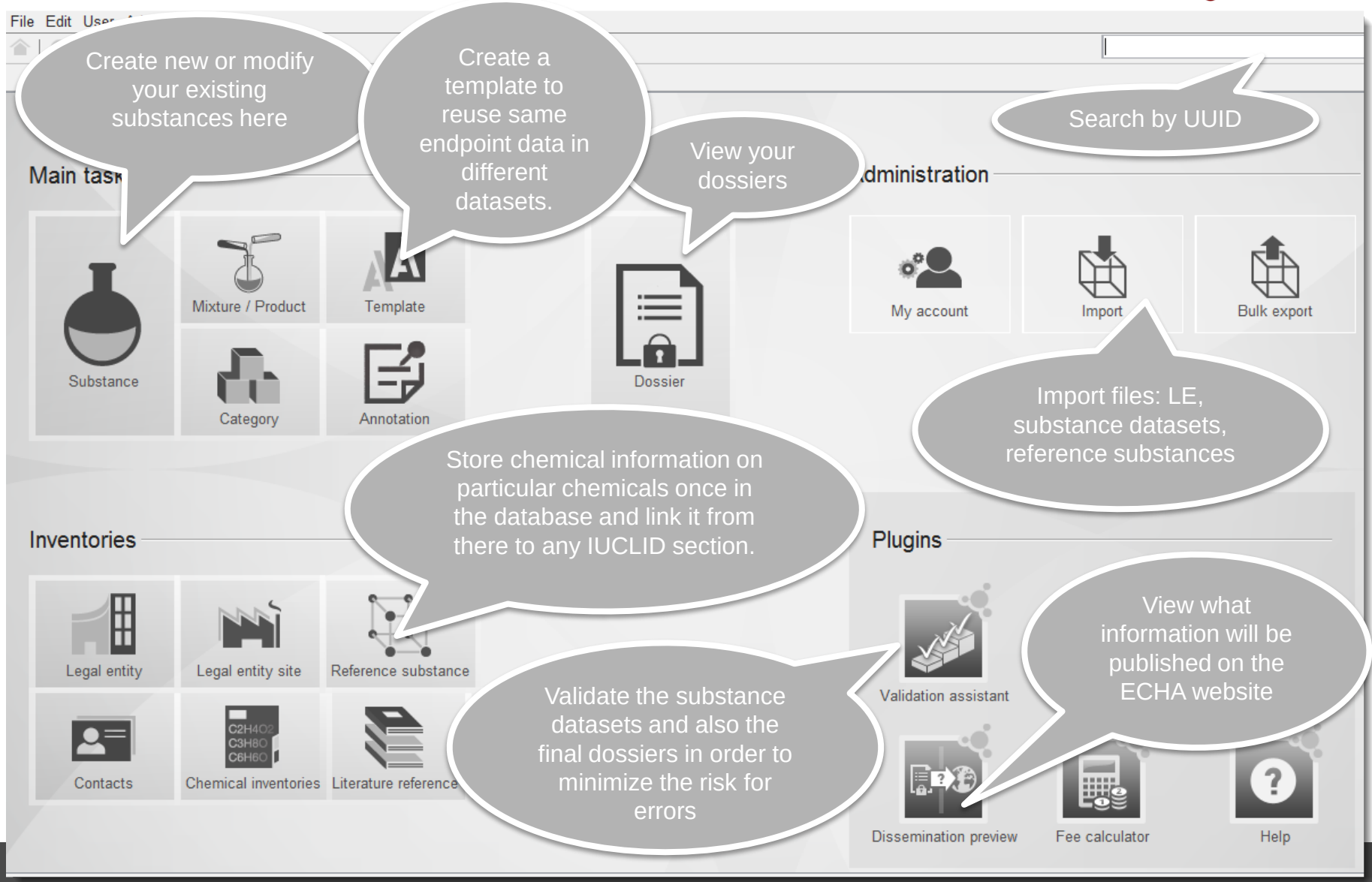
- Questions have been received during the event
- They will be covered during this session
- Please ask the most important questions now

Q&A topics

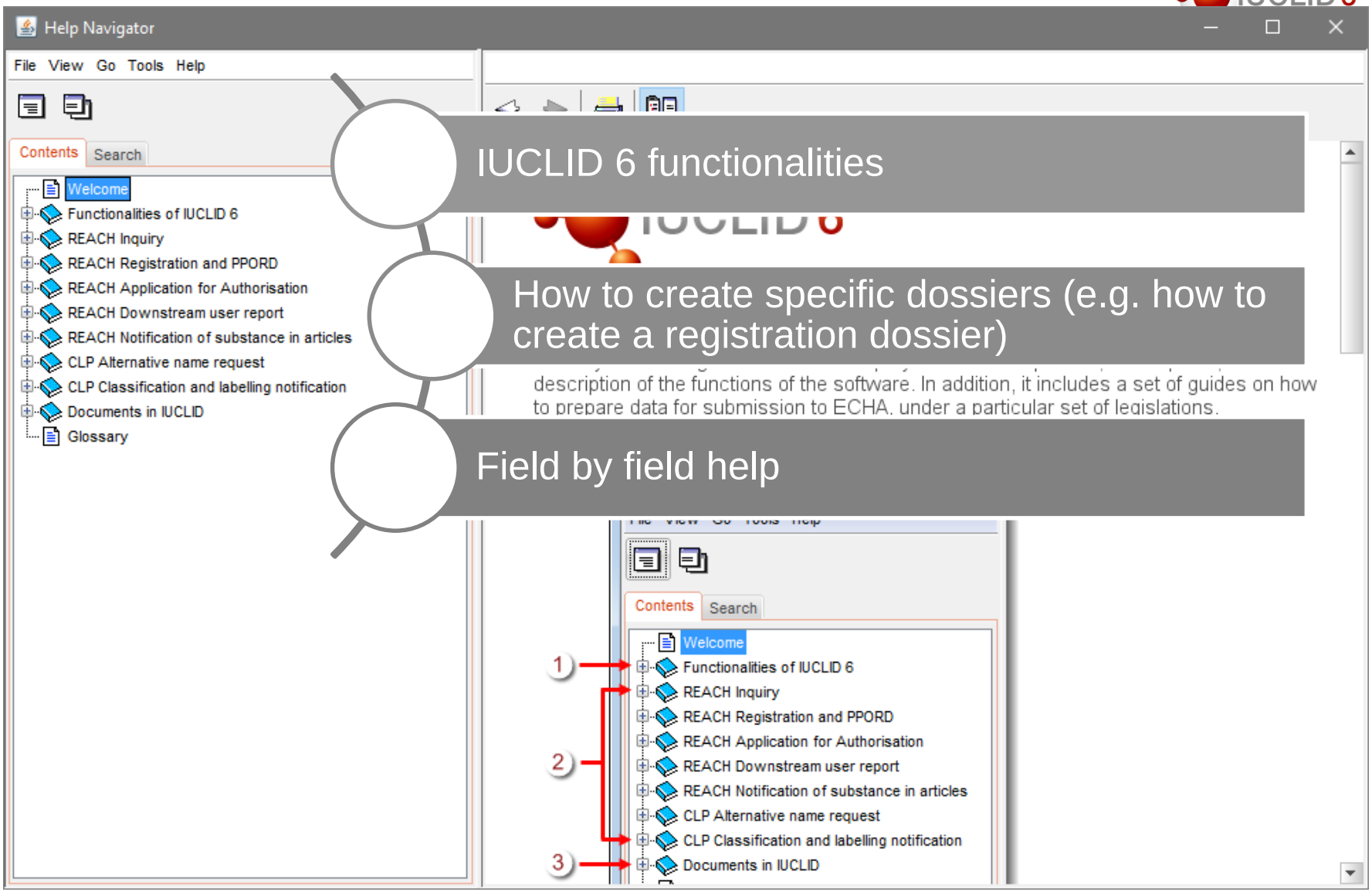
- IUCLID user interface and Help
- Reporting data in IUCLID
  - Dynamic content validation*
  - Substance identity
  - Read across
  - Waivers
  - PNEC calculator*
  - DNEL calculator*
  - Opt-out
  - Changes between IUCLID 5 and IUCLID 6
- IUCLID features
  - Validation assistant
  - Print*
  - Report 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*

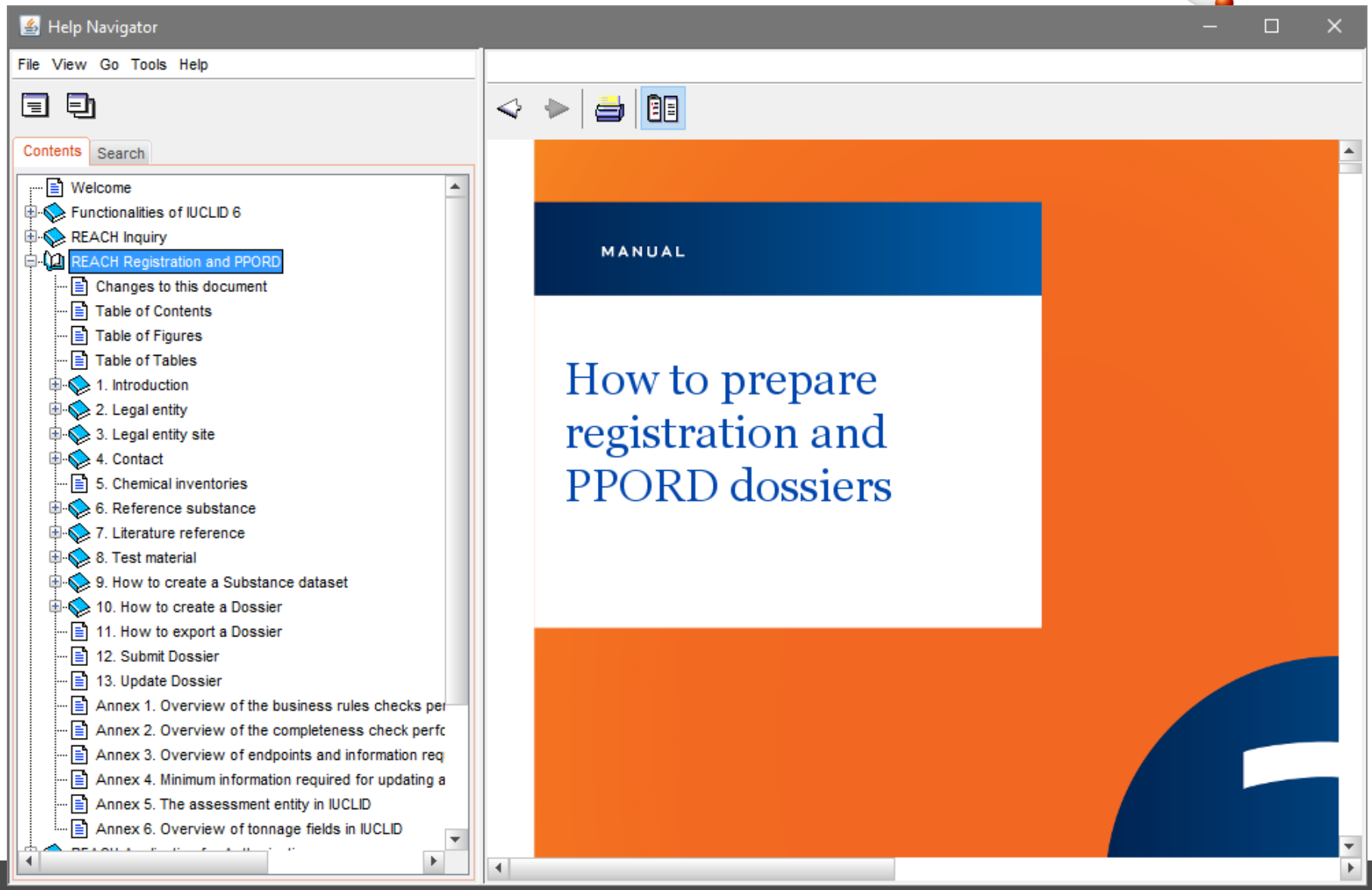
IUCLID user interface and Help


File Edit
Create new or modify your existing substances here
Create a template to reuse same endpoint data in different datasets.
View your dossiers
Search by UUID
Main tasks
Substance
Mixture / Product
Template
Category
Annotation
Dossier
Administration
My account
Import
Bulk export
Import files: LE, substance datasets, reference substances
Store chemical information on particular chemicals once in the database and link it from there to any IUCLID section.
Inventories
Legal entity
Legal entity site
Reference substance
Contacts
Chemical inventories
Literature reference
Plugins
Validation assistant
Validate the substance datasets and also the final dossiers in order to minimize the risk for errors
View what information will be published on the ECHA website
Dissemination preview
Fee calculator
Help

Embedded Help System (press F1)



Embedded Help System (F1)



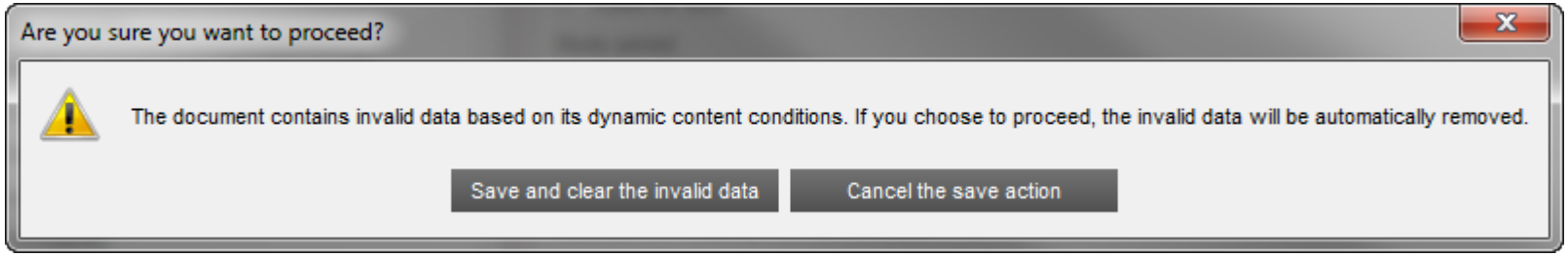
Reporting data in IUCLID

Dynamic content validation

Data reporting in IUCLID 6

Dynamic content validation (1)

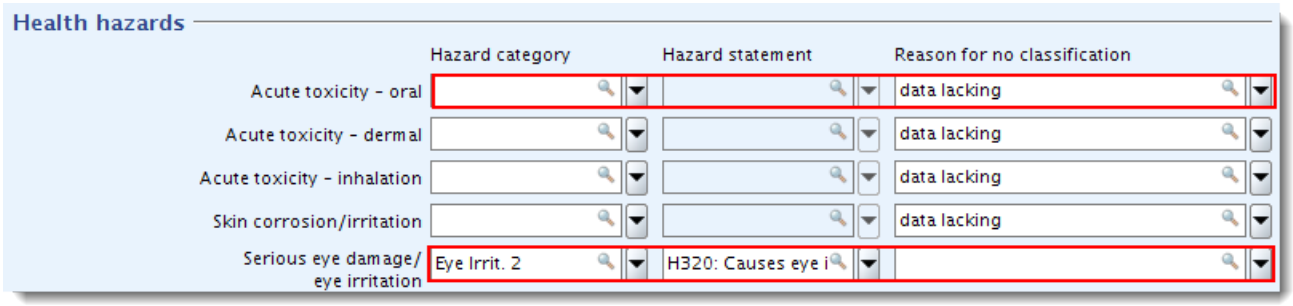
- **What?**
  - When the user makes selections in a field that is subject to dynamic content validation, this causes the incompatible fields to become inactive
- **Why?**
  - To support the user in not entering conflicting information in the application.
- **How?**
  - When the user makes selections 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.



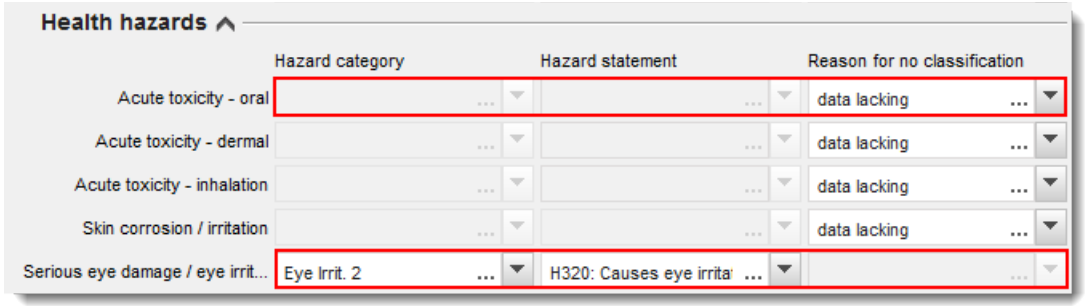
Data reporting in IUCLID 6

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



IUCLID 5

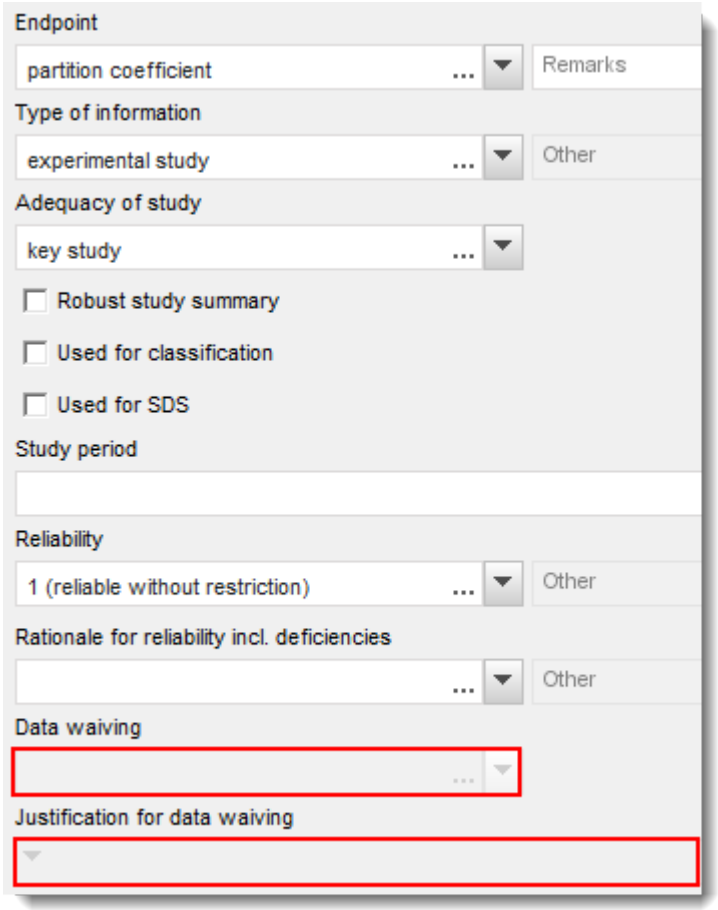


IUCLID 6

Data reporting in 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

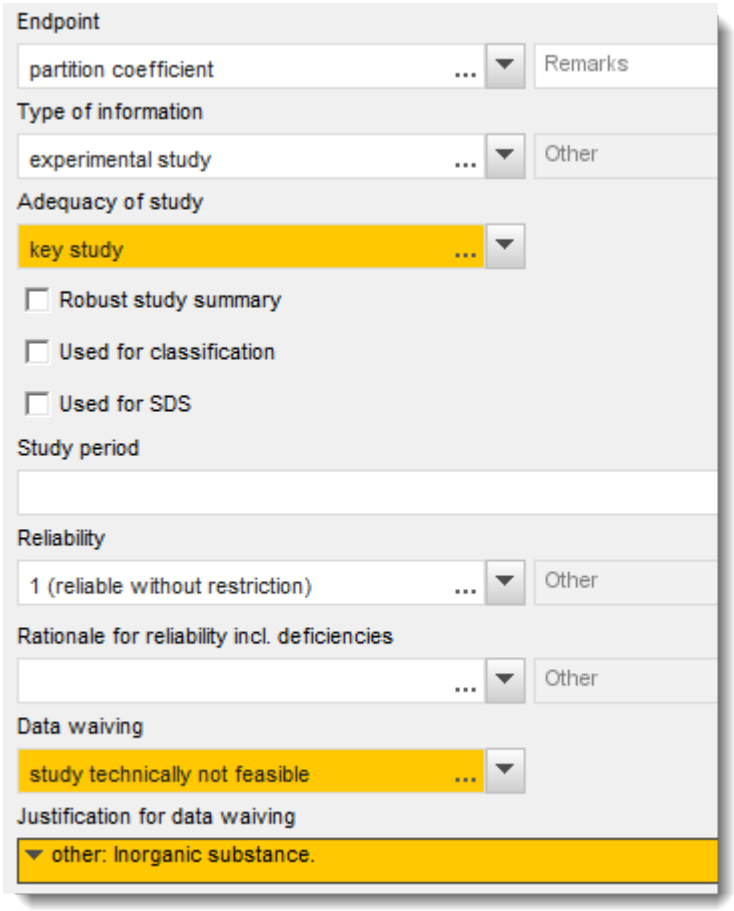


IUCLID 6: Section 4.7, new endpoint study record

Data reporting in IUCLID 6

Dynamic content validation (4)

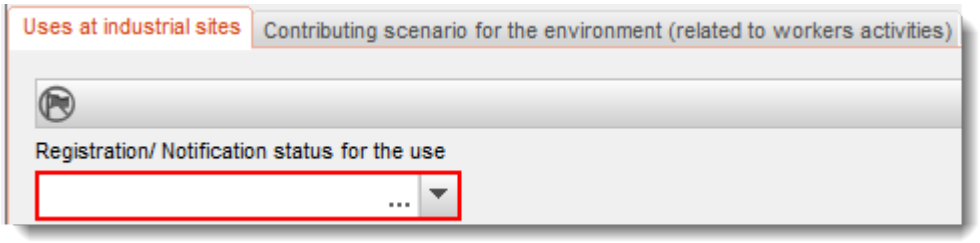
- **Where?**
- Endpoint study record – Administrative data:
  - When an endpoint study record has been migrated from IUCLID 5 and contains conflicting information in fields with dynamic content validation, the fields that contain inconsistent information are highlighted in orange.
  - The conflicting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



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.

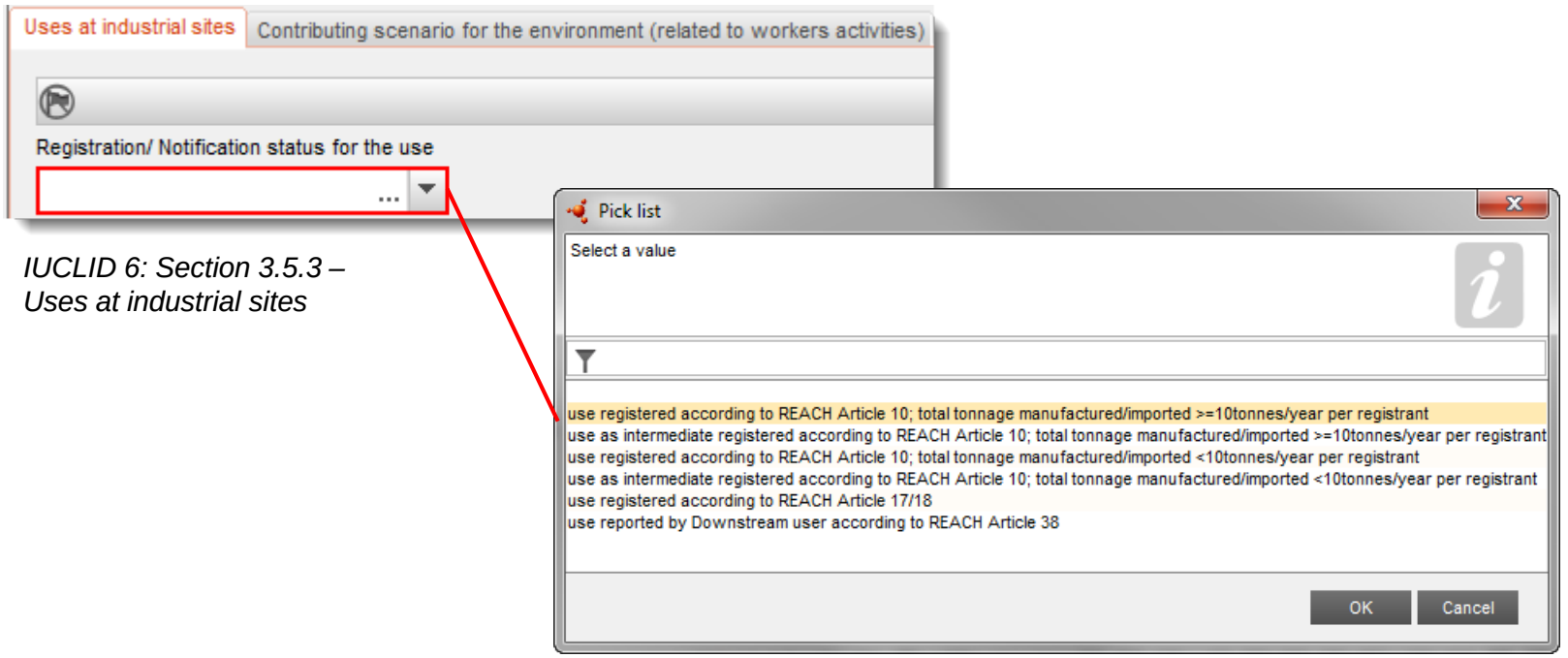


IUCLID 6: Section 3.5.3 – Uses at industrial sites

Data reporting in IUCLID 6

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.



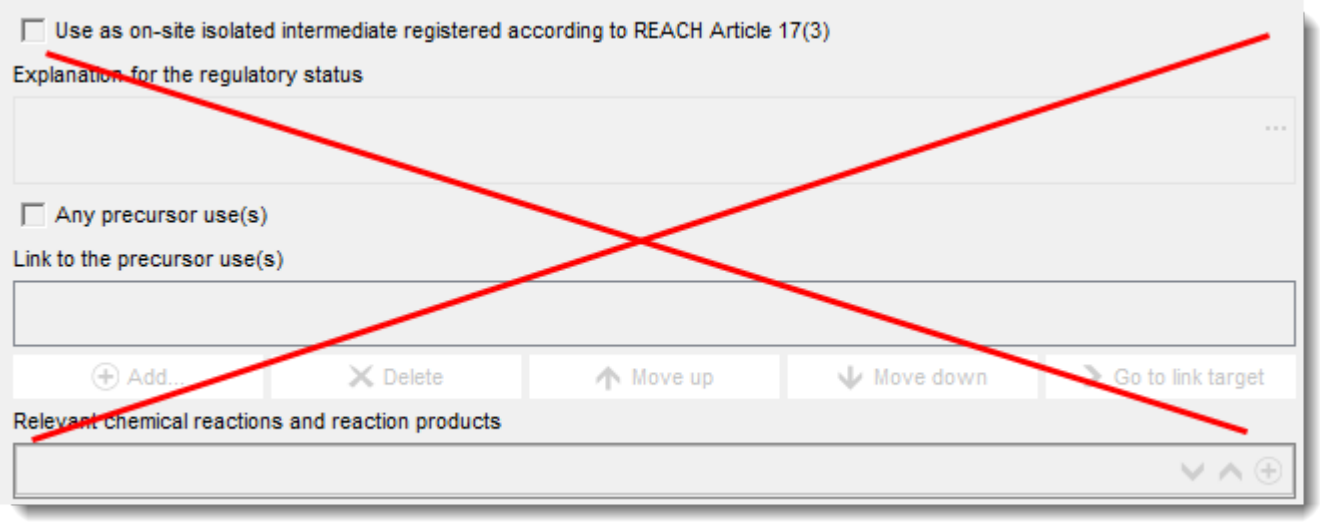
IUCLID 6: Section 3.5.3 – Uses at industrial sites

Data reporting in IUCLID 6

Dynamic content validation (7)

- **Where?**
- Section 3.5.3 – Uses at industrial sites:
  - **use registered according to REACH Article 10; total tonnage manufactured/imported >=10tonnes/year per registrant**.

  → Fields for reporting information on intermediates are inactive



IUCLID 6: Section 3.5.3 – Uses at industrial sites

Data reporting in IUCLID 6

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

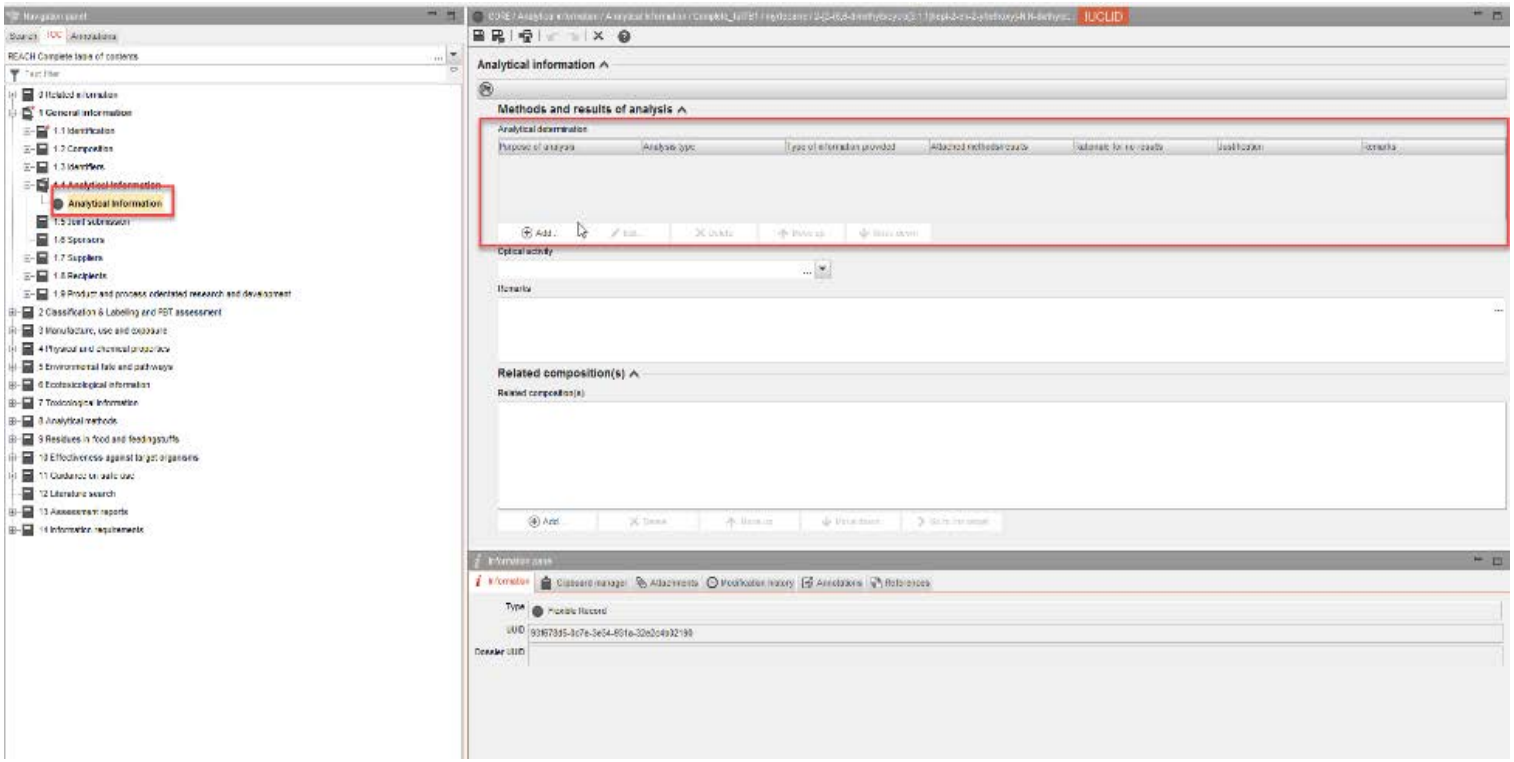
IUCLID 6: Section 3.5.3 – Uses at industrial sites

Reporting data in IUCLID

Substance Identity

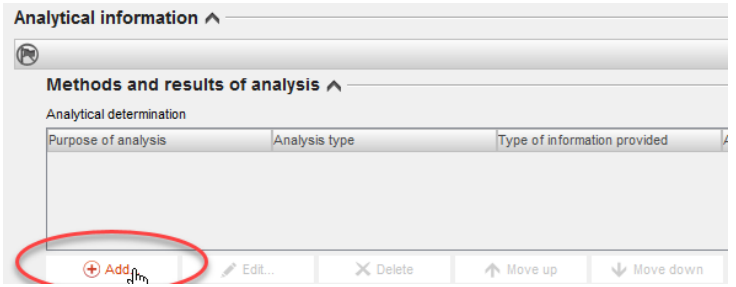
Tips based on experience – Substance ID

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

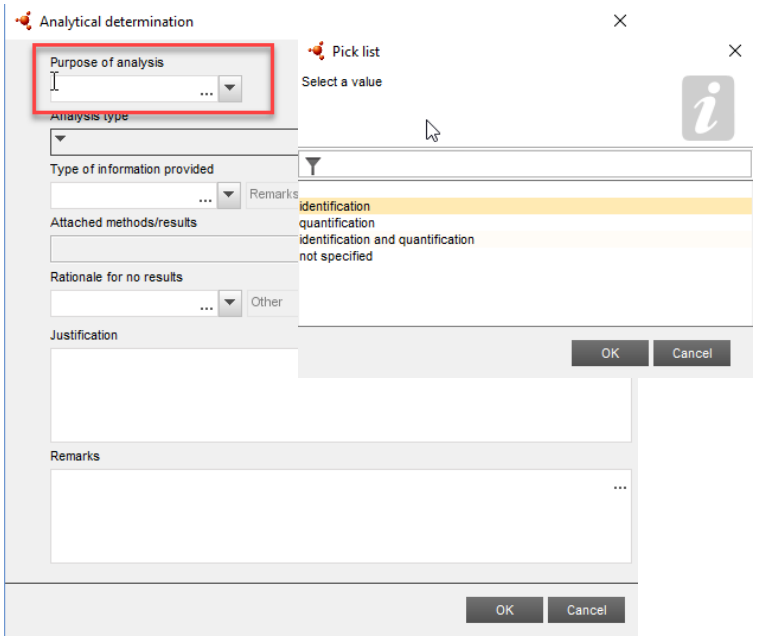


Tips based on experience – Substance ID

- Add row

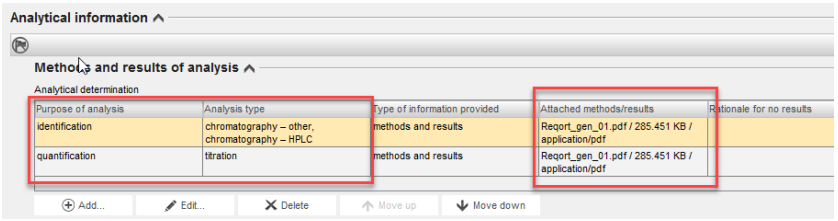


- 'Purpose of the analysis' picklist

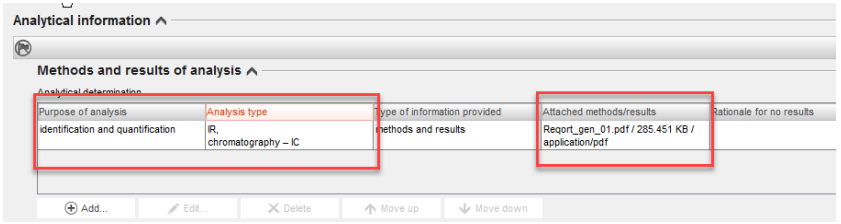


Tips based on experience – Substance ID

‘Identification’ and ‘Quantification’



‘Identification and Quantification’

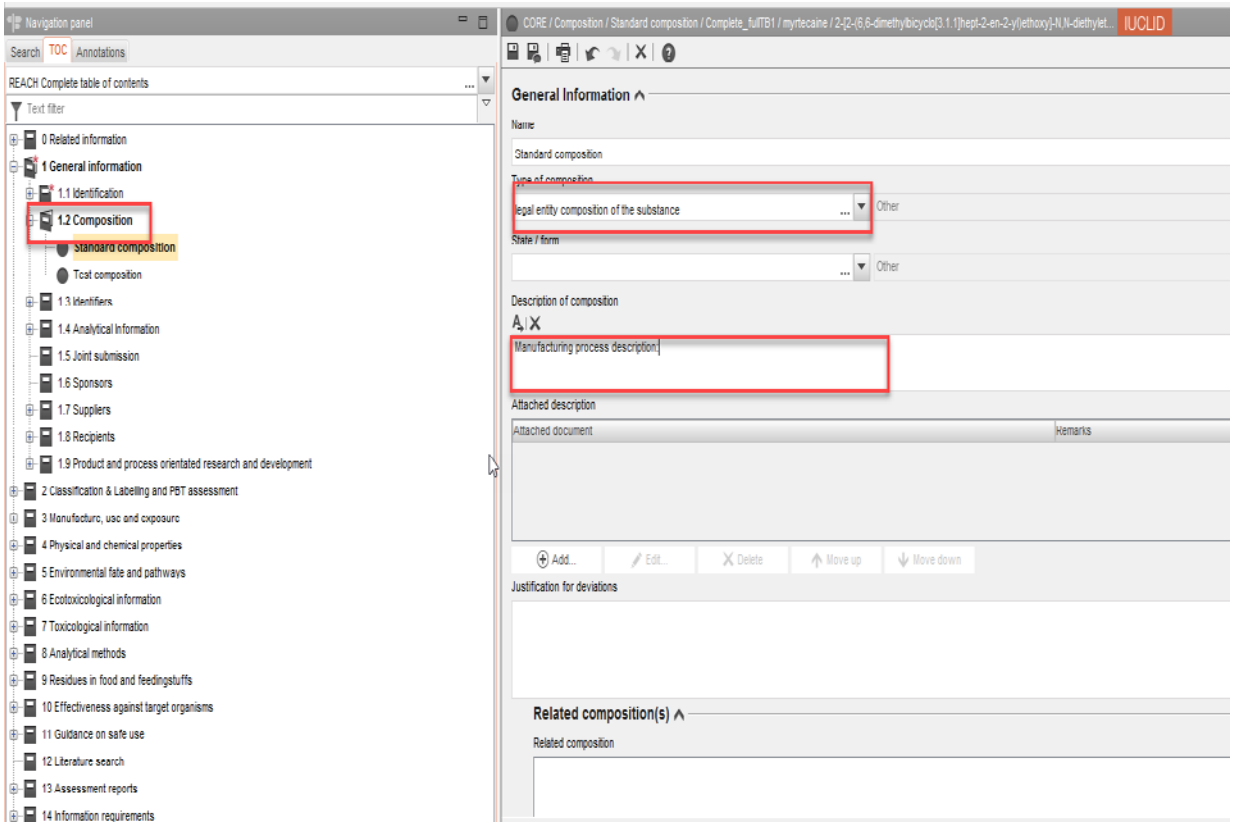


Tips based on experience – Substance ID

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

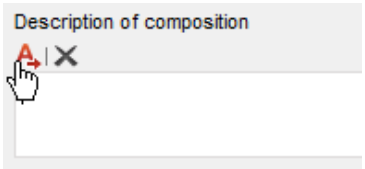
Tips based on experience – Substance ID

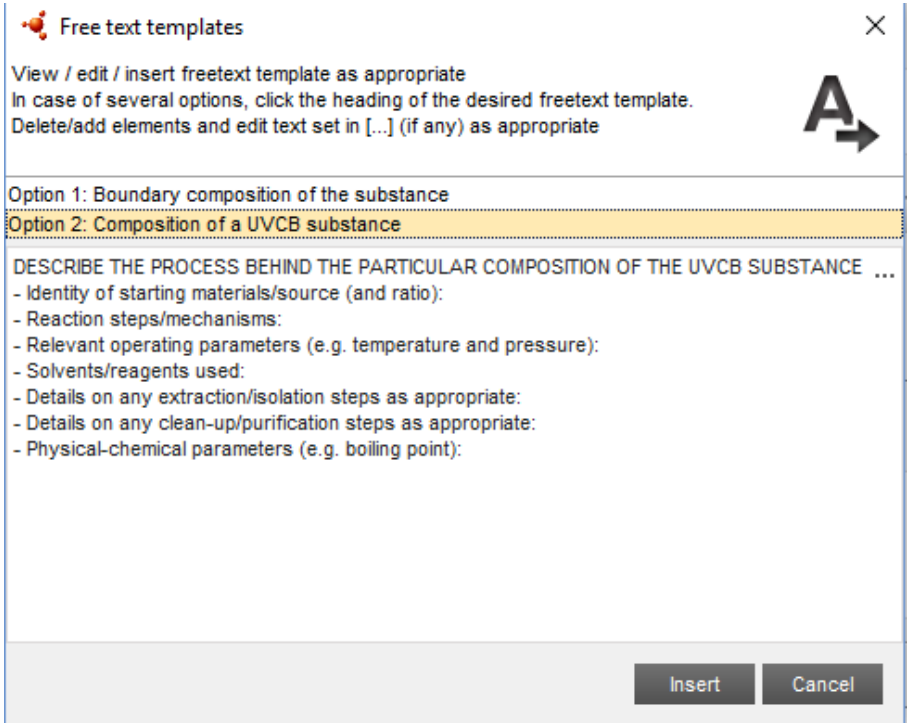
- UVCB substances:
  - Manufacturing process description should be provided for the **registered substance**
  - IUCLID section 1.2



Tips based on experience – Substance ID

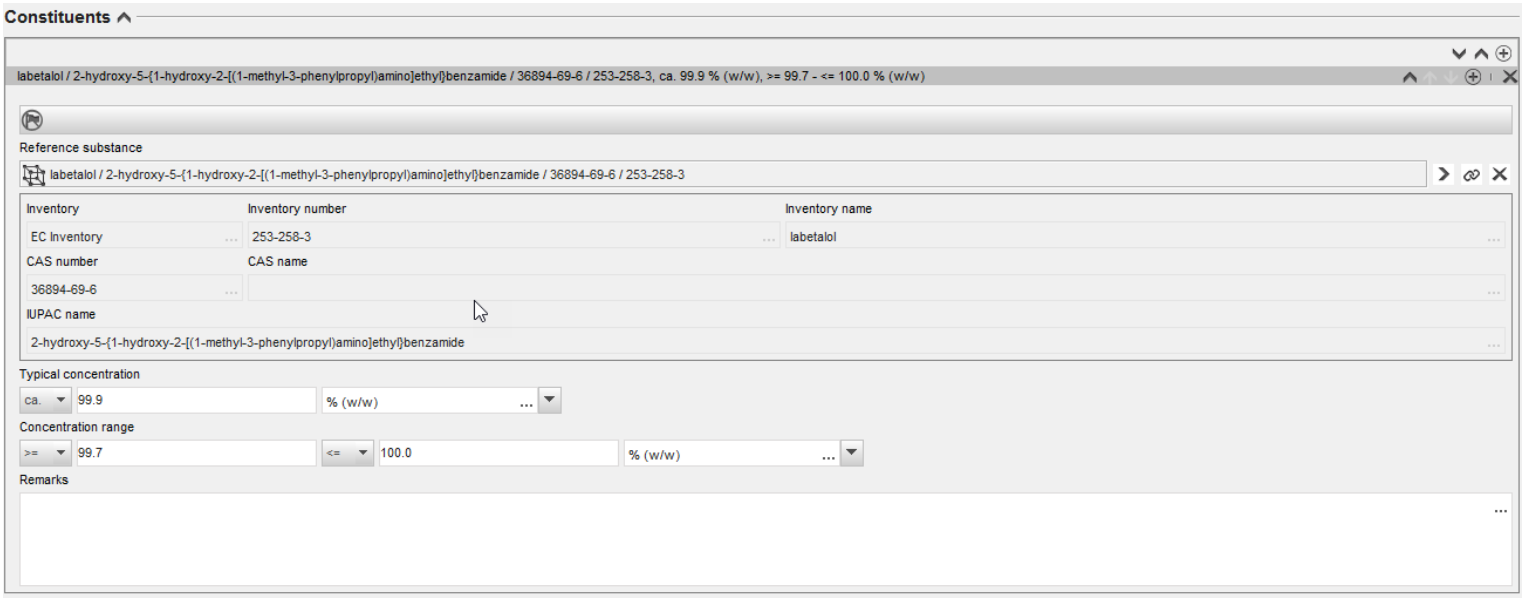
- UVCB substances:
  - Use the Text template
  - Address all the points





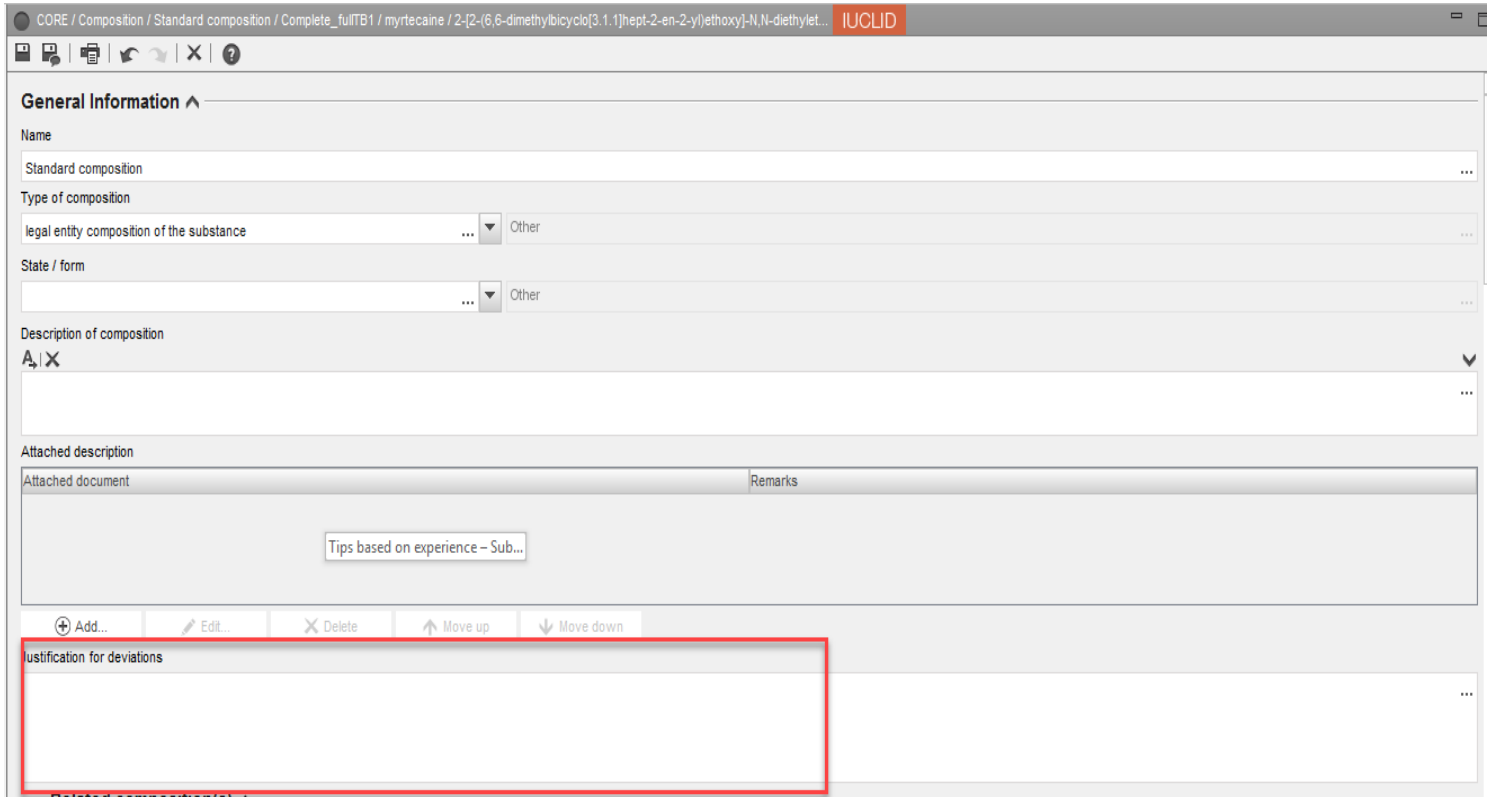
Tips based on experience – Substance ID

- 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



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



Reporting data in IUCLID

Read across

Data reporting in IUCLID 6

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.

Data reporting in IUCLID 6

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).

Data reporting in IUCLID 6

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).

Data reporting in IUCLID 6

Reporting of read-across information (4)

2. Analogue / supporting substance approach:

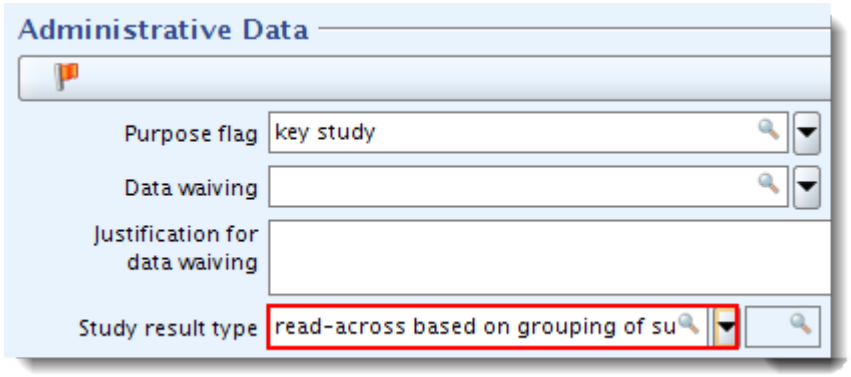
	Endpoint study record	Source record	Target record
i	Administrative data	X	X
	Endpoint	X	X
	Type of information	X	X
	Adequacy of study	X	X
	Robust study summary Used for classification Used for SDS	X	X
	Study period	X	
	Reliability	X	
	Rationale for reliability incl. deficiencies	X	
	Data waiving		
	Justification 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*

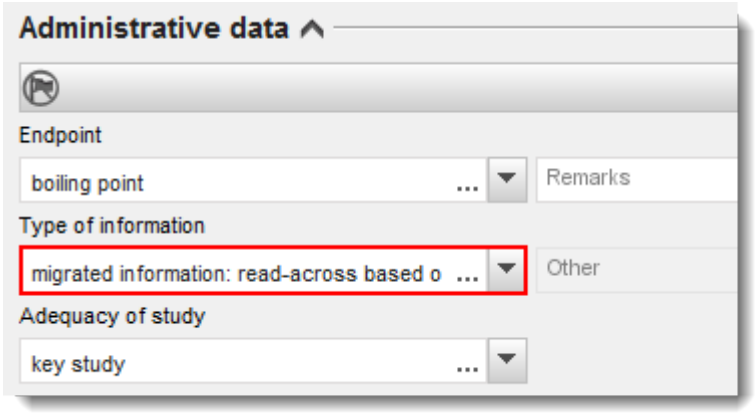
Reporting of read-across information (5)

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 clarify and data quality, to move to the new approach whenever possible.



IUCLID 5: read-across record



IUCLID 6: migrated read-across record

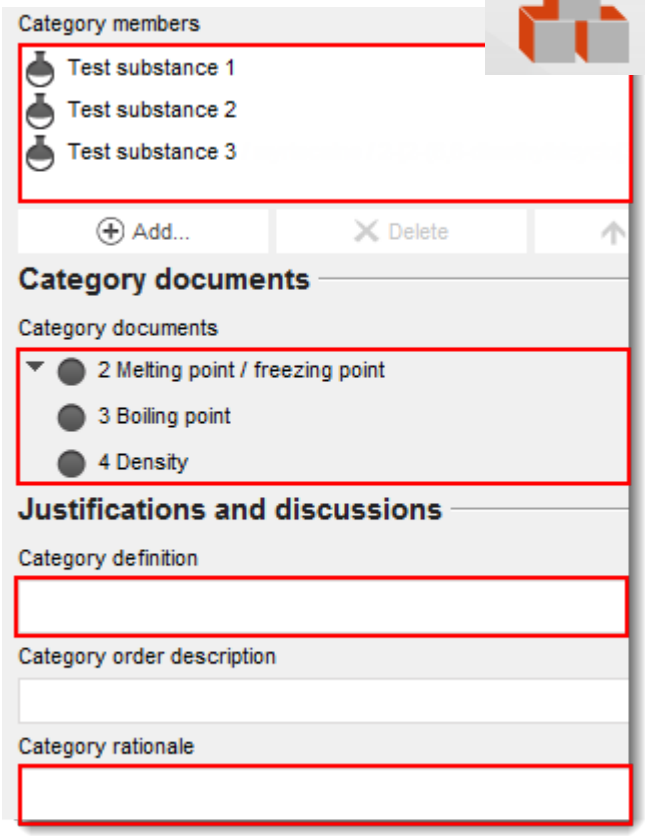
Data reporting in IUCLID 6

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



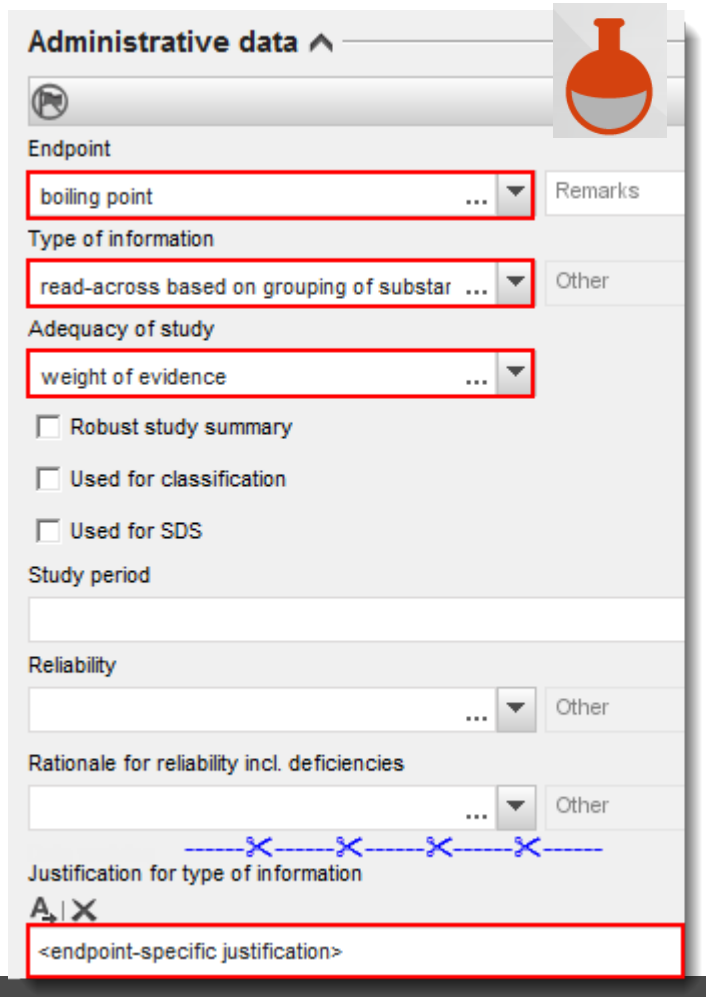
Data reporting in IUCLID 6

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



Data reporting in IUCLID 6

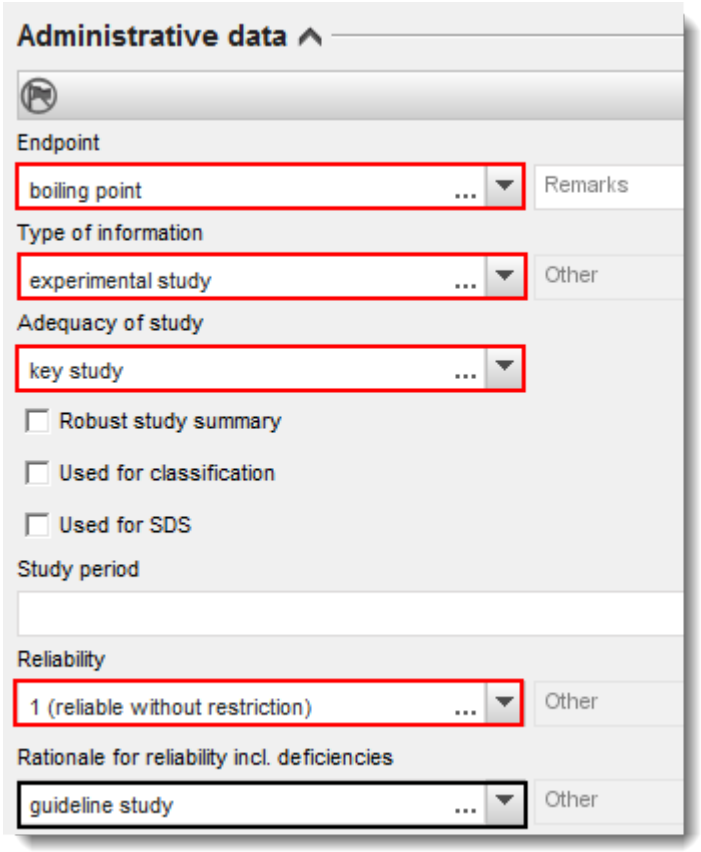
Reporting of read-across information (8)

Migrated data – checklist for analogue approach:

- Split the read-across information into source and target data.

- <u>The source record</u>
  - 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



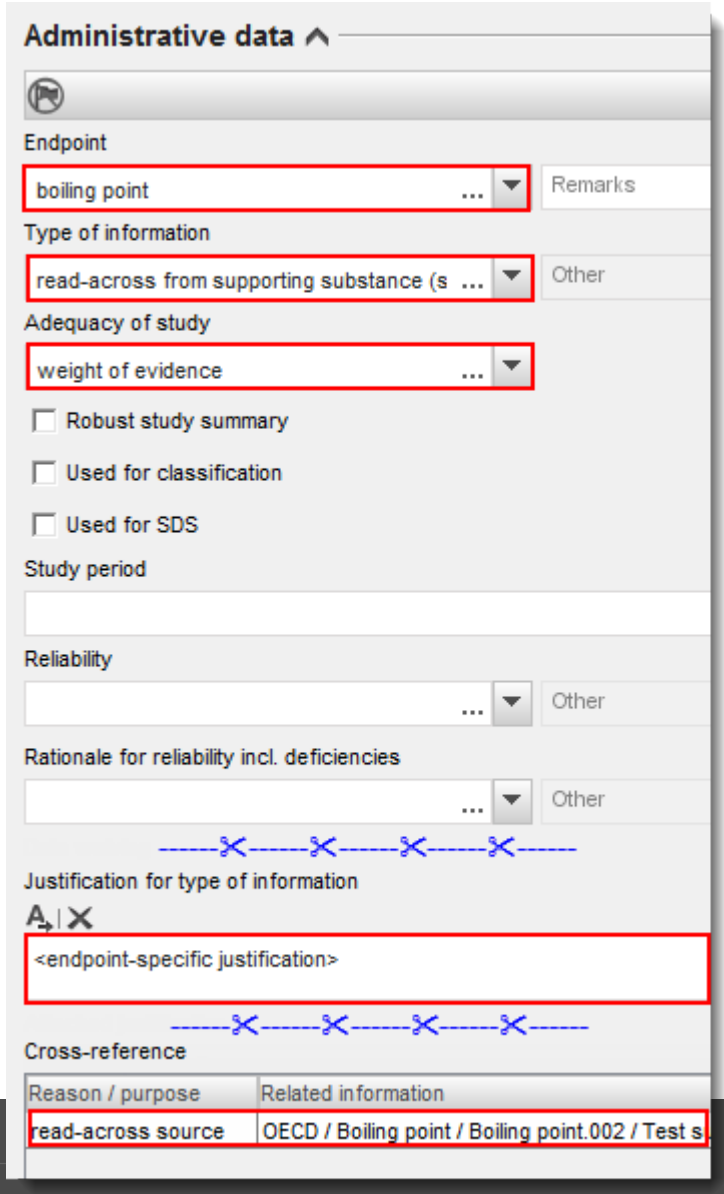
Data reporting in IUCLID 6

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



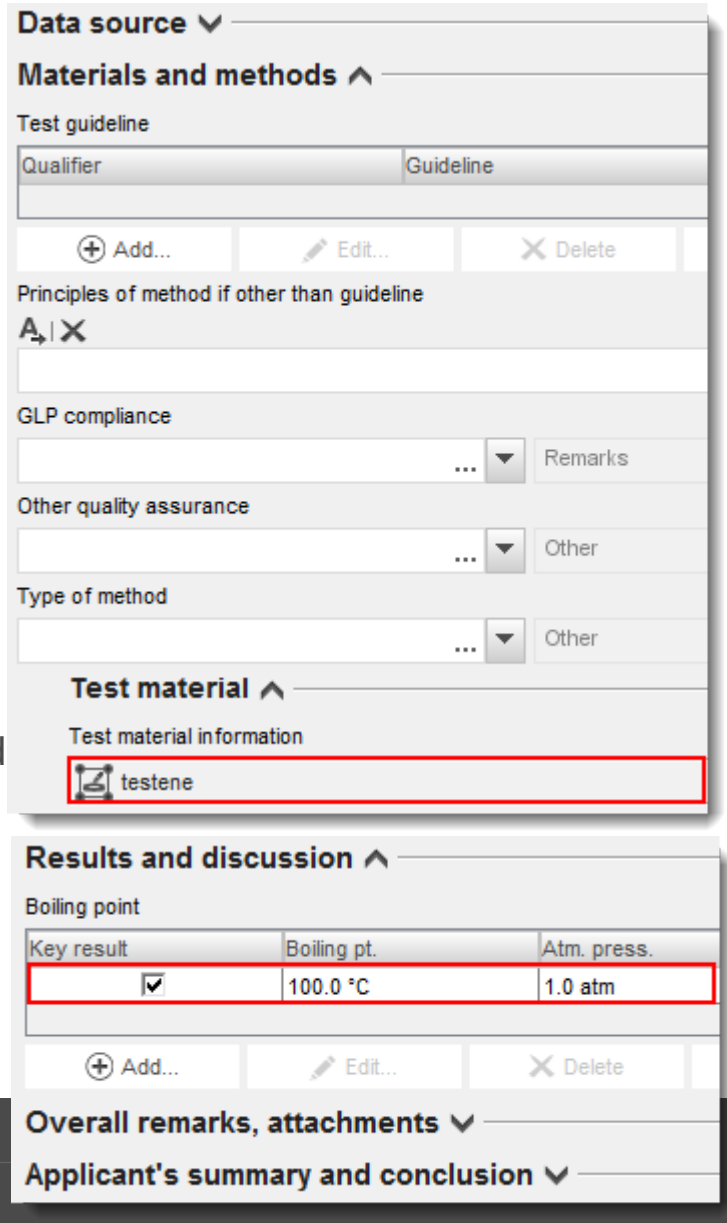
Data reporting in IUCLID 6

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).

Target data: read-across record



Data reporting in IUCLID 6

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.)
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.

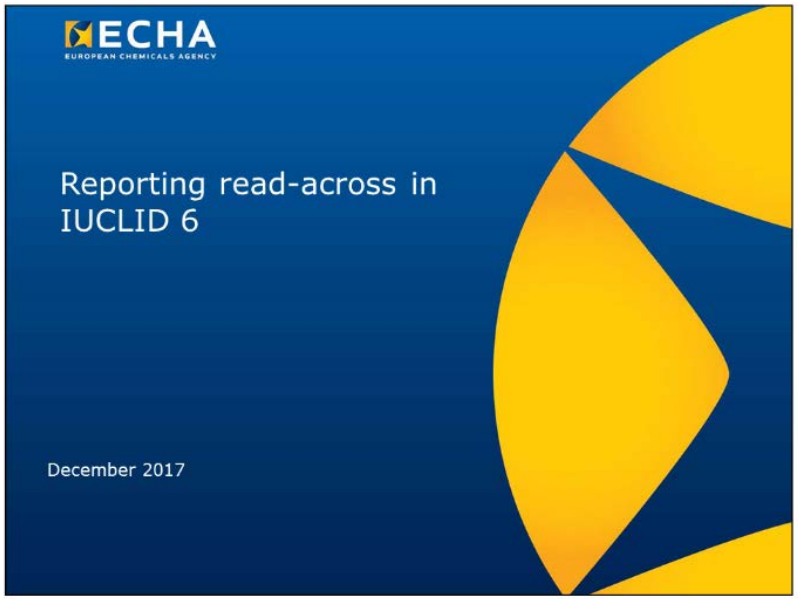
Read-across

- 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)

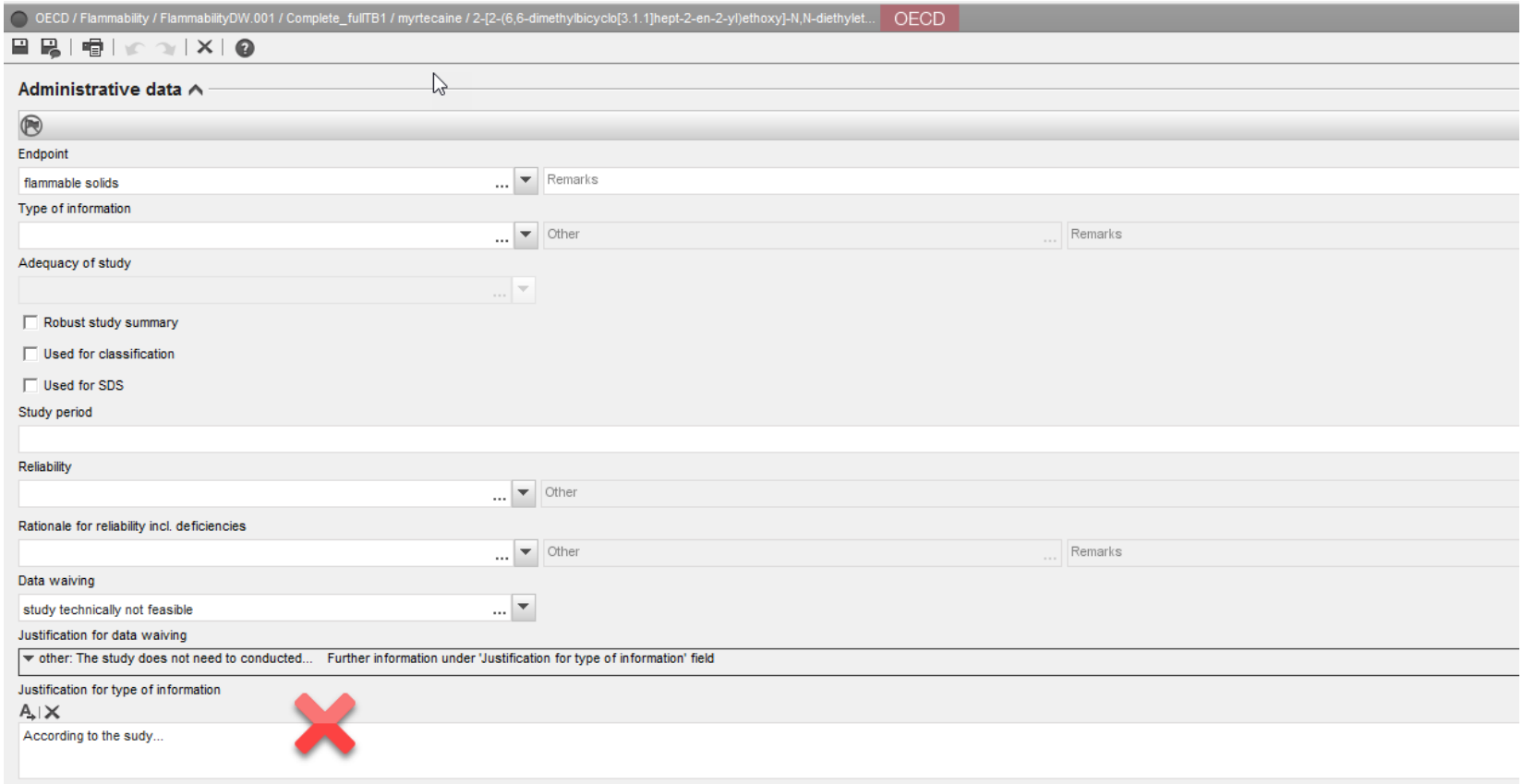


Reporting data in IUCLID

Data waivers

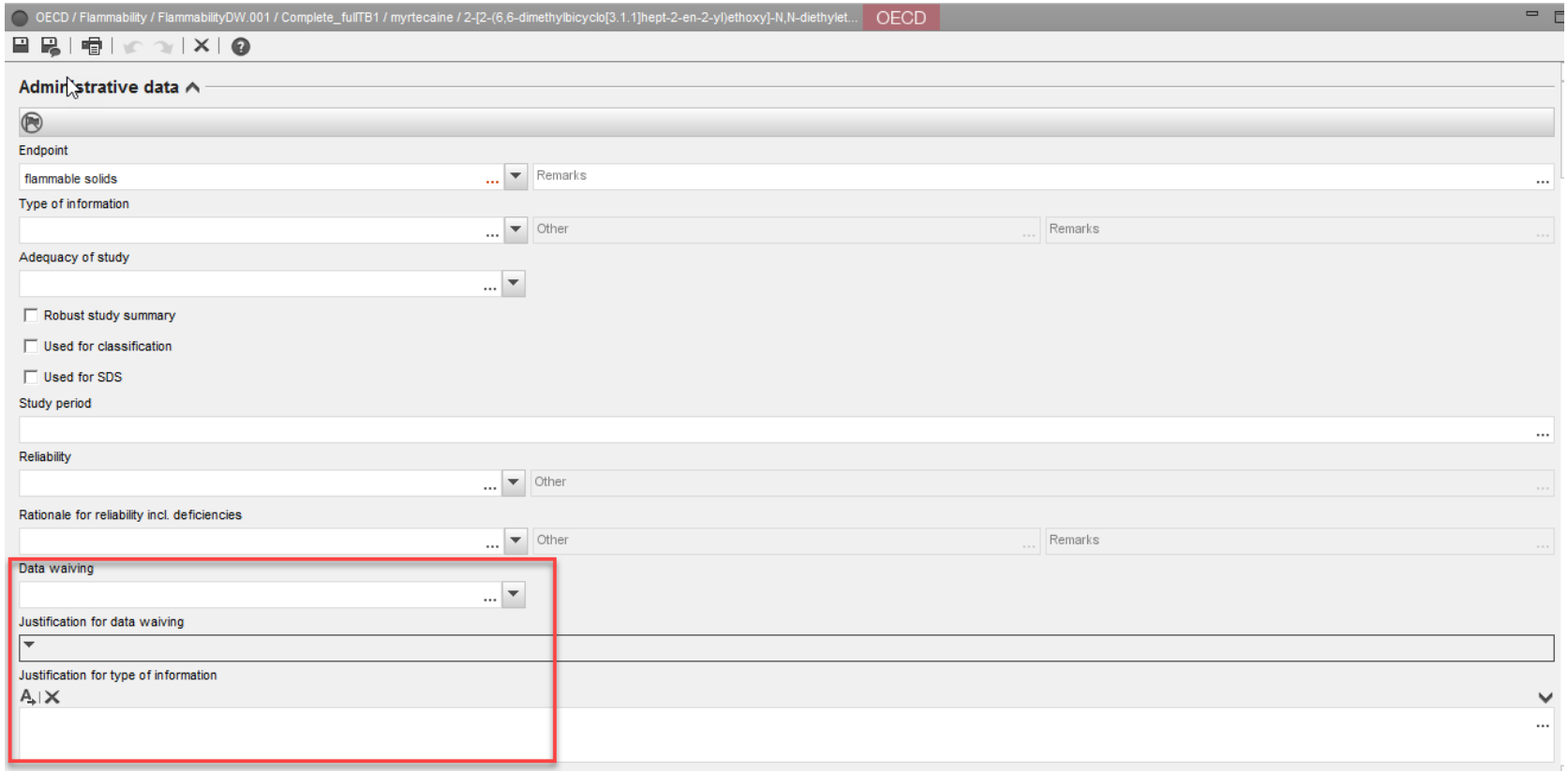
Tips based on experience – Data waivers

- Do not report study results as data waivers



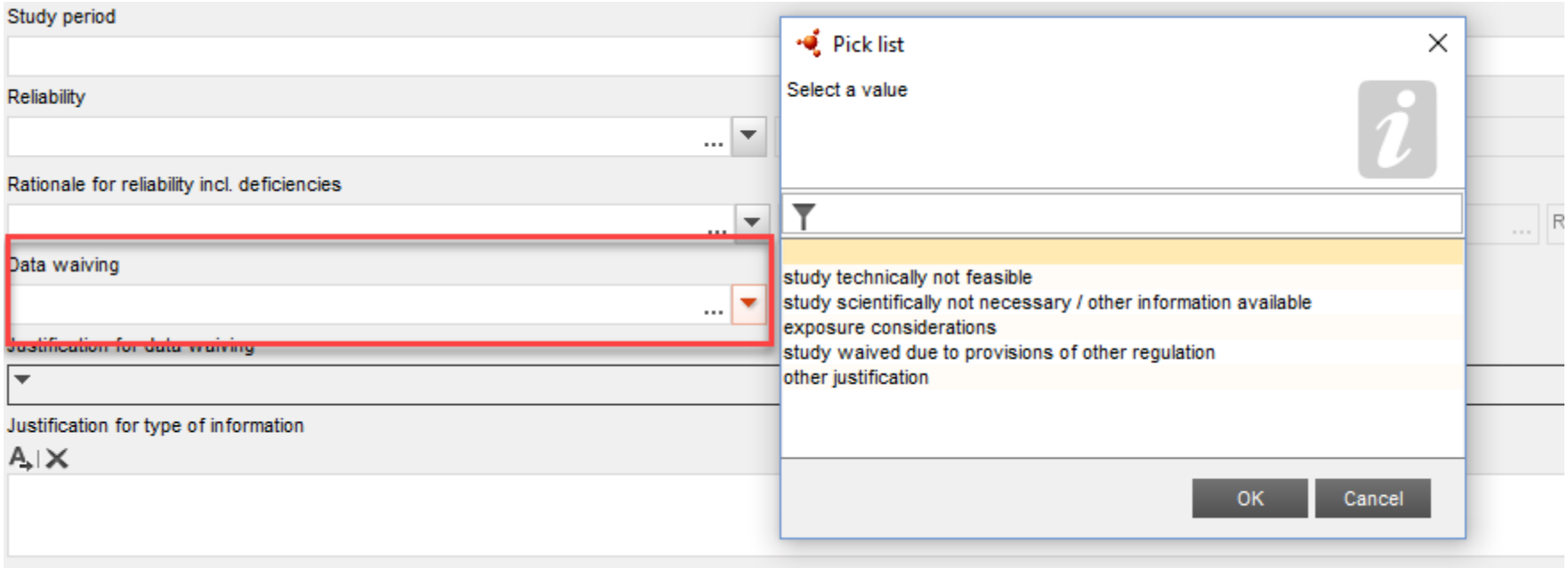
Tips based on experience – Data waivers

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



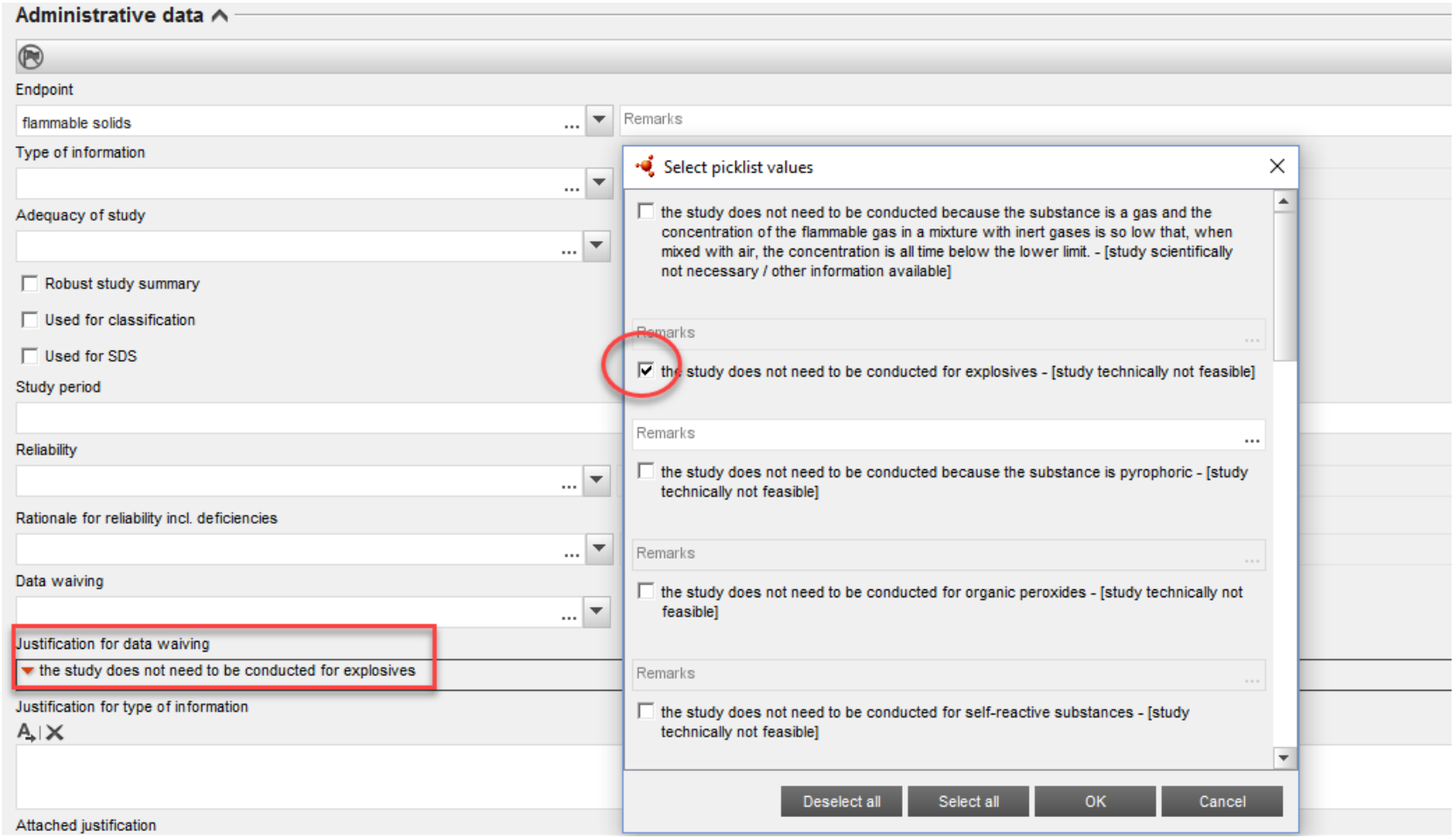
Tips based on experience – Data waivers

- ‘Data waiving’ picklist



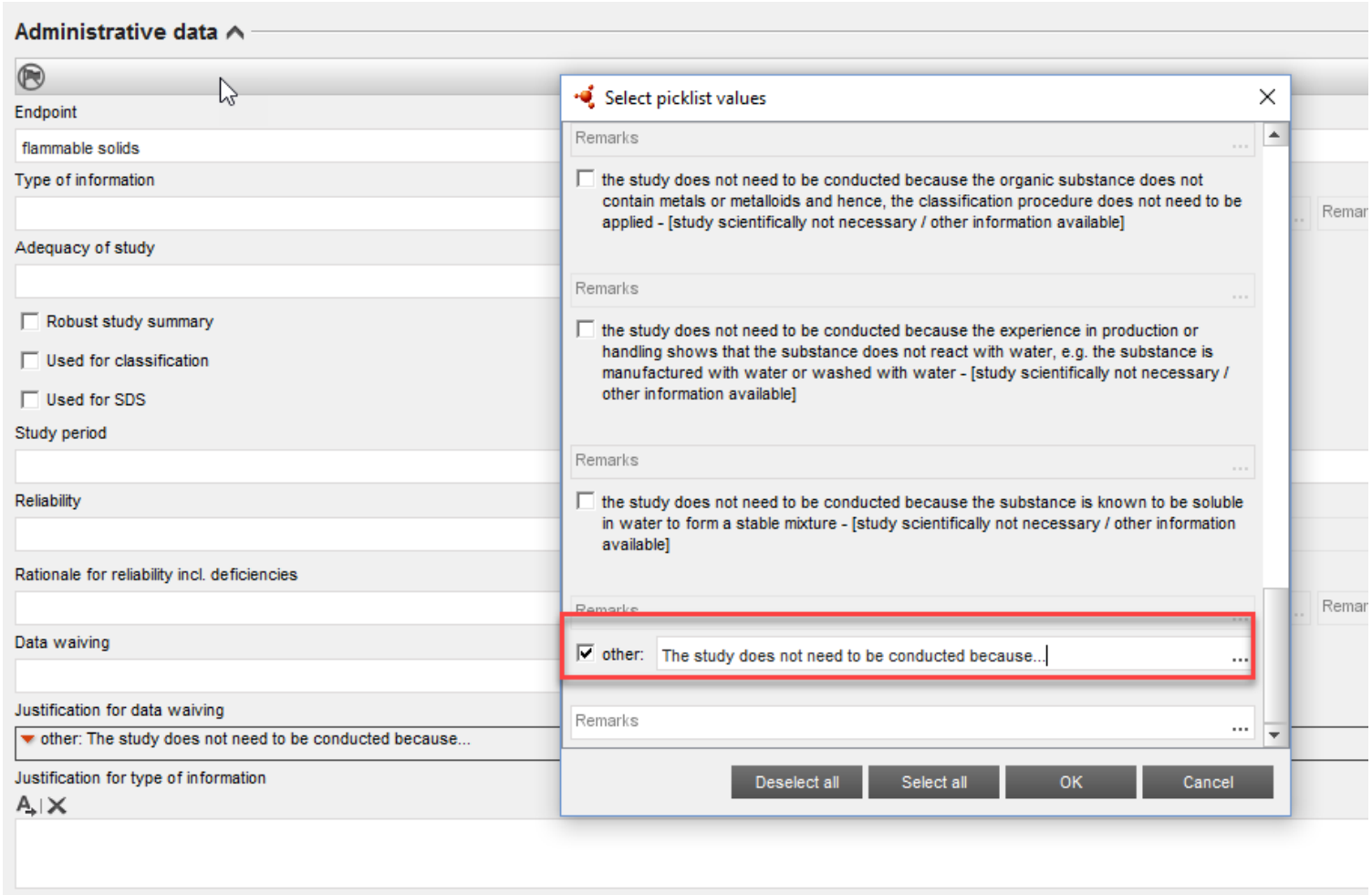
Tips based on experience – Data waivers

- Use the existing justifications if applicable



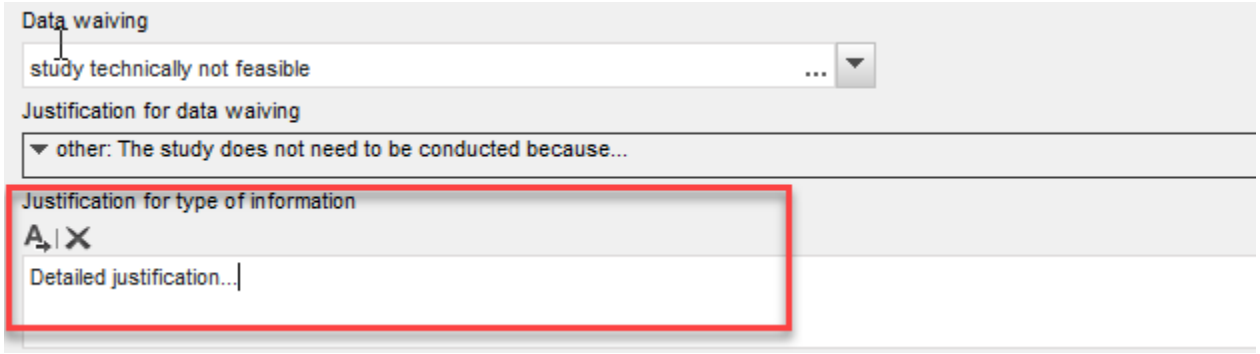
Tips based on experience – Data waivers

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



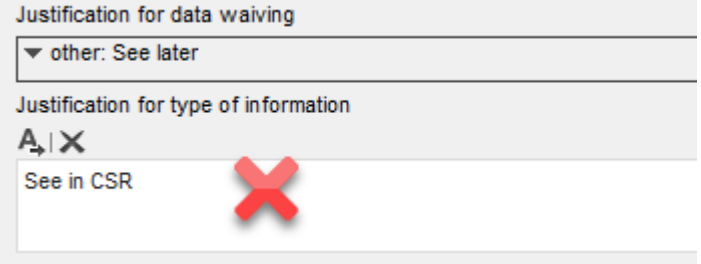
Tips based on experience – Data waivers

- If needed a detailed justification in the highlighted textbox



Tips based on experience – Data waivers

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



- The justification should be in the right place!

Reporting data in IUCLID

PNEC calculator

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.

PNEC calculator

Purpose

- PNEC derivation is a key element for the risk characterisation of a chemical substance.

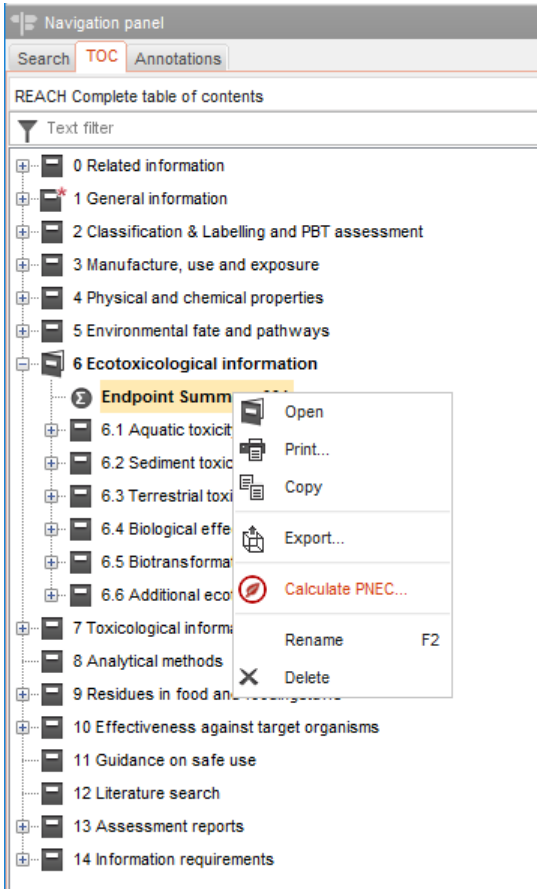
- The PNEC calculator allows you to derive PNECs automatically from the data already available in the **endpoint summaries** (IUCLID sections 5.4.1 (Adsorption / desorption), 6.1.1 to 6.1.6 (Aquatic toxicity), 6.2 (Sediment toxicity) and 6.3.1 to 6.3.4 (Terrestrial toxicity)) **of a substance dataset 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 PNECoral used for the assessment of secondary poisoning.

PNEC calculator

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 addressed 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.

PNEC calculator

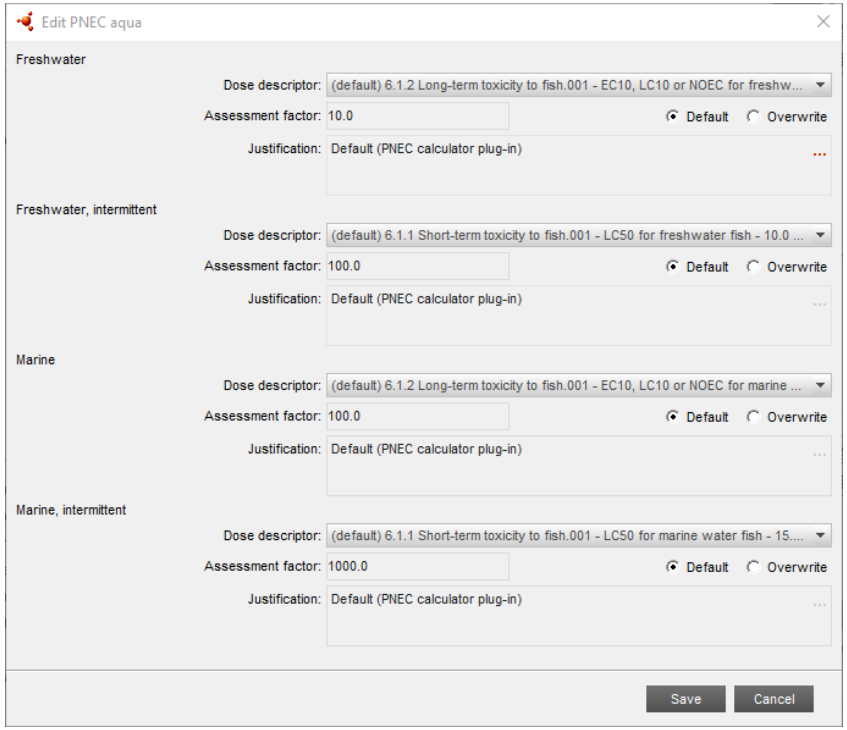
Overview – how it works?

- 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.

PNEC calculator

Overview – how it works?

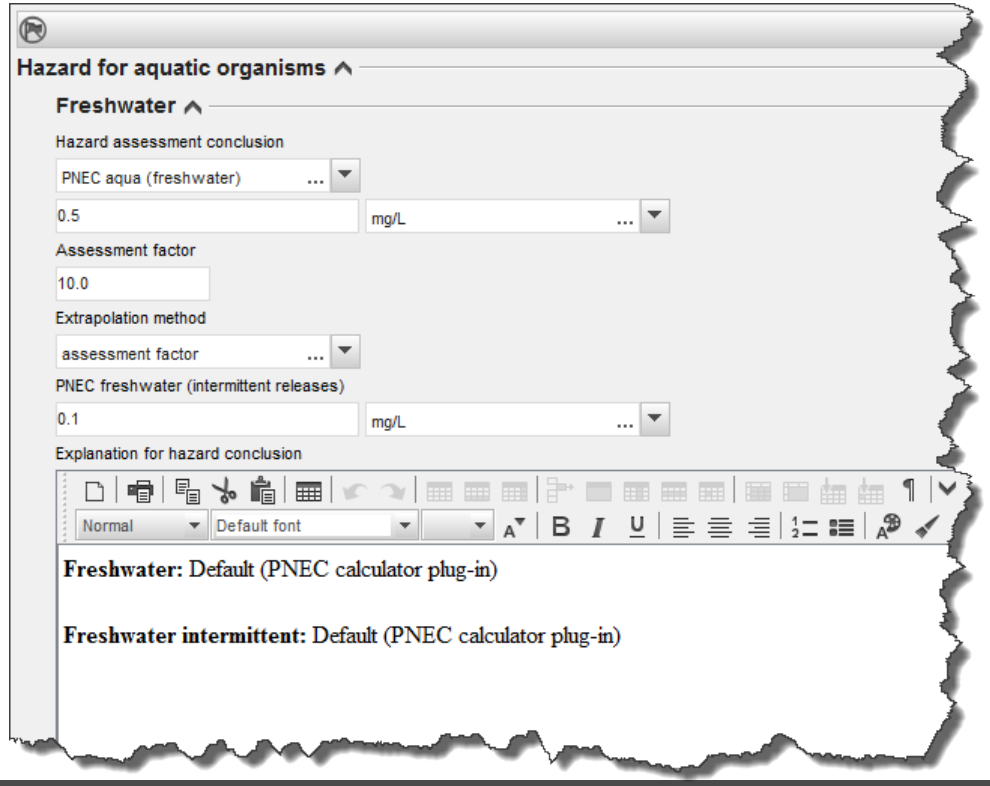
- Edit mode
  - Allows the user to:
    - select a different dose descriptor as starting point,
    - use non-default assessment factors,
    - use another extrapolation method (for sediment and soil).
  - Any modification from default requires the user to provide a justification.



PNEC calculator

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.



Reporting data in IUCLID

DNEL calculator

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

DNEL calculator

Purpose

- DNEL derivation is a key element for the risk characterisation of a chemical substance.

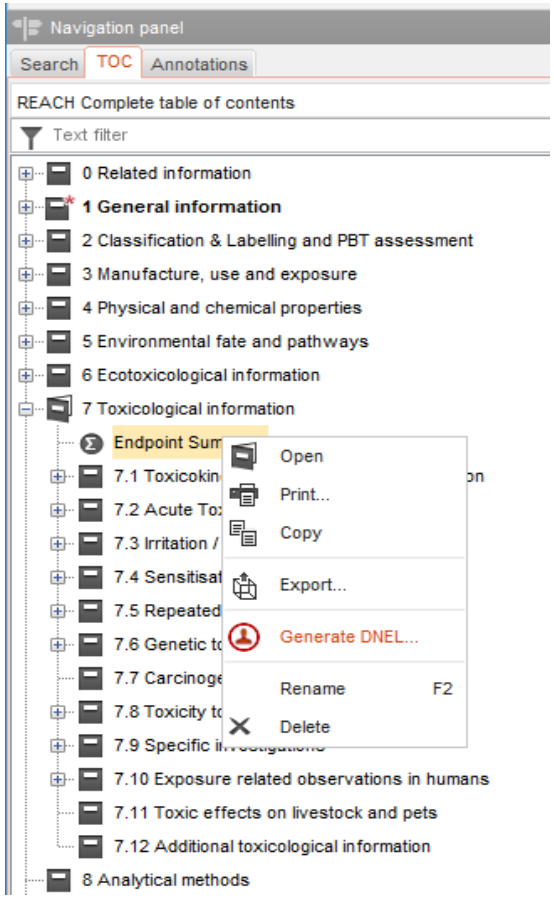
- The DNEL generator allows you to derive DNELs automatically from the data already available in the **endpoint summaries (sections 7.1, 7.5 and 7.8) of a substance dataset or template** and report them back in the corresponding endpoint summary under section '*7 Toxicological information*'.

- 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.

DNEL calculator

Overview – how it works?

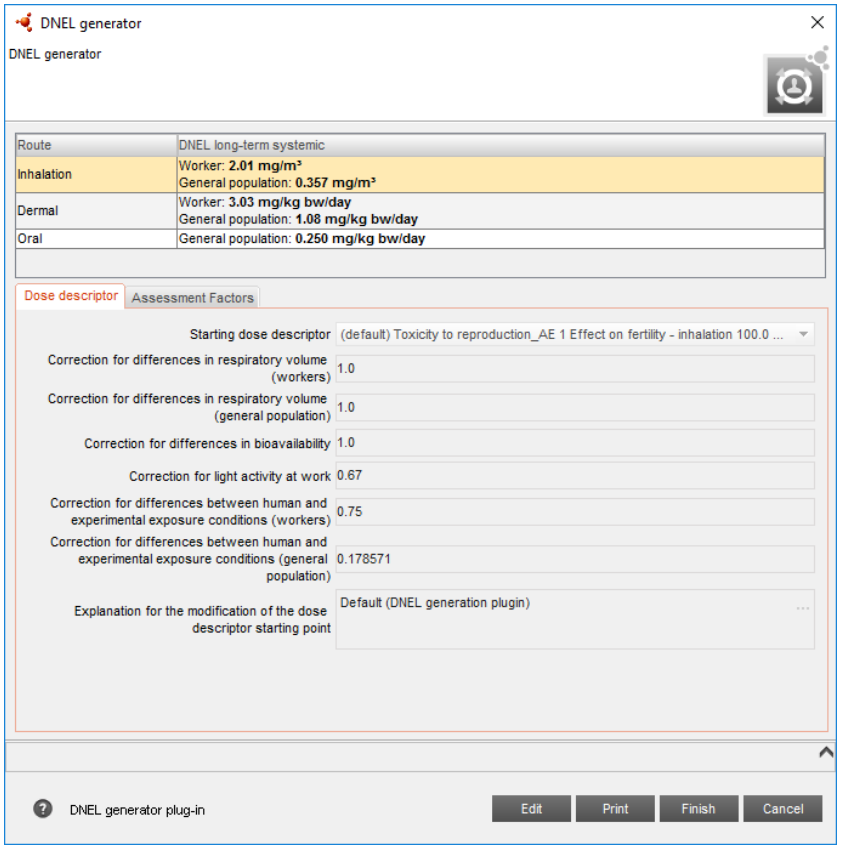
- How to use it?
  - You can use the DNEL calculator by right-clicking the endpoint summary under section '*7 Toxicological information*' and selecting '*Generate DNEL*' from the displayed menu.



DNEL calculator

Overview – how it works?

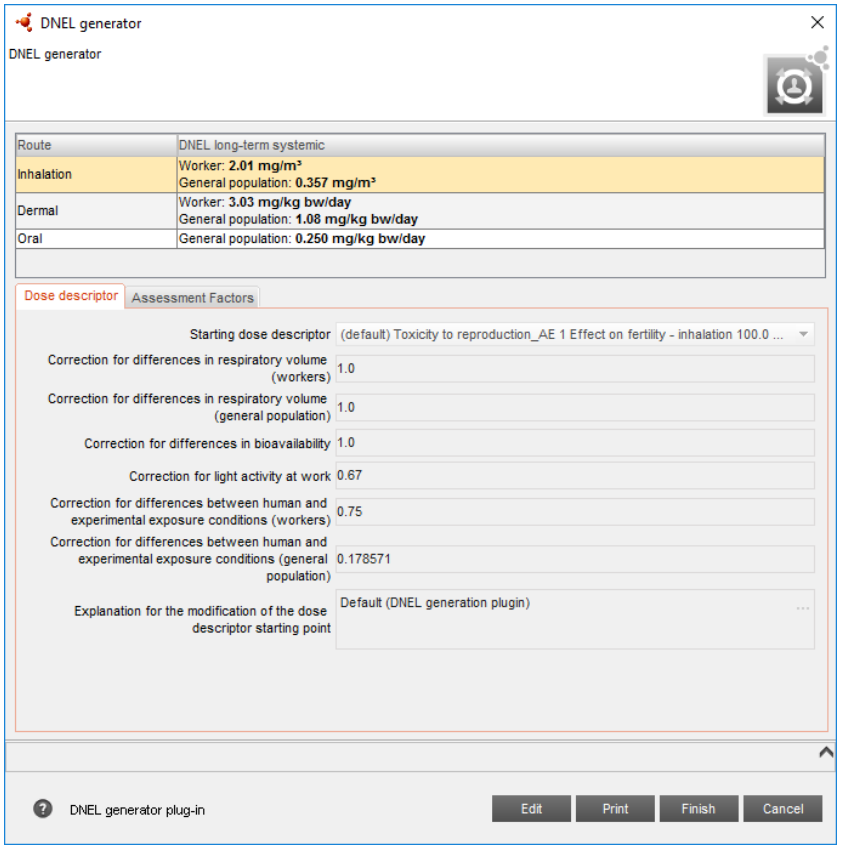
- Outcome
  - The results (DNELs calculated according to the Guidance R8) are displayed in a tabular format by route.
  - The dose descriptor used as starting point for the selected route and the parameters used to correct it are set by the tool and displayed in the tab called '*Dose descriptor*' as 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.



DNEL calculator

Overview – how it works?

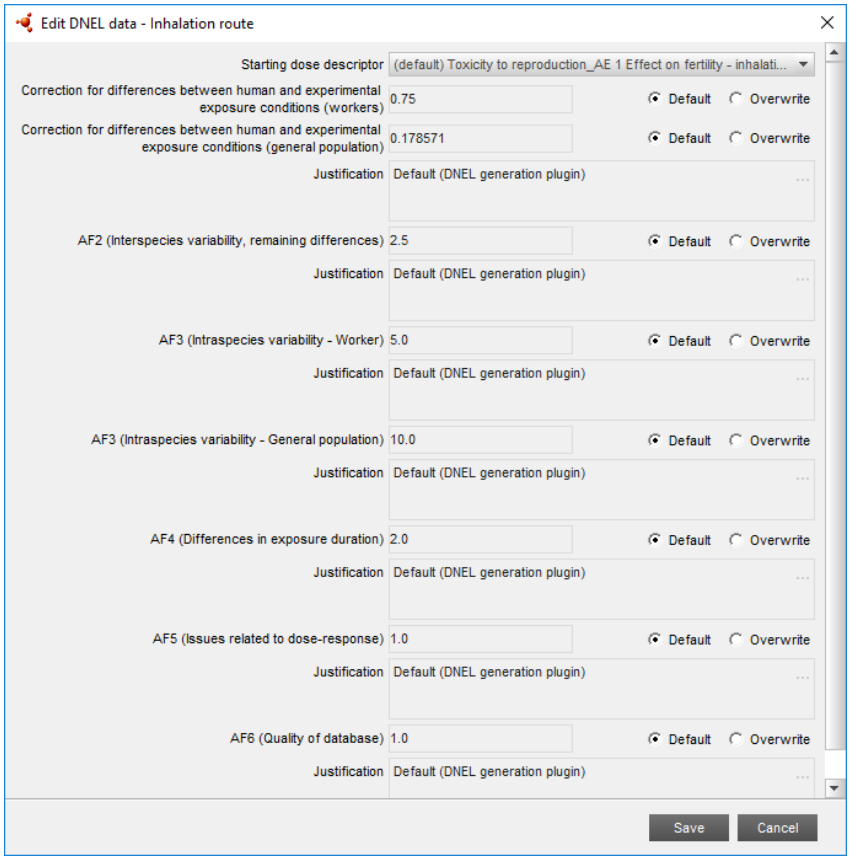
- Functionalities
  - **Edit button** enables to change the selection of the initial dose descriptor and some parameters used to derive the DNELs in a pop-up window.
  - **Print button** generates a report in a .rtf format containing the derived DNELs information as in section 5.11 of the CSR.
  - **Finish 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.



DNEL calculator

Overview – how it works?

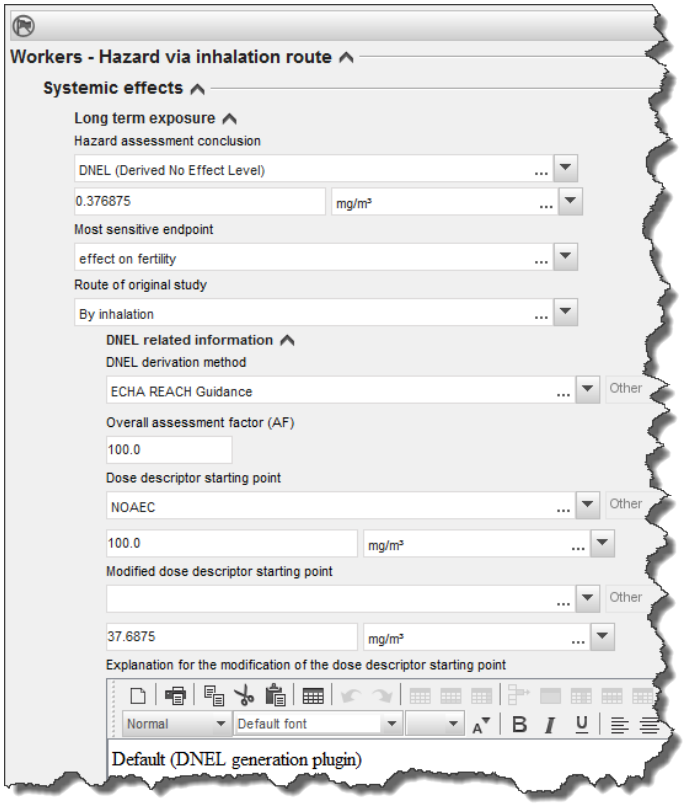
- Edit mode
  - Allows the user to:
    - select a different dose descriptor as starting point,
    - use non-default correction factors for differences between human and experimental exposure conditions,
    - use non-default assessment factors.
  - Any modification from default requires the user to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

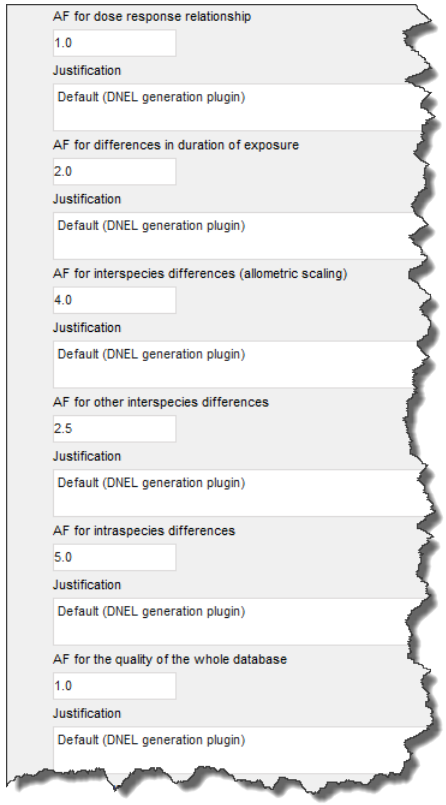


DNEL calculator

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.





DNEL calculator

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 stardard respiratory volume for humans (per kg bw) and applying the corresponding allometric scaling factor.

DNEL calculator

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:

sRV(human, 8h) = 6.7 m3/person/8h

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

- For workers (70 kg)

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

- For general population (60 kg)

  sRV(human, 8h) = 6.7 / 60 kg = 0.1117 m3/kg bw/8h

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

sRV(rat, 8h) = sRV(human, 8h) x allometric scaling factor = 0.0957 x 4 = 0.38 m3/kg bw/8h for workers

sRV(rat, 8h) = sRV(human, 8h) x allometric scaling factor = 0.1117 x 4 = 0.45 m3/kg bw/8h for general population

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

sRV(rat, 24h) = sRV(rat, 8h) x 24/8 = 1.35 m3/kg bw/24h for general population

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

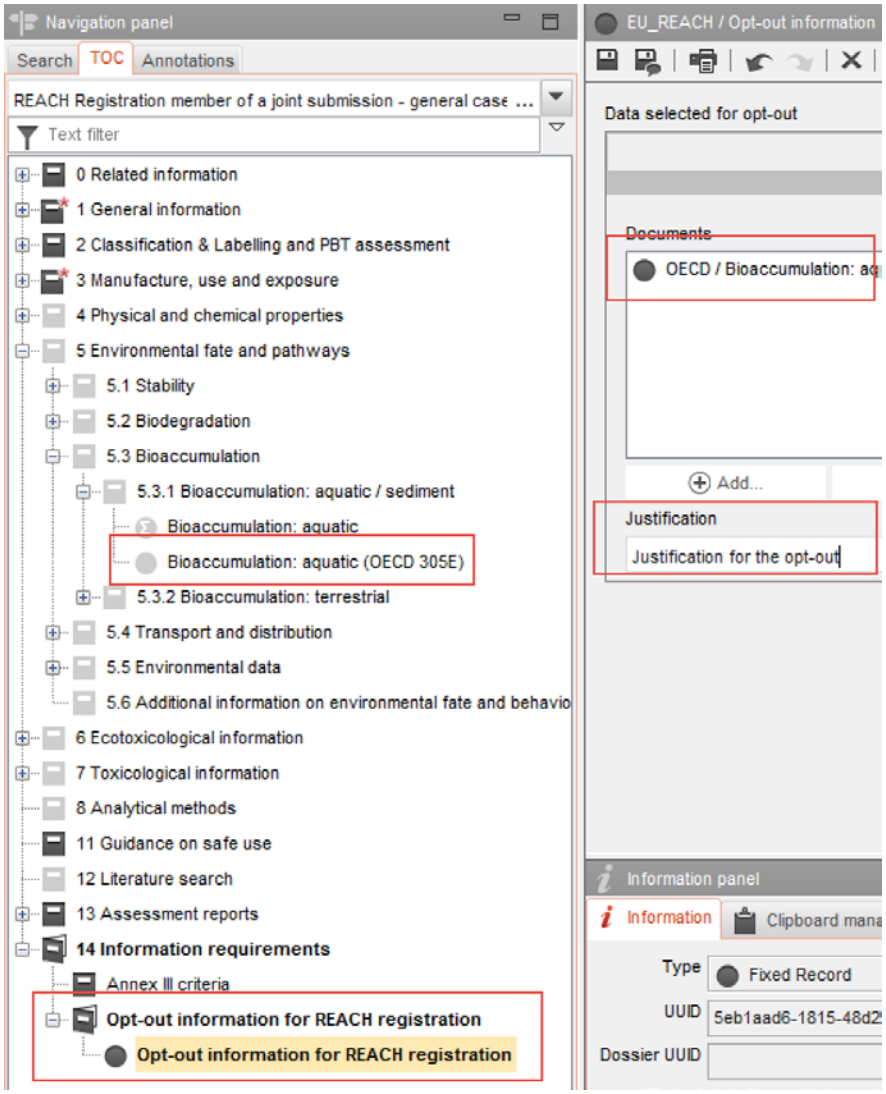
Feedback from users

REACH opt-outs

- Prepare your dataset

    1. Enter the data

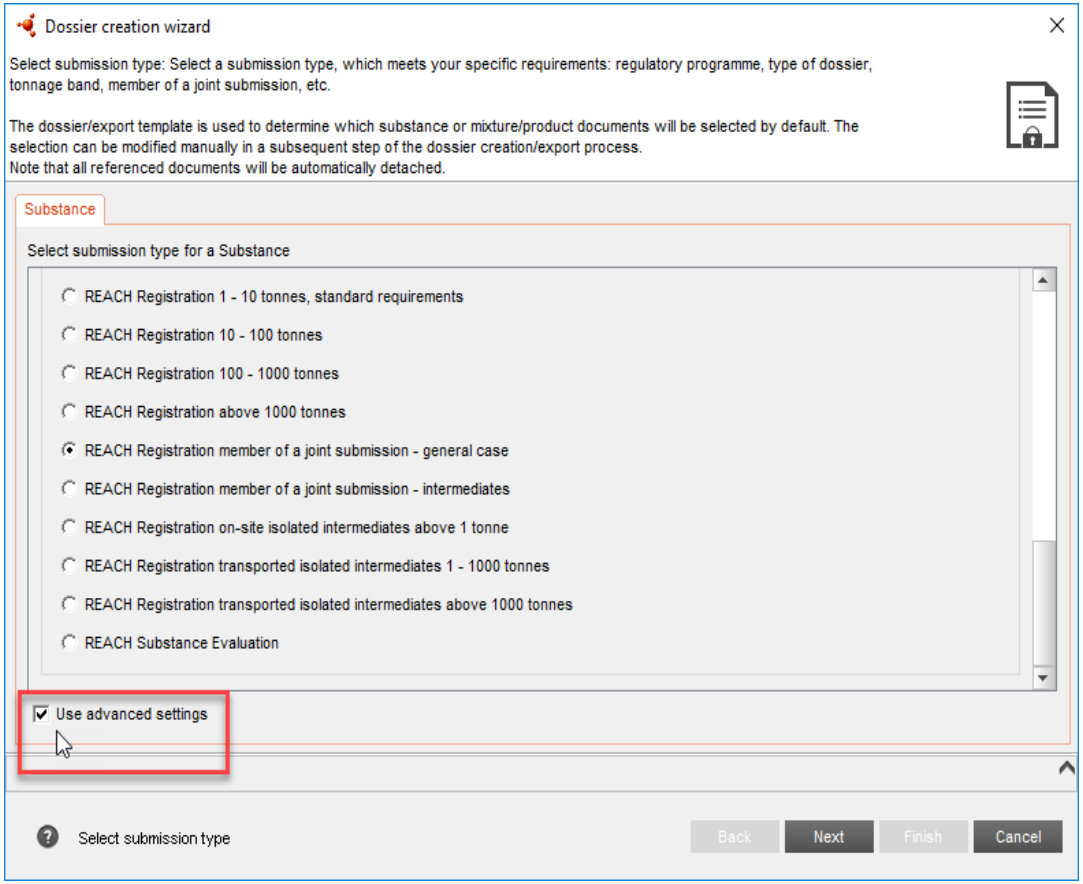
    2. Indicate the opt-outs and the justifications under section 14



Feedback from users

REACH opt-outs

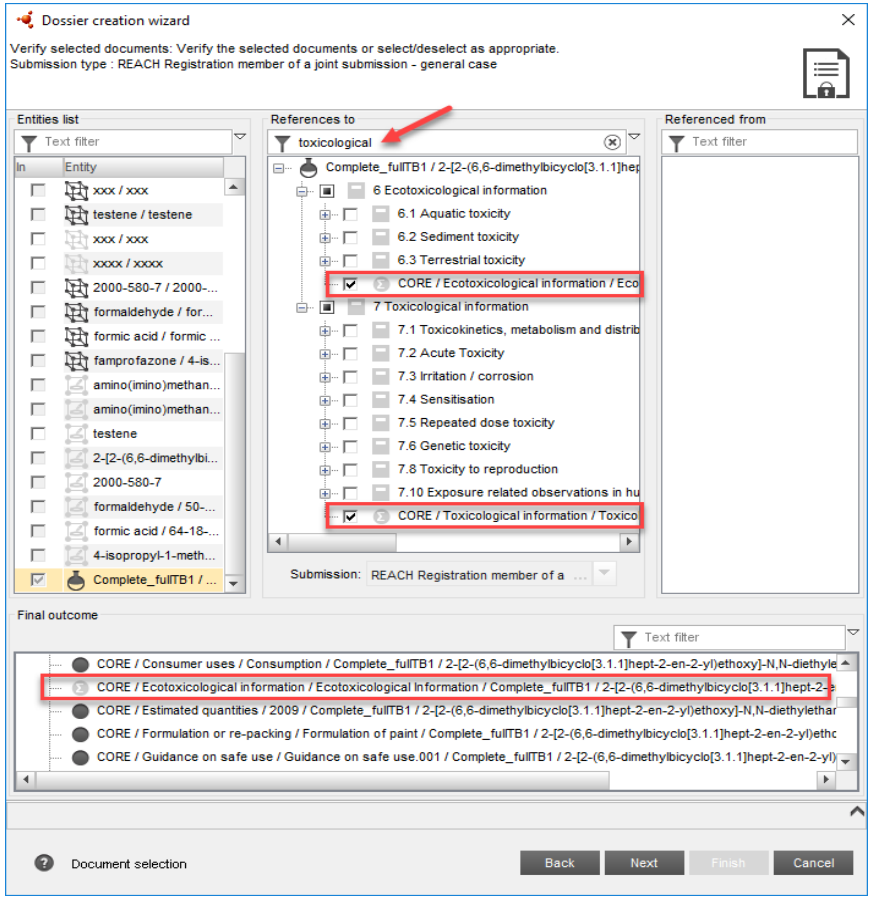
- Create your REACH registration dossier as a member of a joint submission
- An opt-out is done as part of a joint submission
- Activate the advanced settings of dossier creation



Feedback from users

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.



Reporting data in IUCLID

Changes between IUCLID 5 and 6

Data reporting in IUCLID 6

Amendment to REACH Annexes VII and VIII (1)

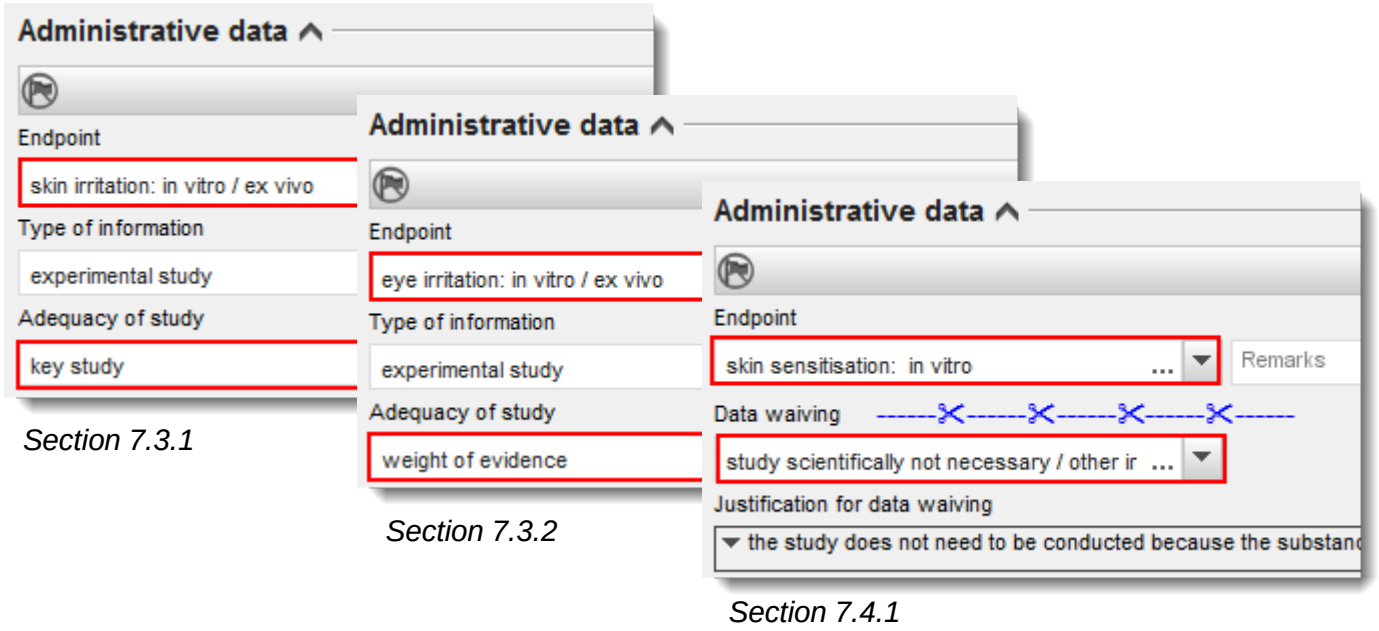
- **What?**
  - Information requirements on skin corrosion/irritation and serious eye damage/eye irritation amended; entered into effect on **June 21, 2016**.
  - Amendment makes the *in vitro* studies the standard information requirement at Annexes VII and VIII; *in vivo* studies to be considered only 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=

Data reporting in IUCLID 6

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.



Data reporting in IUCLID 6

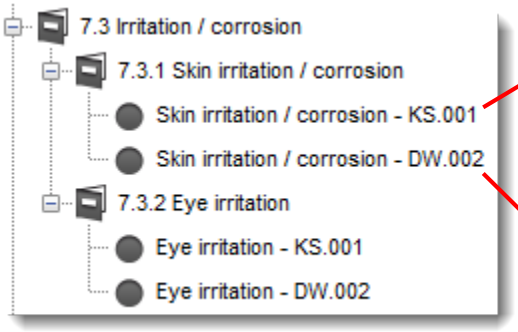
Amendment to REACH Annexes VII and VIII (3)

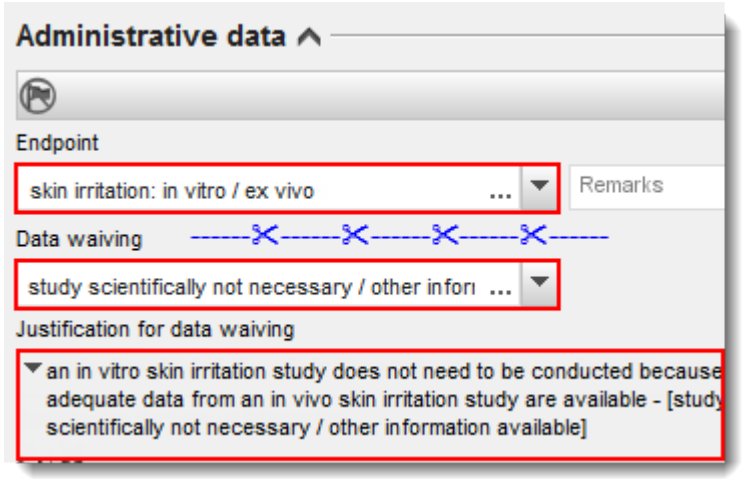
- **Consequence for reporting in IUCLID?**
  - **If an *in vivo* study exists** that was carried out or initiated before the Annex amendment took effect, this should be reported as an endpoint study record with the appropriate 'Adequacy of study', and the 'Endpoint' selection "… in vivo".
  - **In addition**, 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)

Data reporting in IUCLID 6

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





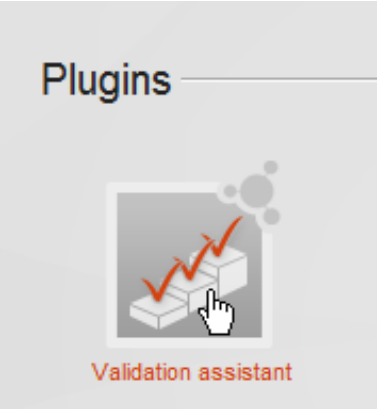
Add a link in the 'Cross reference' table of DW record to the KS record, to show where the in vivo information is provided.

IUCLID features

Validation assistant

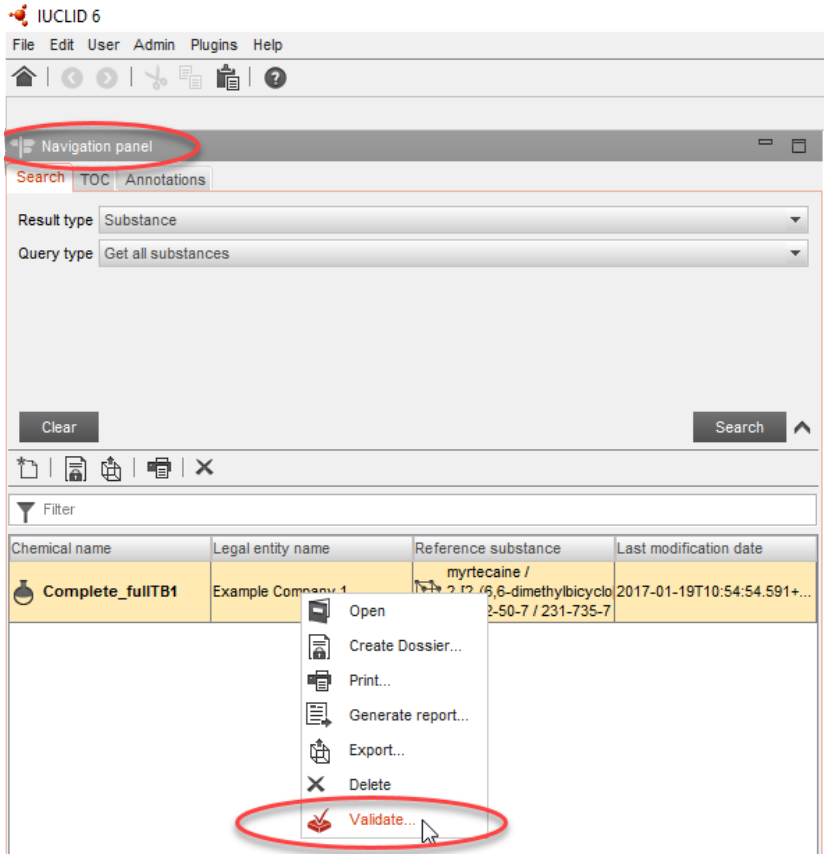
Tips for REACH registrants - general

- Validation Assistant plug-in



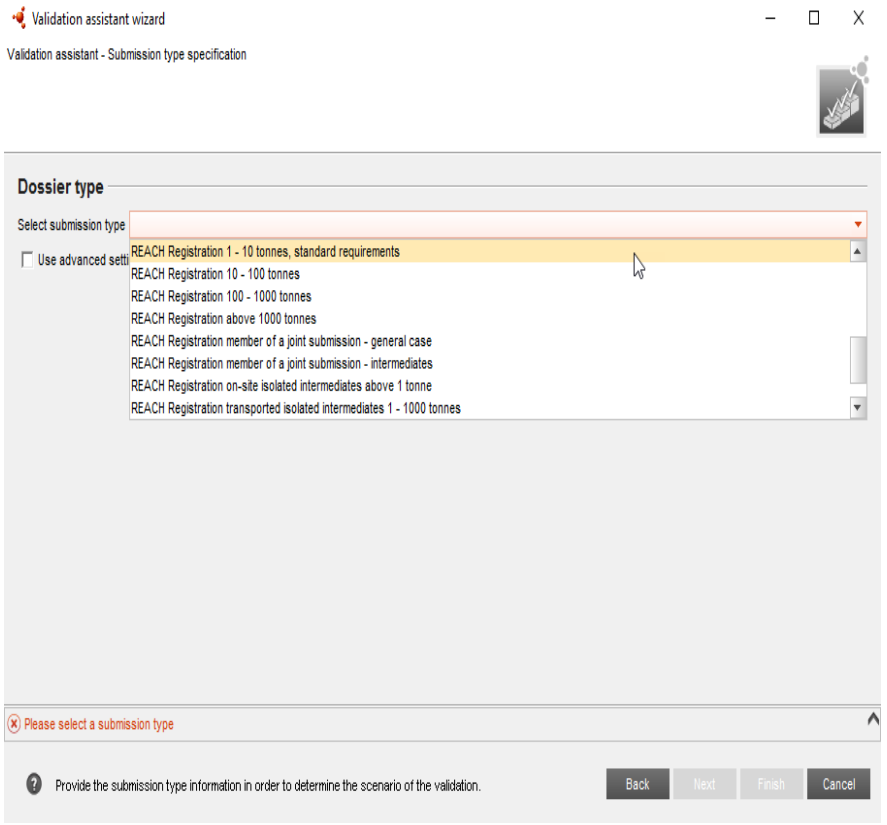
Using the Validation Assistant

- Use the Validation Assistant on your substance dataset



Using the Validation Assistant

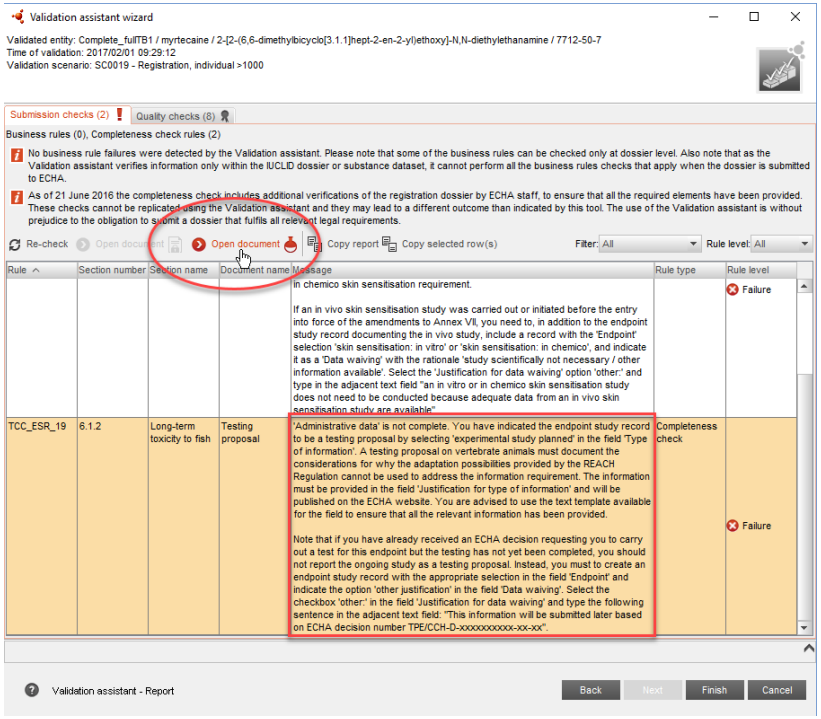
- Select the scenario that applies to your substance



Using the Validation Assistant

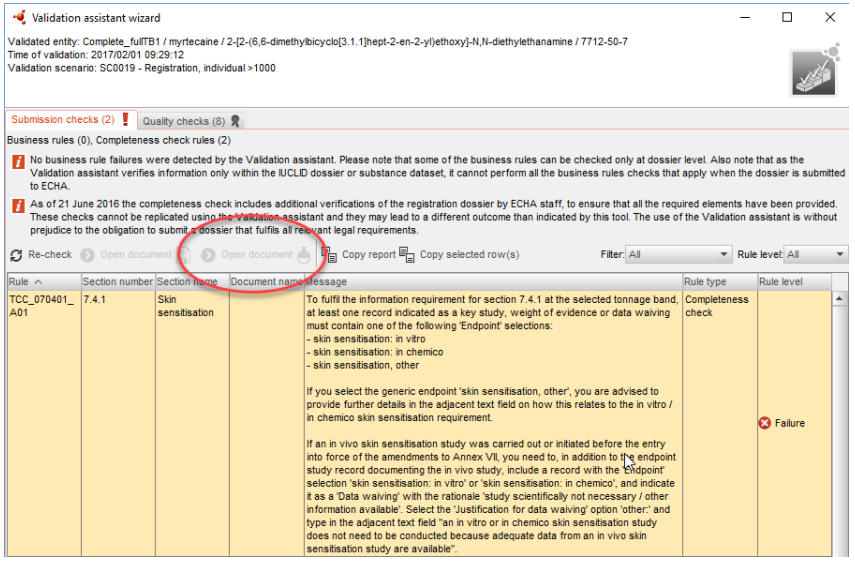
Click on the failure

- Open document in substance dataset



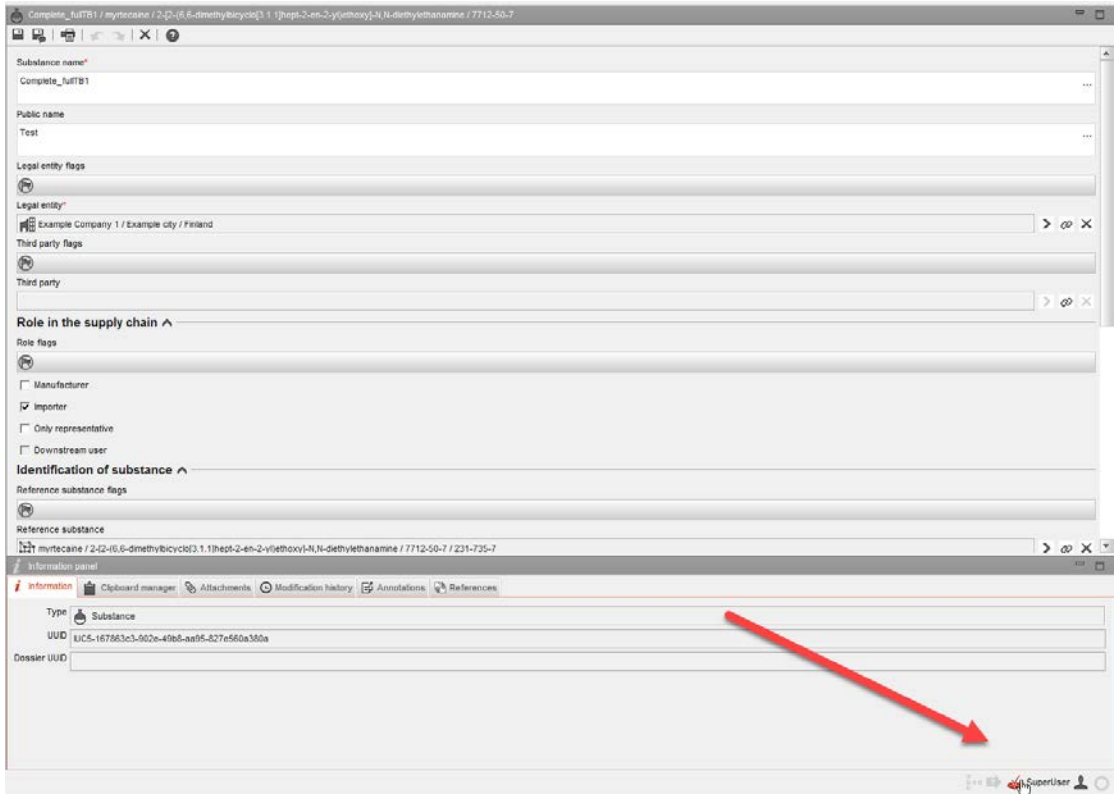
Click on the failure

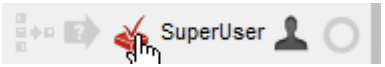
- Open document in substance dataset is unavailable



Using the Validation Assistant

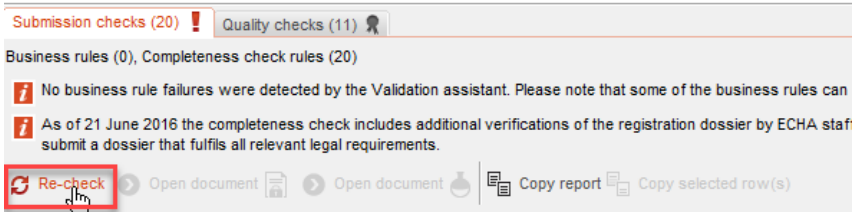
- Correct the failure in the substance dataset and unhide the VA report



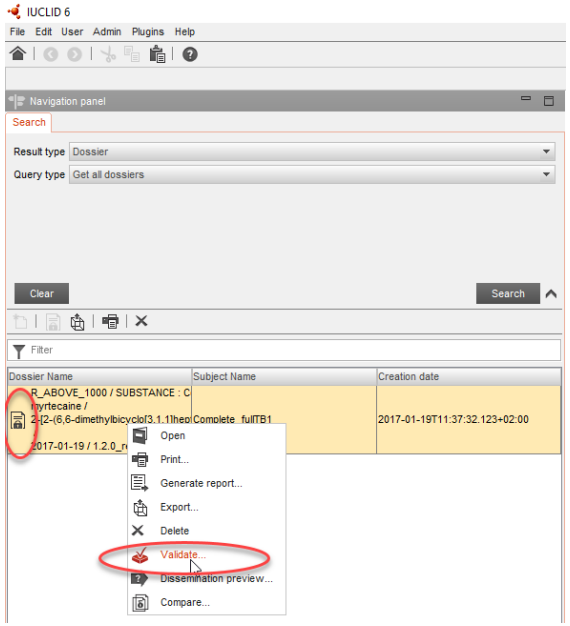


Using the Validation Assistant

- Re-check the substance dataset



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

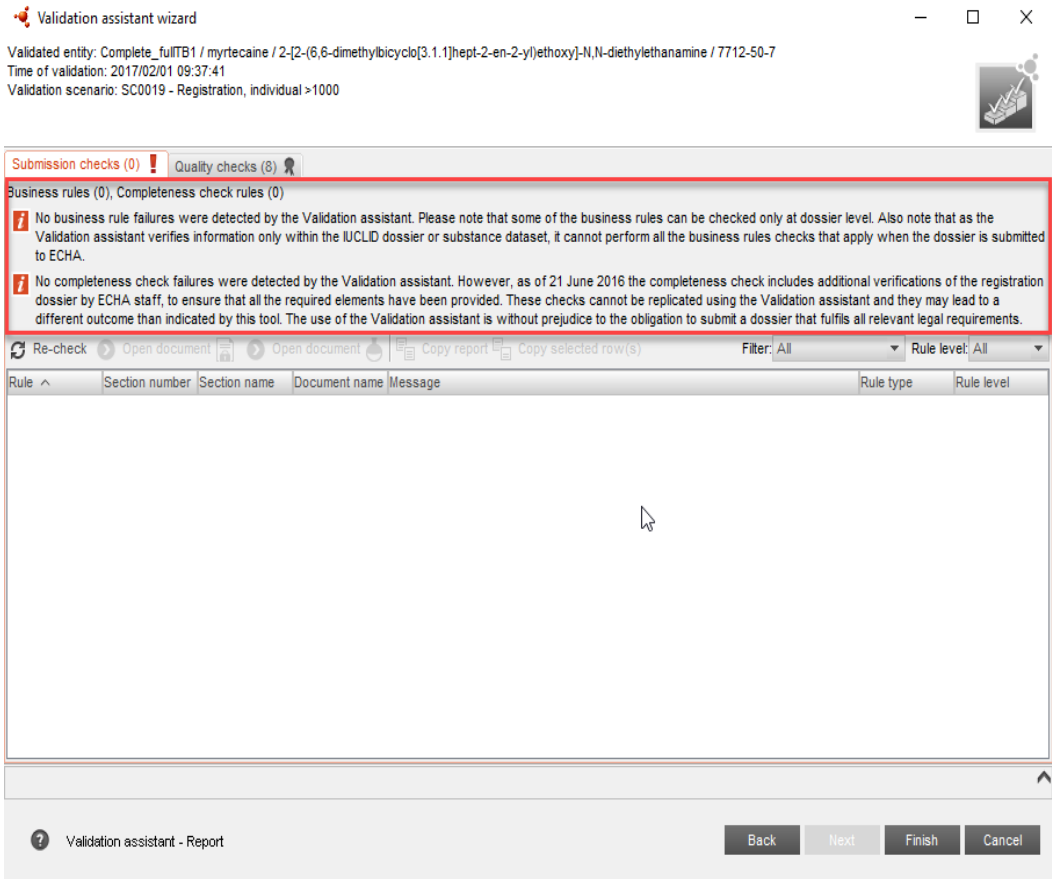


Using the Validation Assistant

- Note the disclaimers!

They tell what the results mean

- Business rules
- Completeness checks



Manual checks at TCC by ECHA staff

- 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

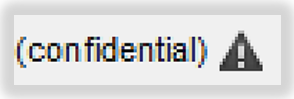
- ECHA Helpdesk

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

Print

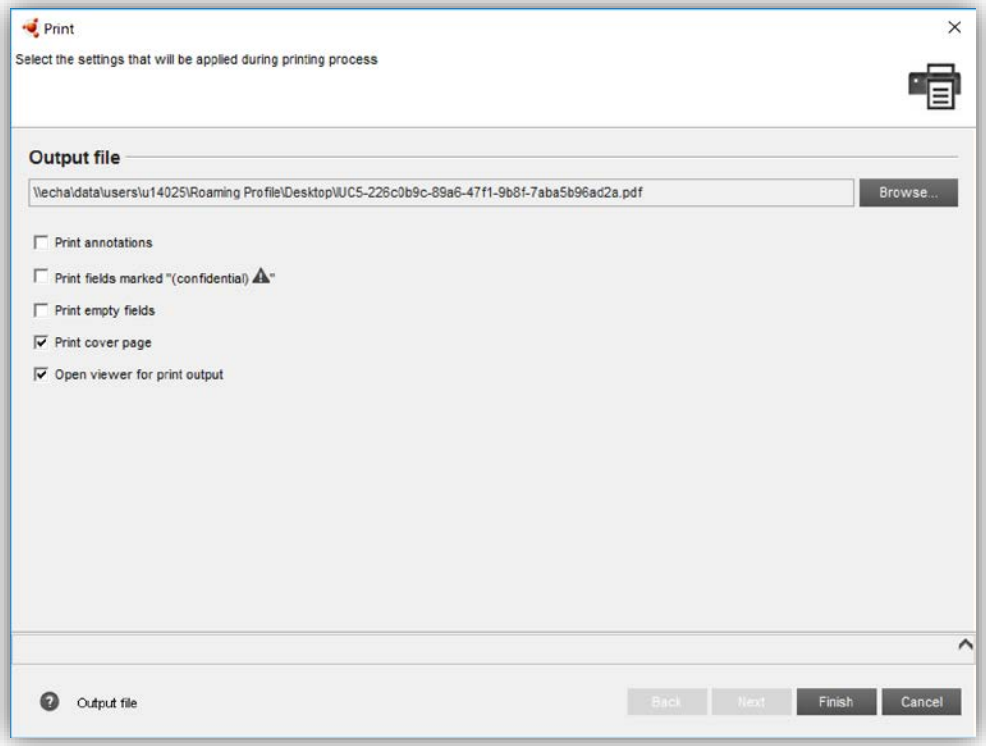
IUCLID 6 version 2.0.0

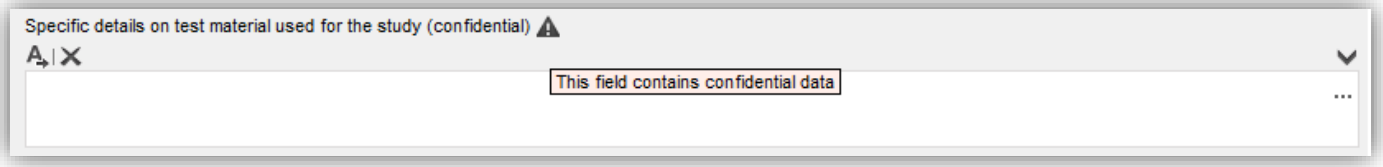
Print option



- 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





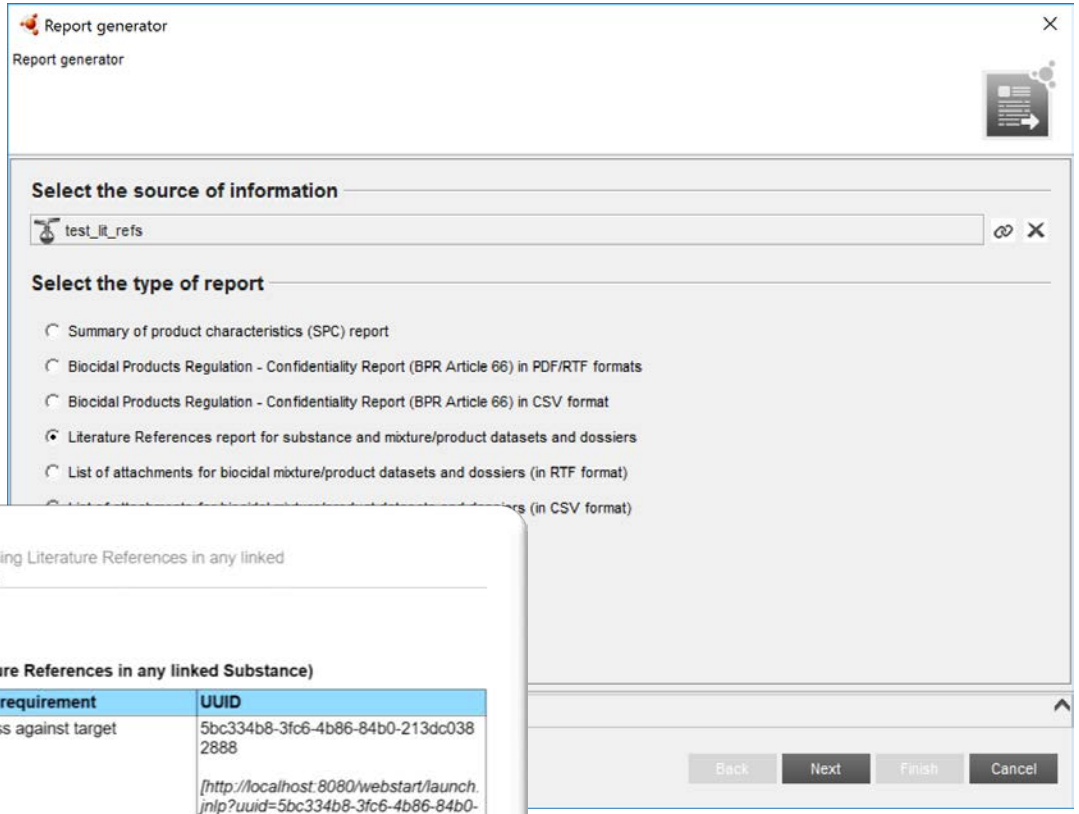
Report generator

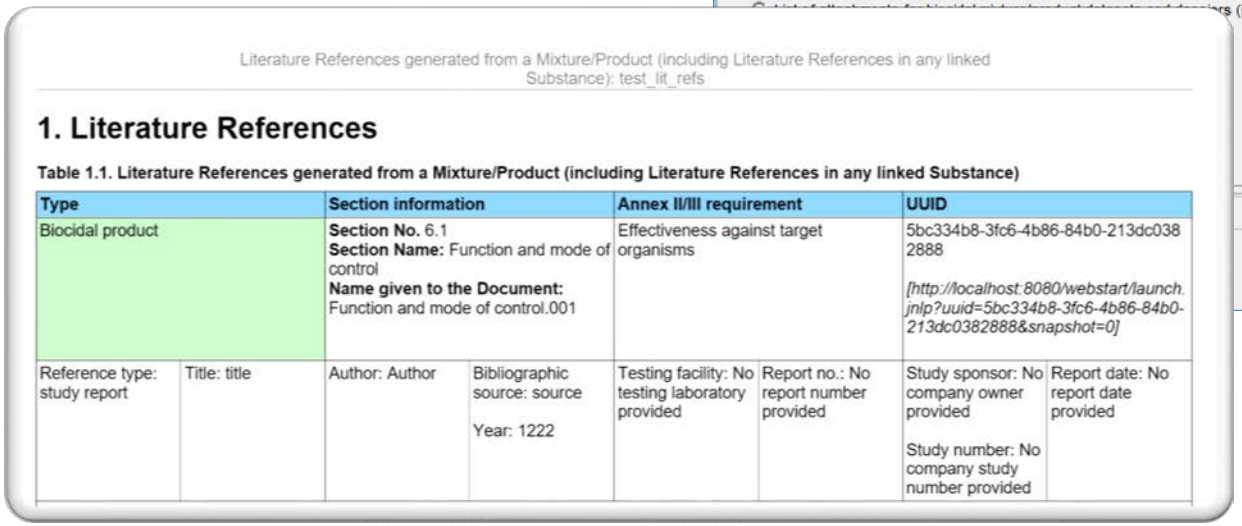
Report generator

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 *[http://localhost:8080/webstart/launch.jnlp?uuid=5bc334b8-3fc6-4b86-84b0-213dc0382888&snapshot=0]*	
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 Study number: No company study number provided	Report date: No report date provided

Report generator

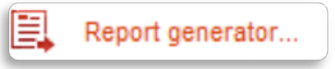
Other reports available and compatible with IUCLID 6.2

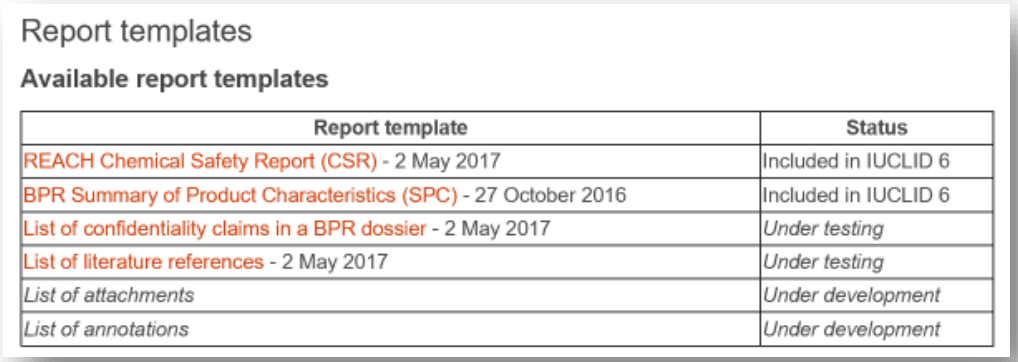
- **S**ummary of **P**roduct **C**haracteristics report (for uploading into SPC Editor)
  - Can be generated from mixture/product datasets/dossiers as an XML
- Literature references report (RTF)
  - Can be generated from both substance and mixture/product datasets/dossiers
- Attachments report for BPR 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

Report Generator

The IUCLID Report Generator - what's new?

- Manage Reports (new feature of the report generator)

- New templates available to store in  and use with the 



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*

Report Generator

Manage reports – what is it used for?

The Manage reports feature allows you to:

- **<u>Upload</u> and <u>Store</u> report templates in your own IUCLID installation and use these with the report generator**

- **<u>Further customise</u> 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

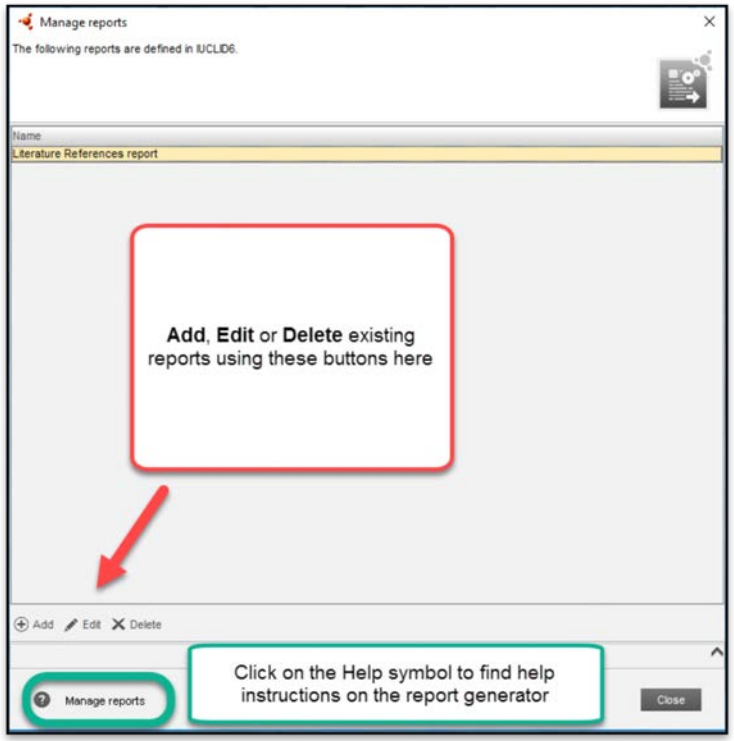
- Go to the IUCLID dashboard
- Left-click on the ‘Report generator’ icon
- Select ‘Manage reports’

Report Generator

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



Report Generator

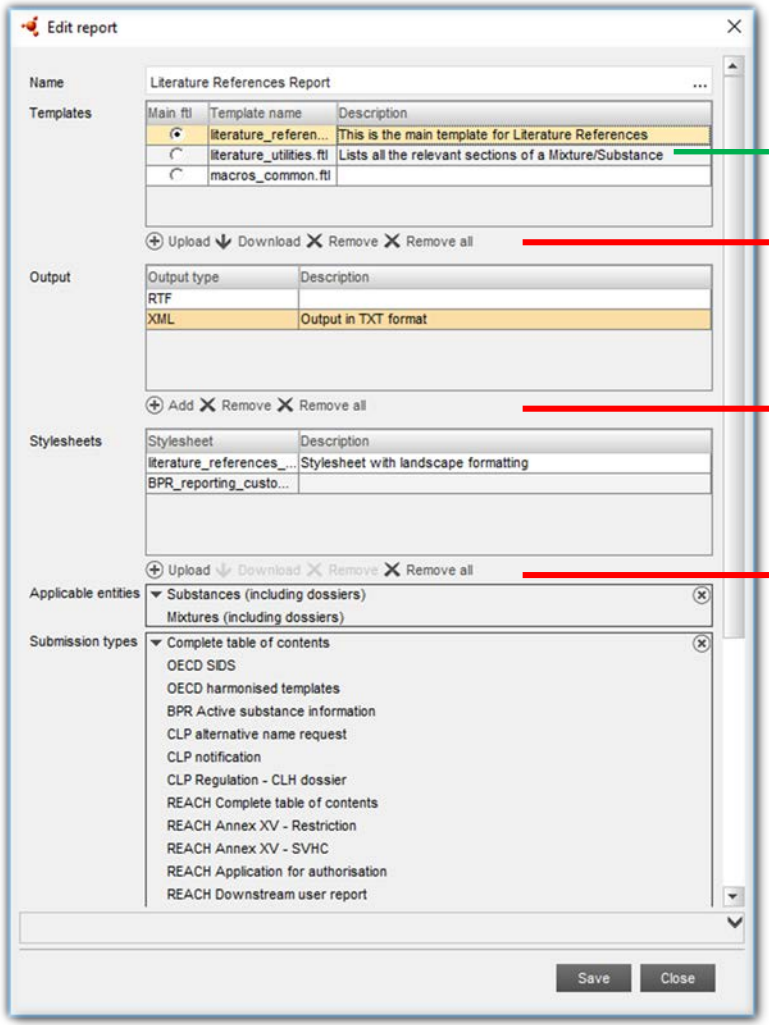
How to store and further customise your report templates

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

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

Report Generator

Editing or adding your report templates



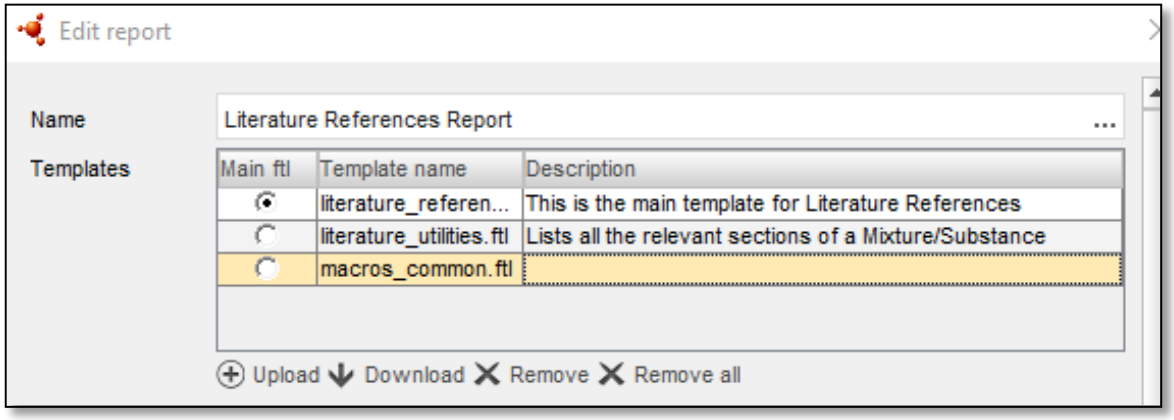
Make short comments about your uploaded files

Upload, download and remove your files

Report Generator

Editing or adding your report templates

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



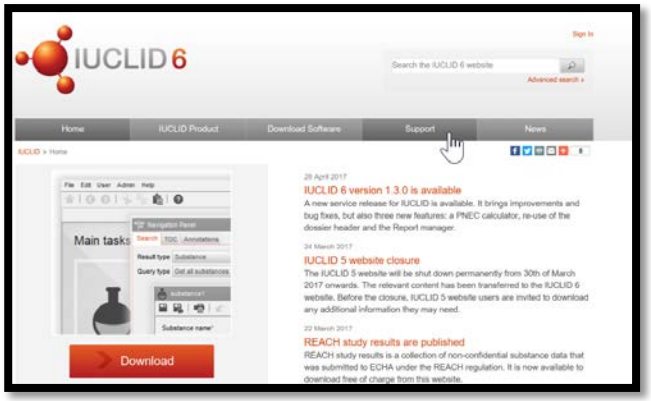
Additional templates are usually uploaded alongside the Main template to help shorten the length and complexity of the Main template or to re-use code which is repeatedly used by the Main template, saving time for the person writing the template and reducing the risk of errors when generating the report.

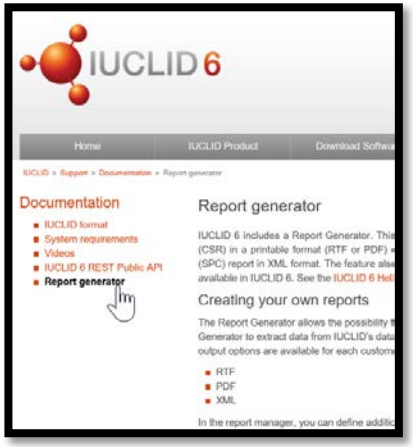
For example, a ‘utilities’ template in the example above lists all the relevant sections in a Substance and Mixture which I wish the Main template to include in the report.

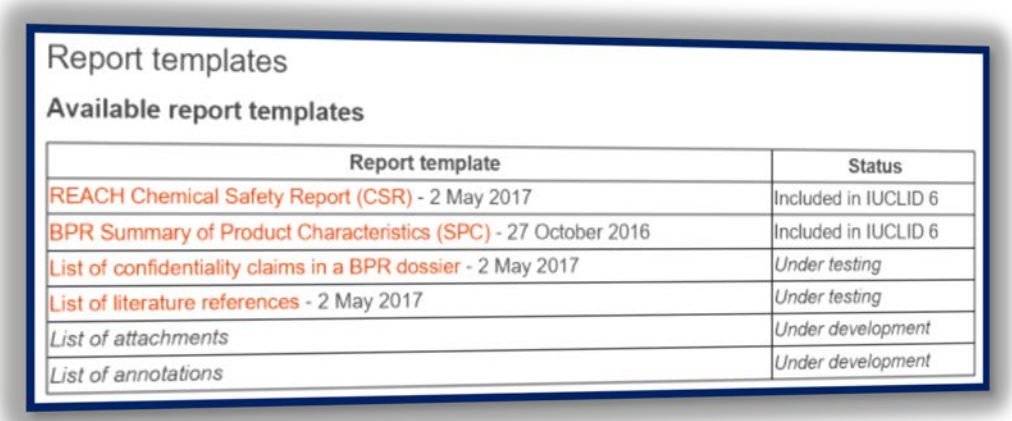
Report Generator

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

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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

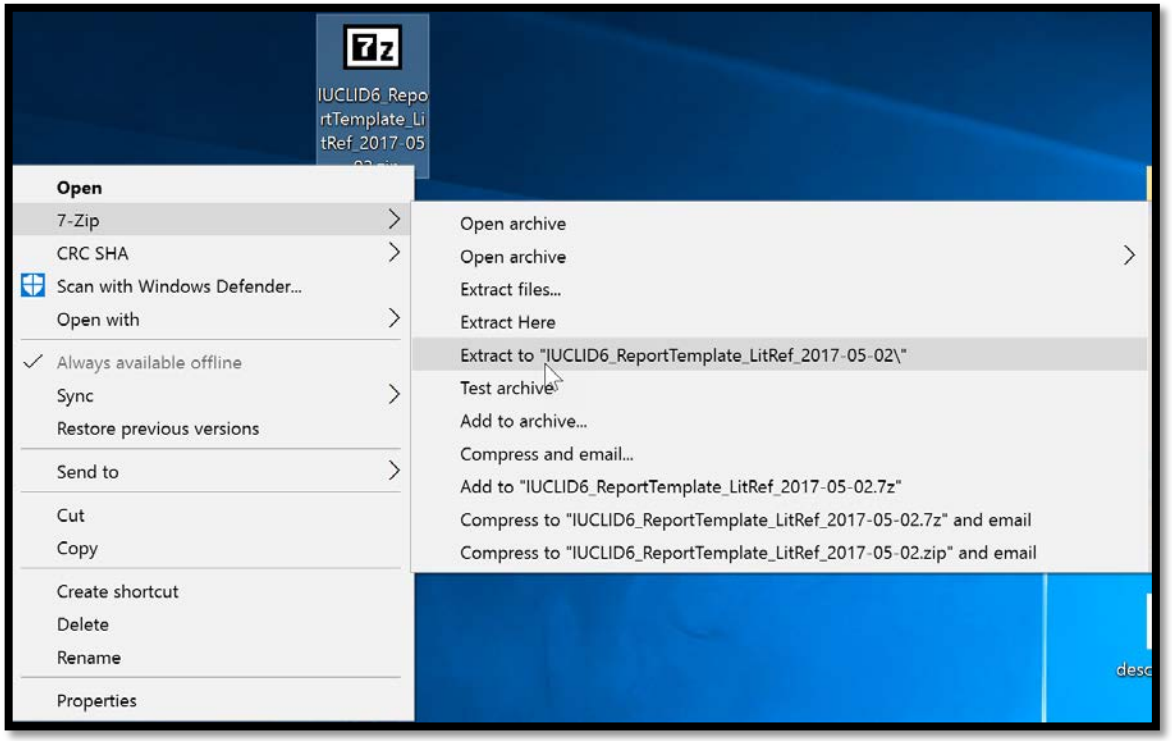
Report Generator

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.

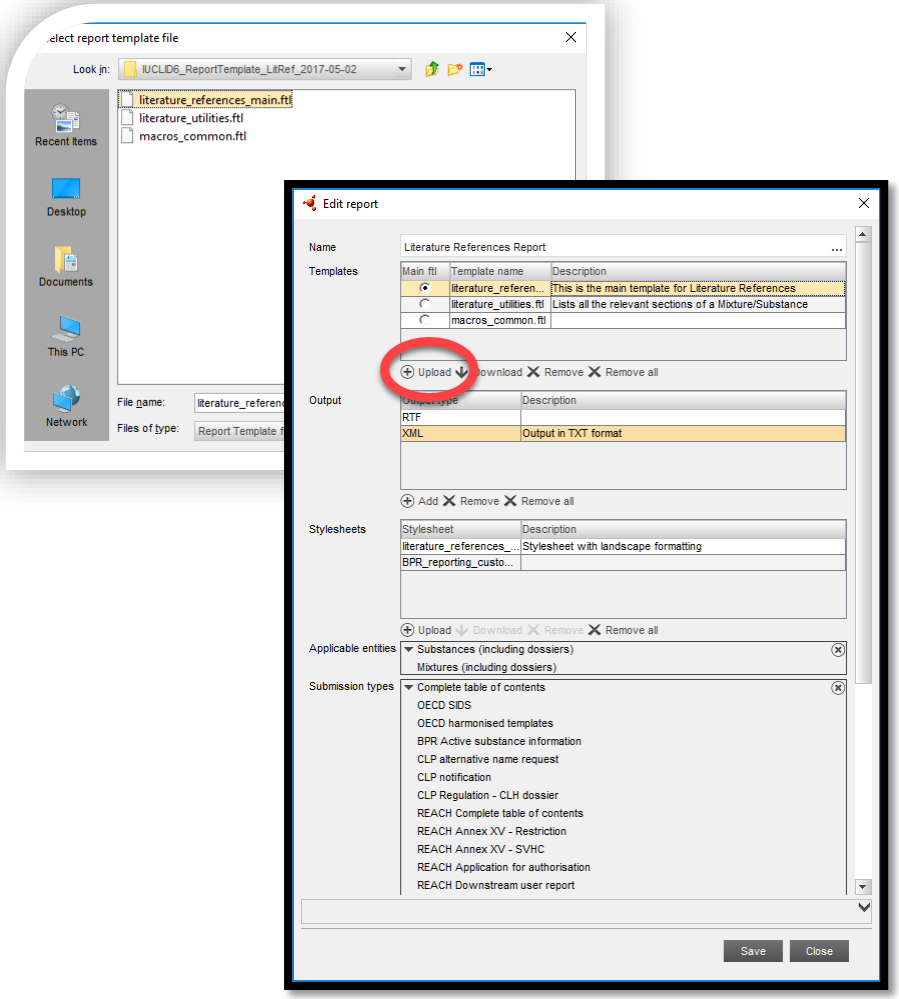
Extract the Zip folder like so:



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

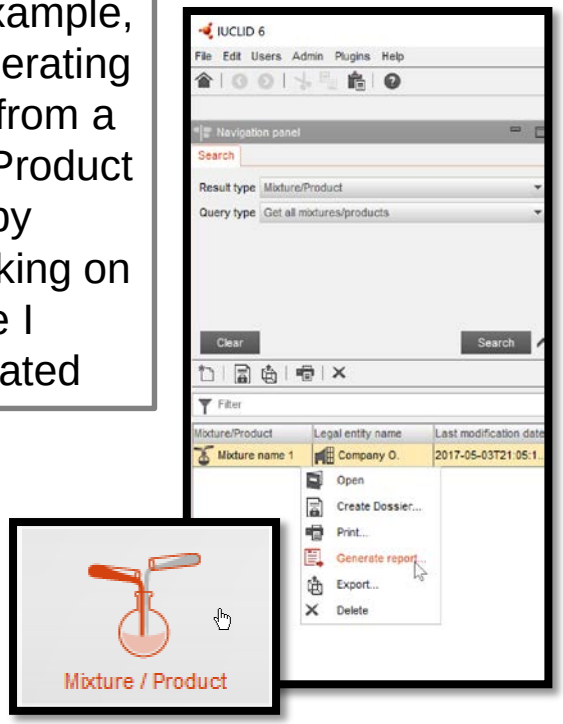
How you choose to customise the report will be reflected in the options presented to you when generating the report

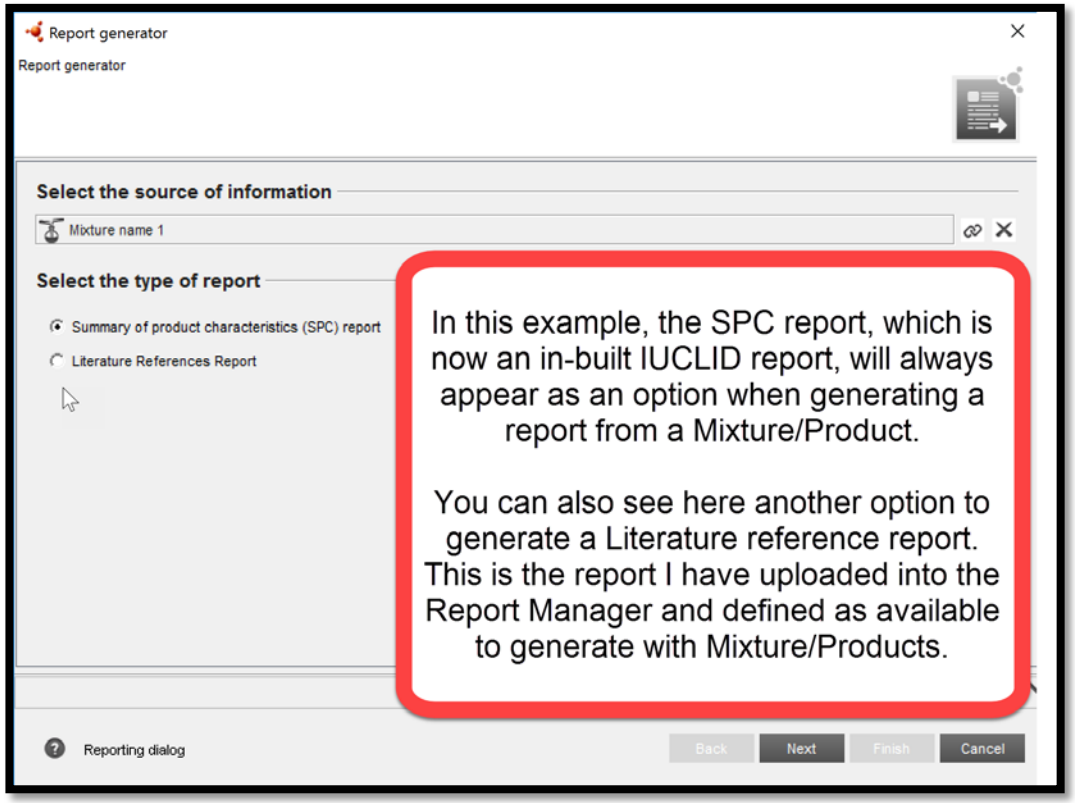
Report Generator

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





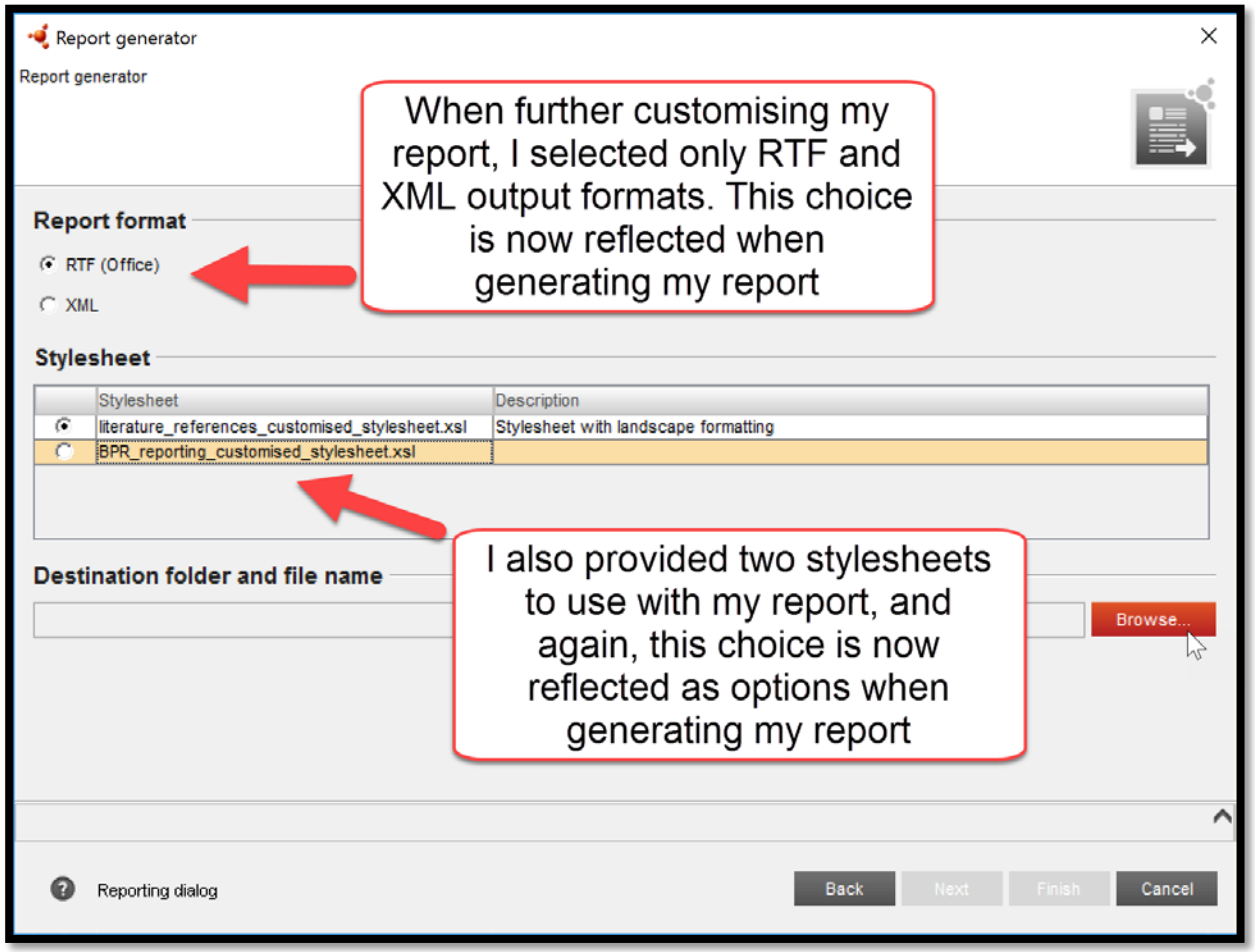
First step of the Report generator wizard

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

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*

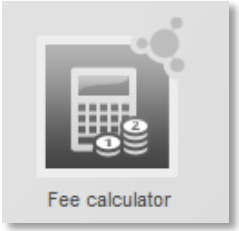
Fee calculator

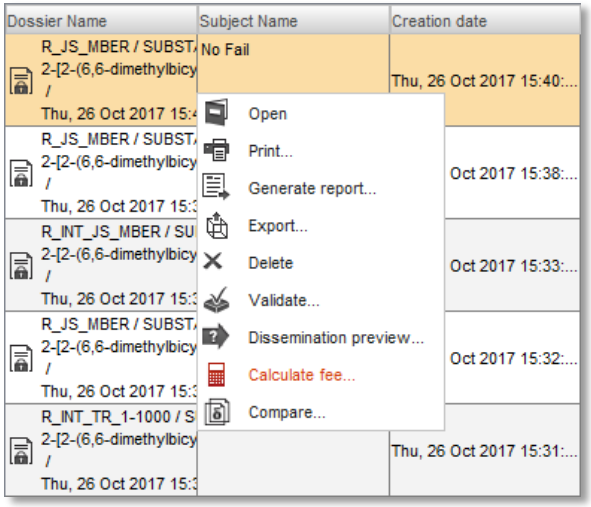
Fee calculator

- 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



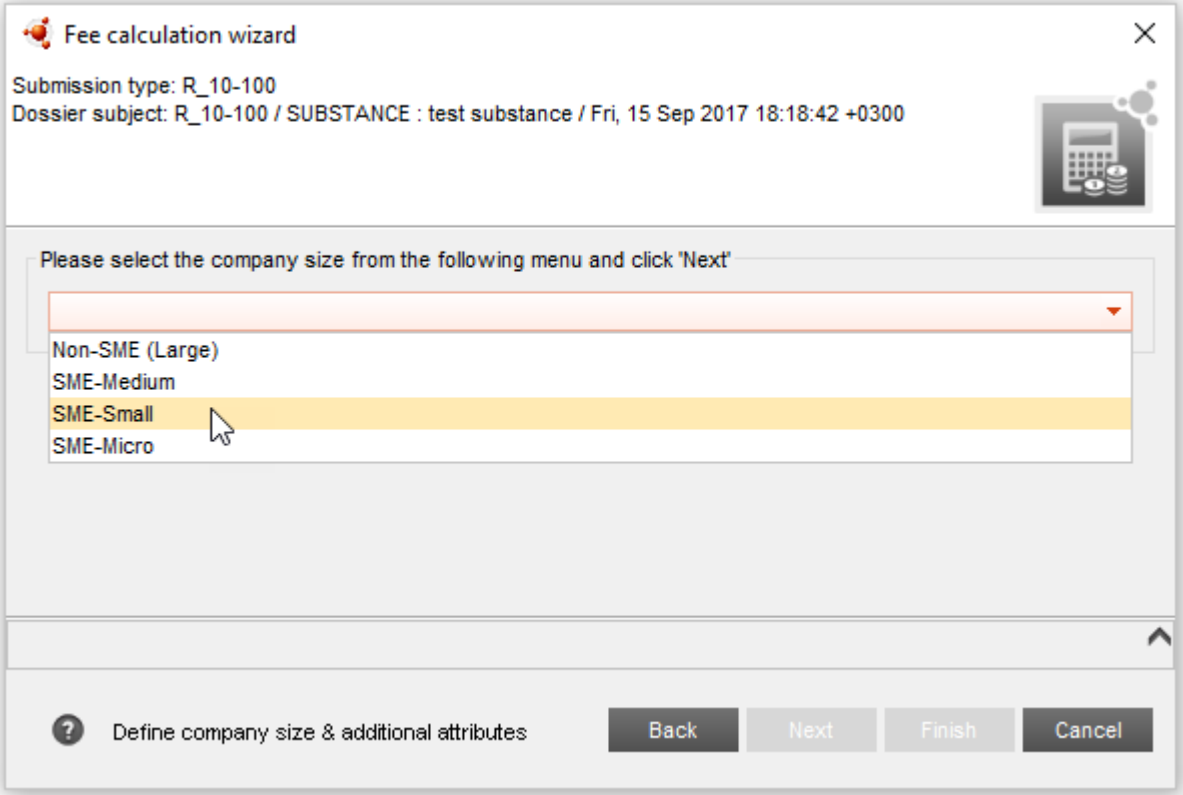


Fee calculator

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 calculator

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

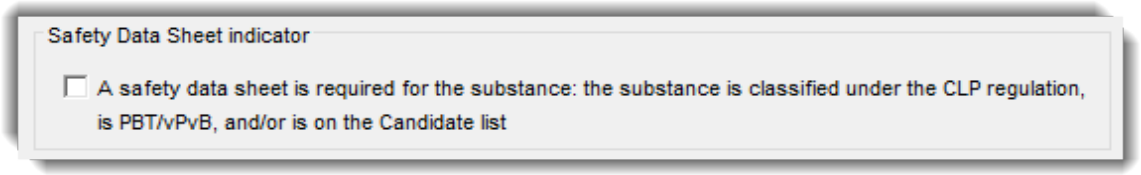
- For calculating the fees of dossiers with tonnage band 1–10 tonnes/year where the fee waiver has been claimed, you will need to indicate whether the substance fulfils the Annex III criteria

Fee calculator

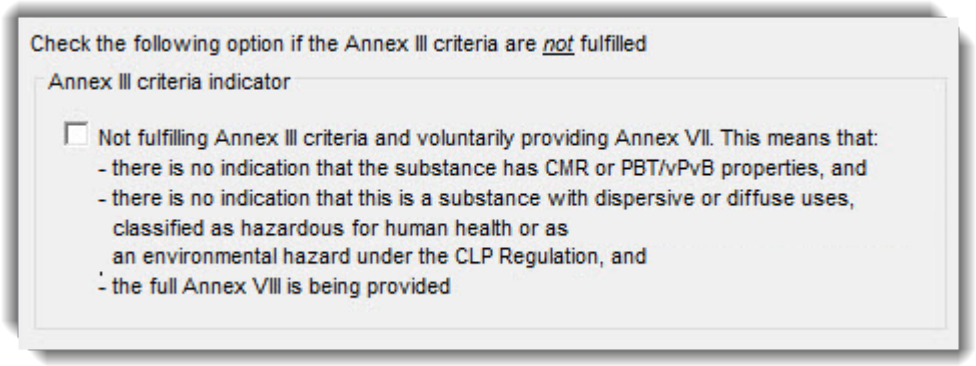
Indicators needed for the fee calculation

- Hazardous substance indicator

- Safety Data Sheet indicator



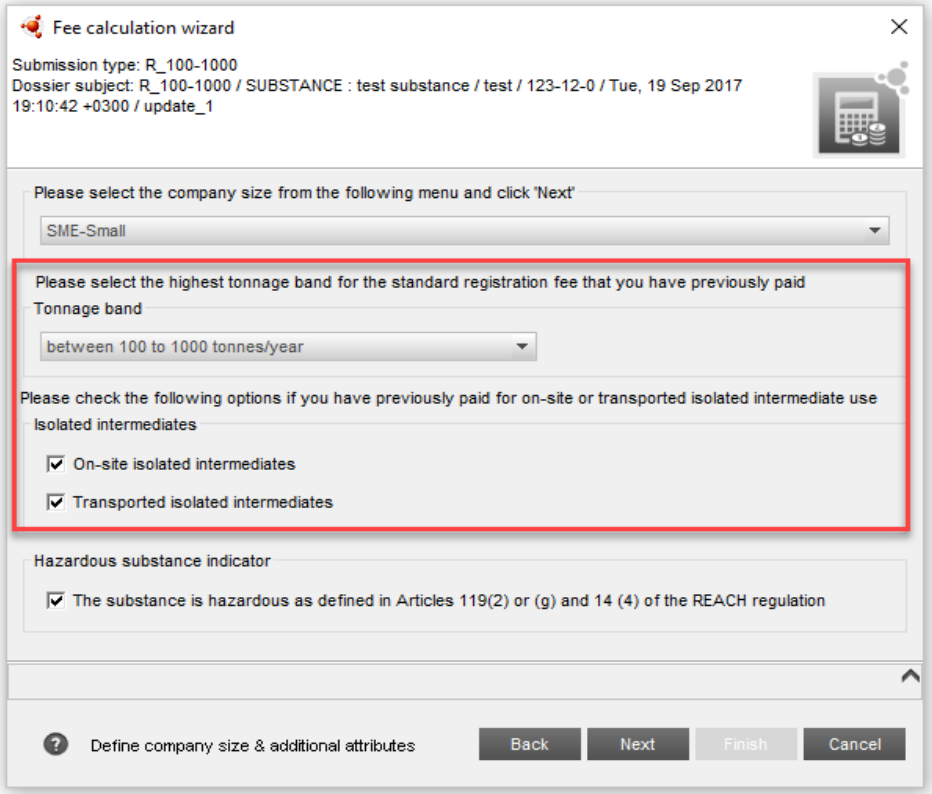
- Annex III criteria indicator



Fee calculator

Calculate the fee of dossier updates

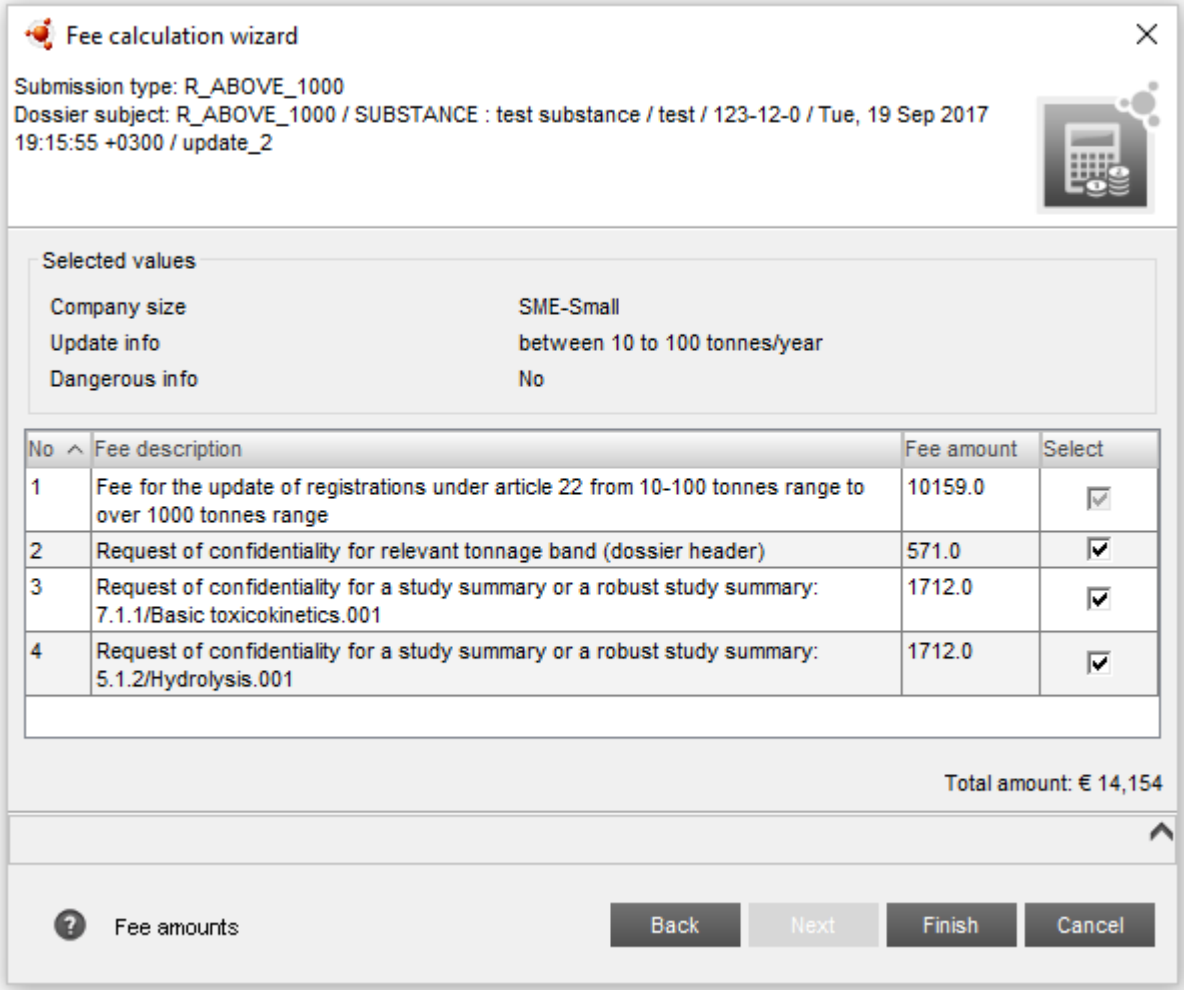
- If the dossier is an update, select the tonnage band of the previous paid submission
- Tick the appropriate box if the on-site or transported intermediate use has been previously paid



Fee calculator

Result window

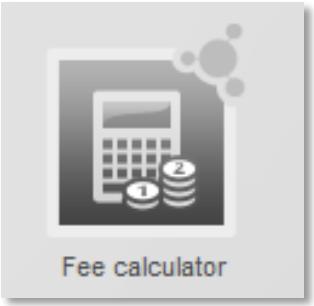
- Fees calculated according to the information contained in the dossier and the information you provided in the indicators
- Table with the description and exact amount charged for each fee applied
- Section of the dossier where the confidentiality has been claimed
- At the bottom of the table: total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



Fee calculator

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

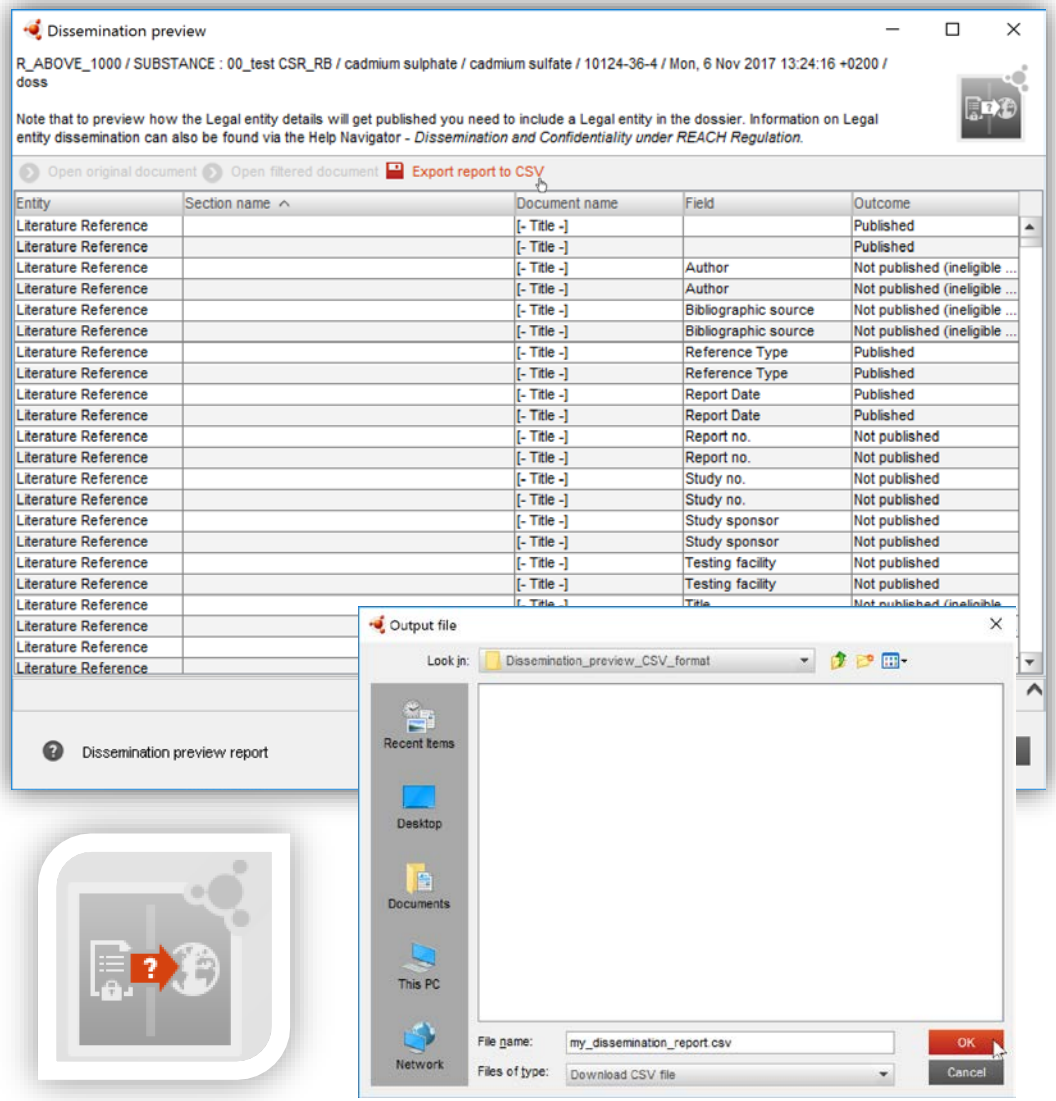


Dissemination preview

IUCLID 6 version 2.0.0

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



Comparison of dossiers

Comparison tool

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

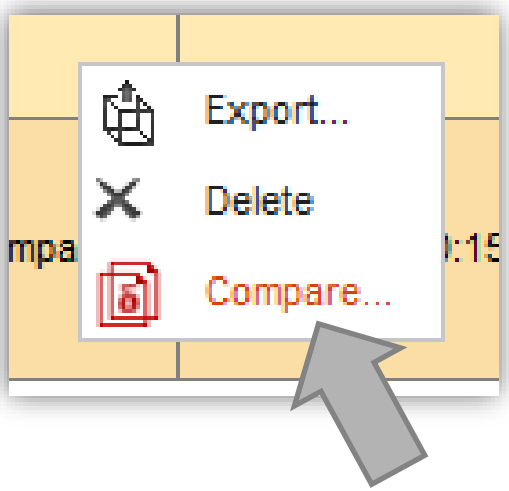
Comparison tool

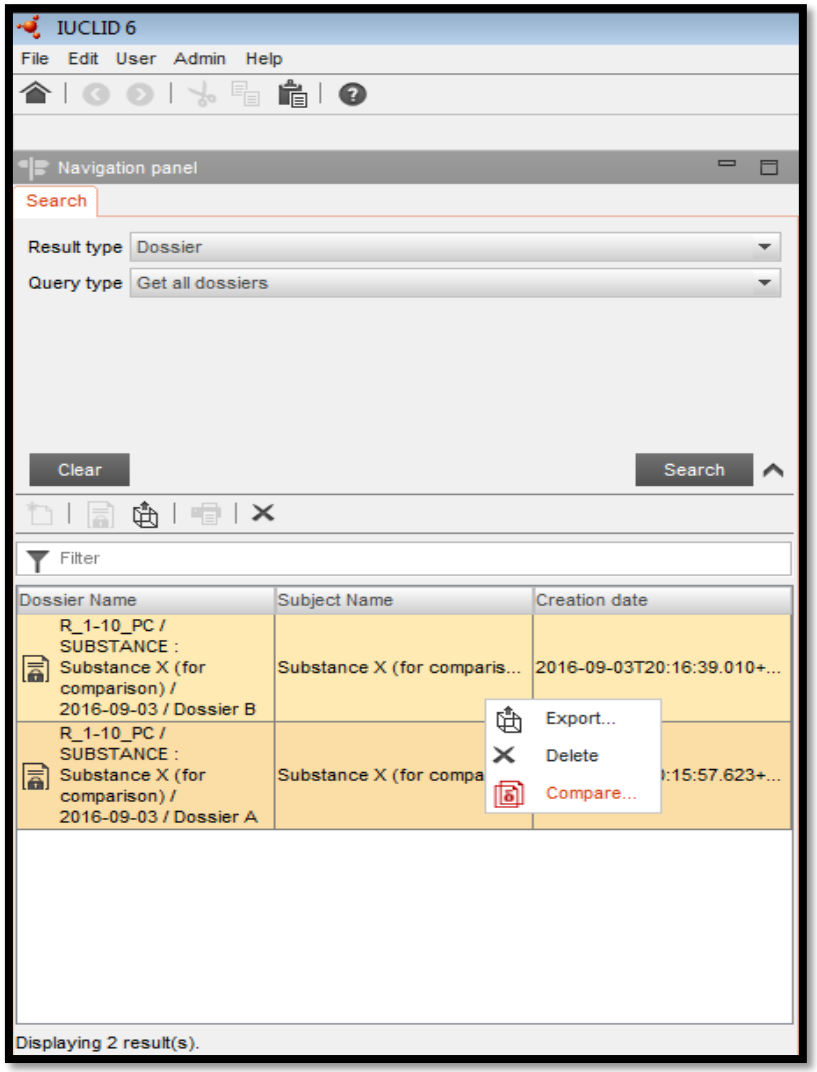
Overview – how it works

- 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

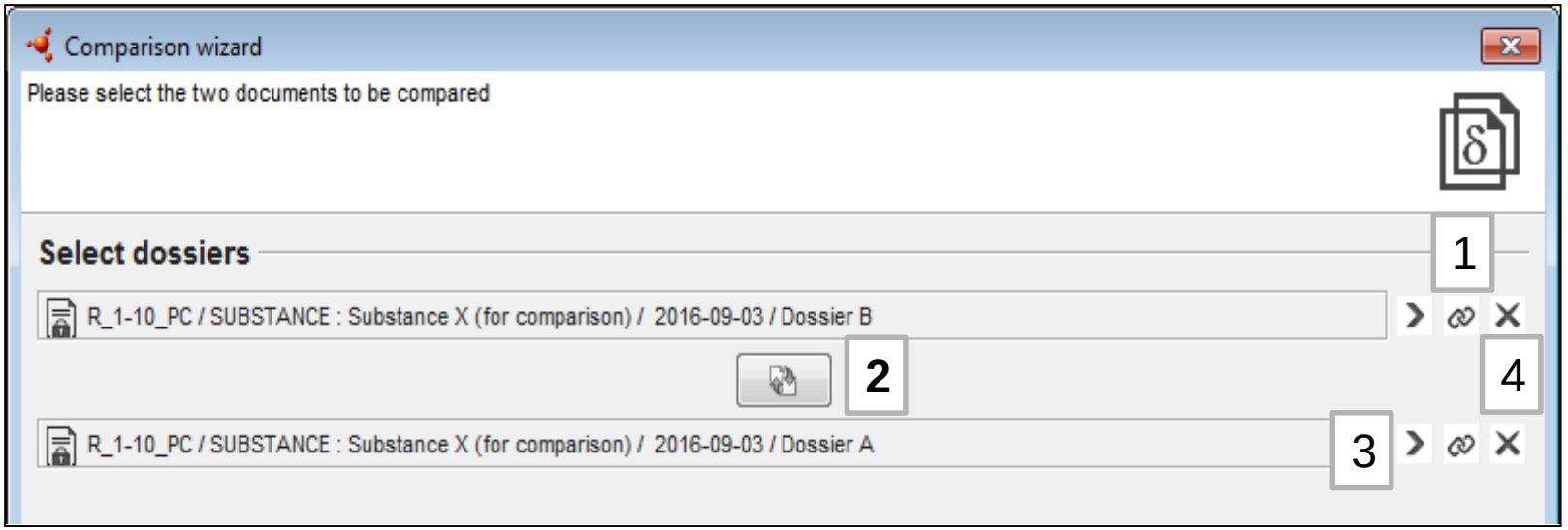




Comparison tool

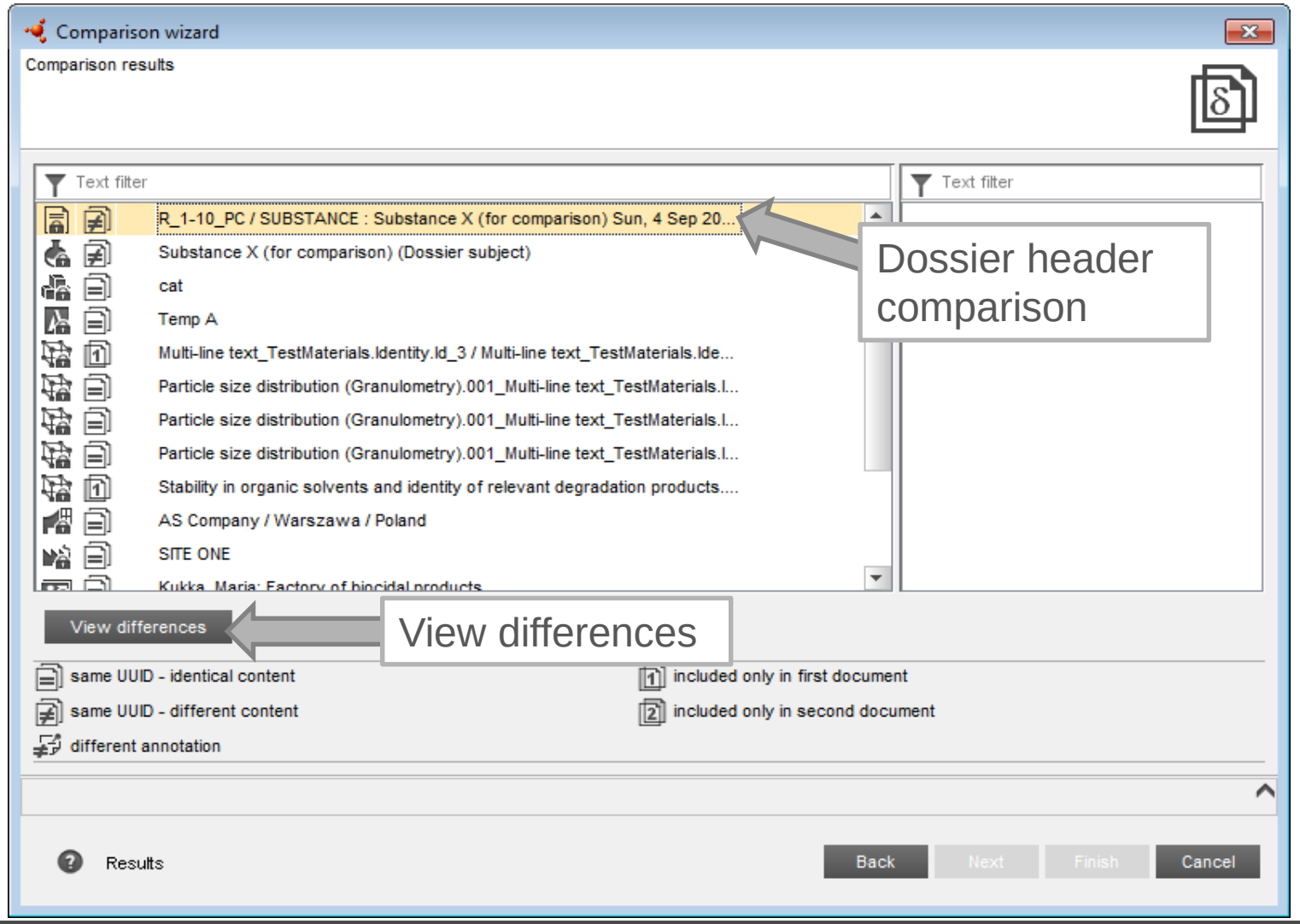
The first step of the Comparison wizard allows you to:

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



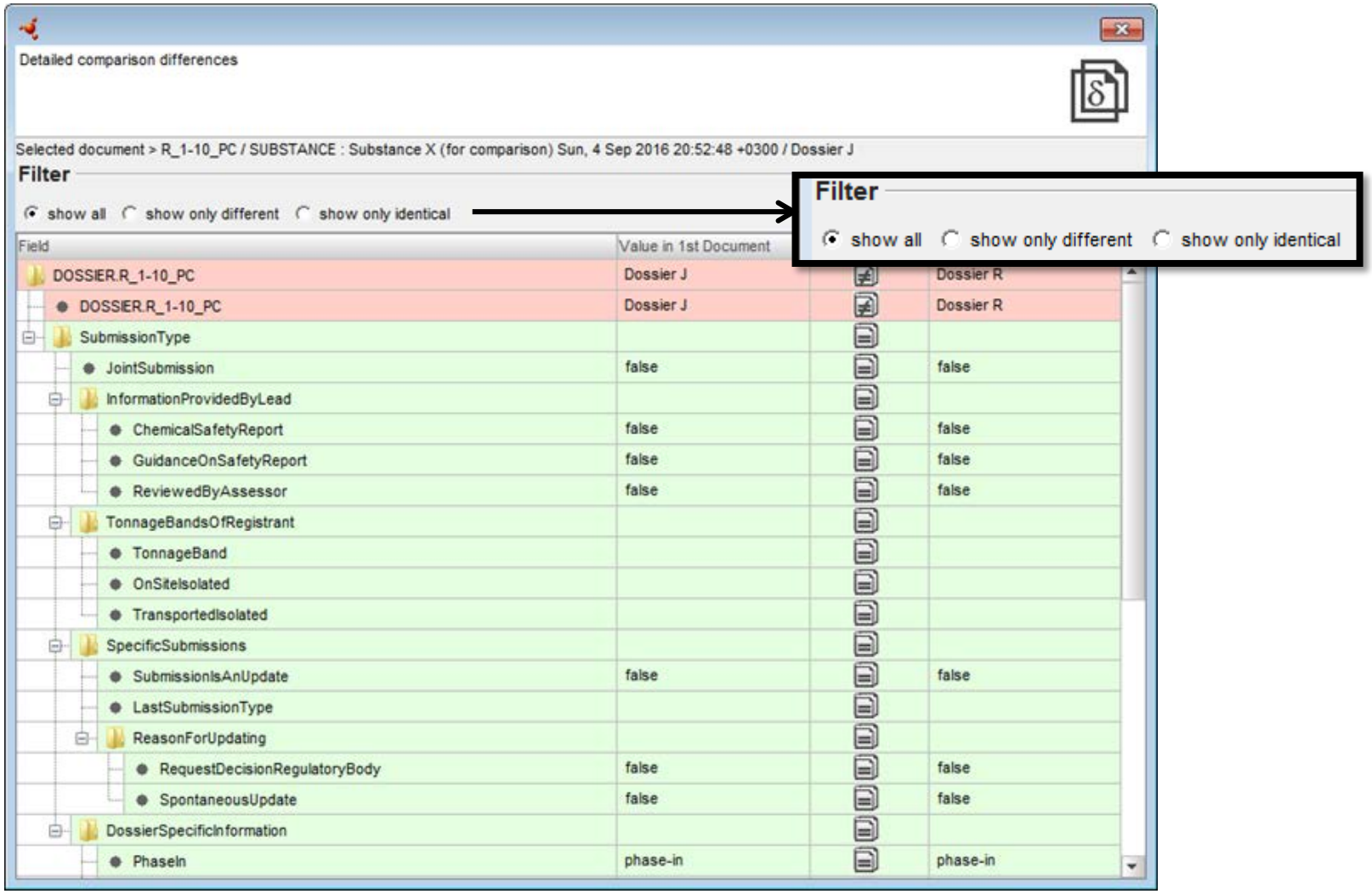
Comparison tool

Final Comparison step

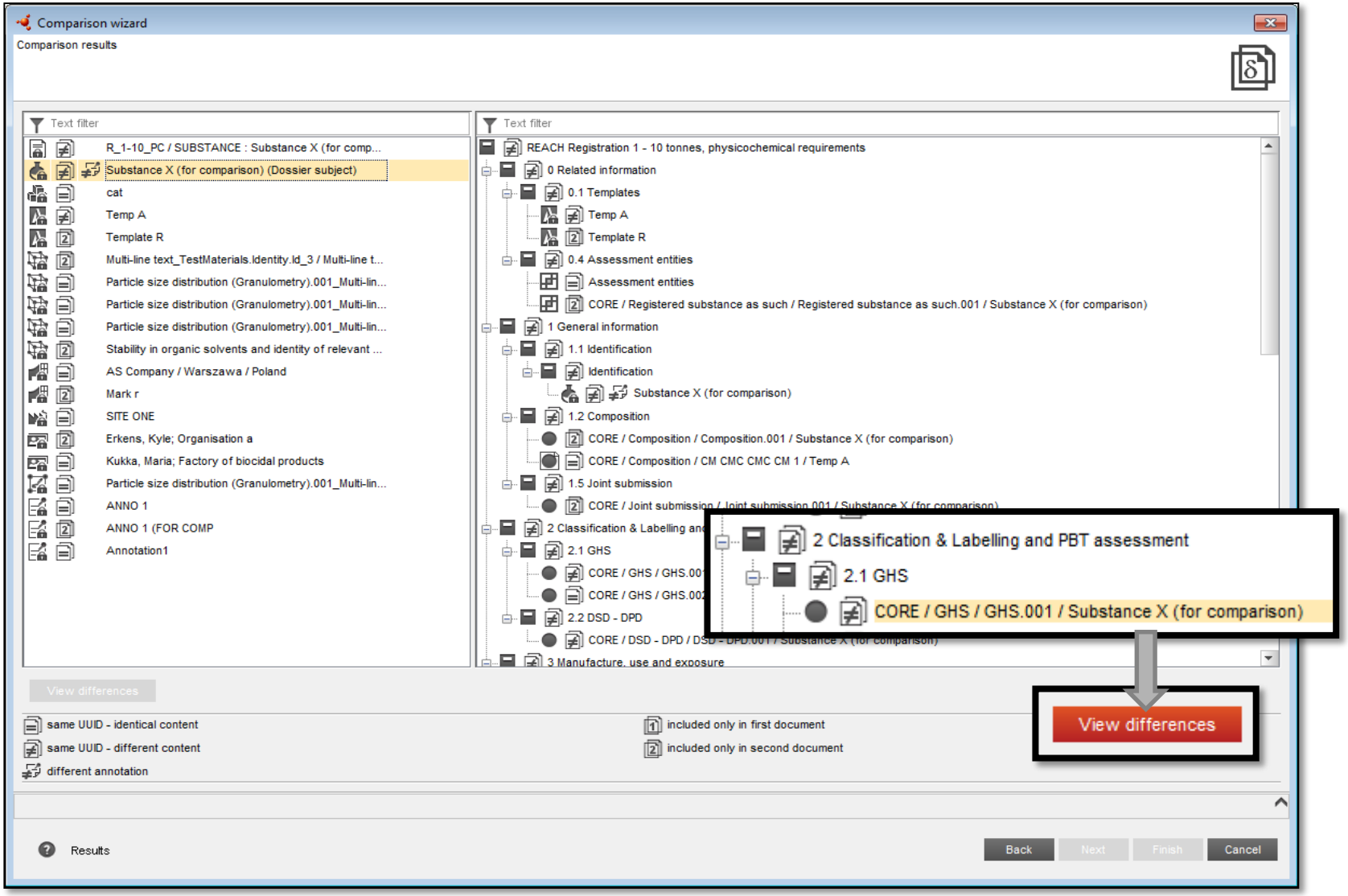


Comparison tool

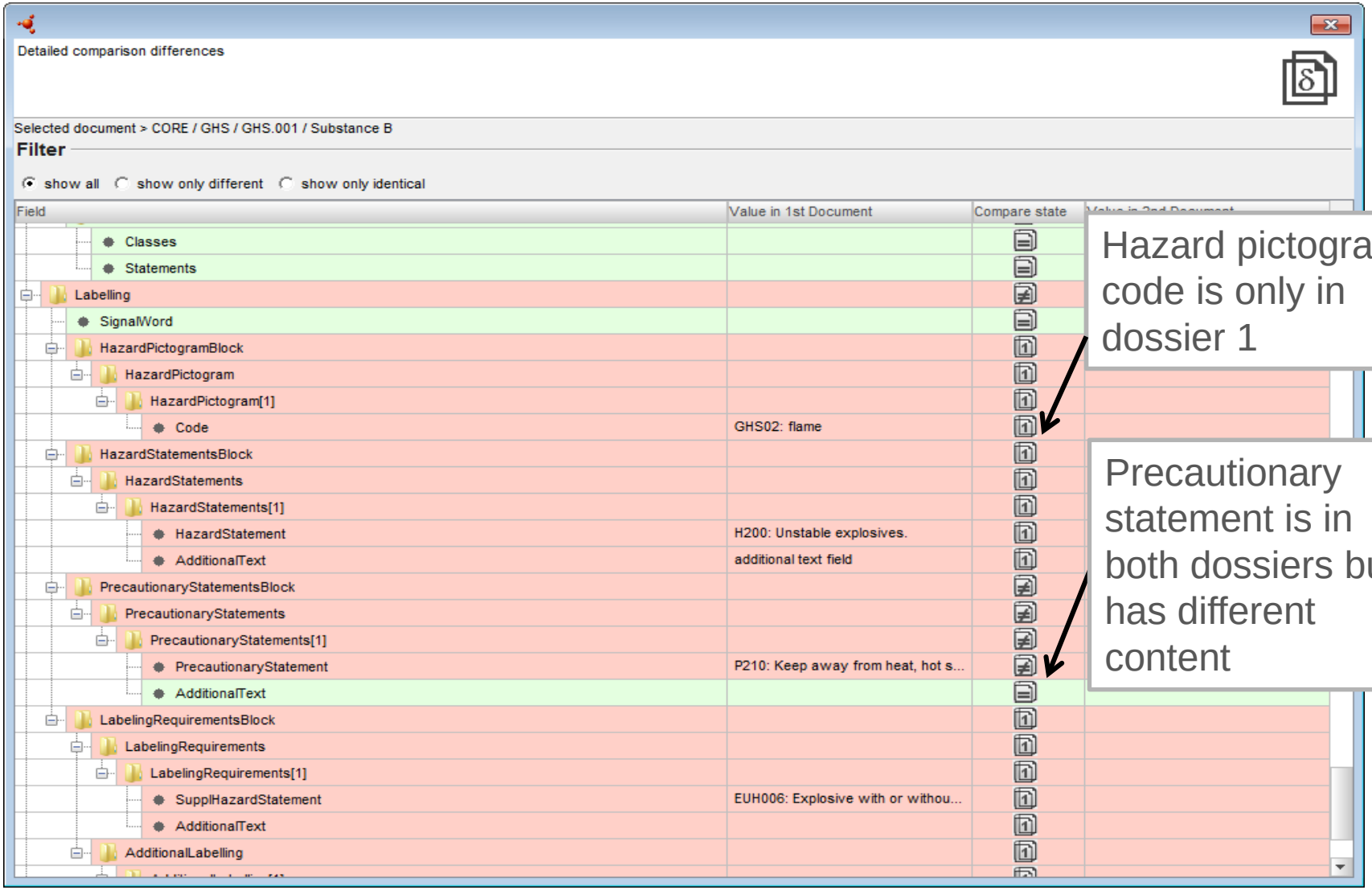
View Differences results table



Comparison tool



Comparison tool



Inventory management

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’

Inventory Management

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.

Inventory Management

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

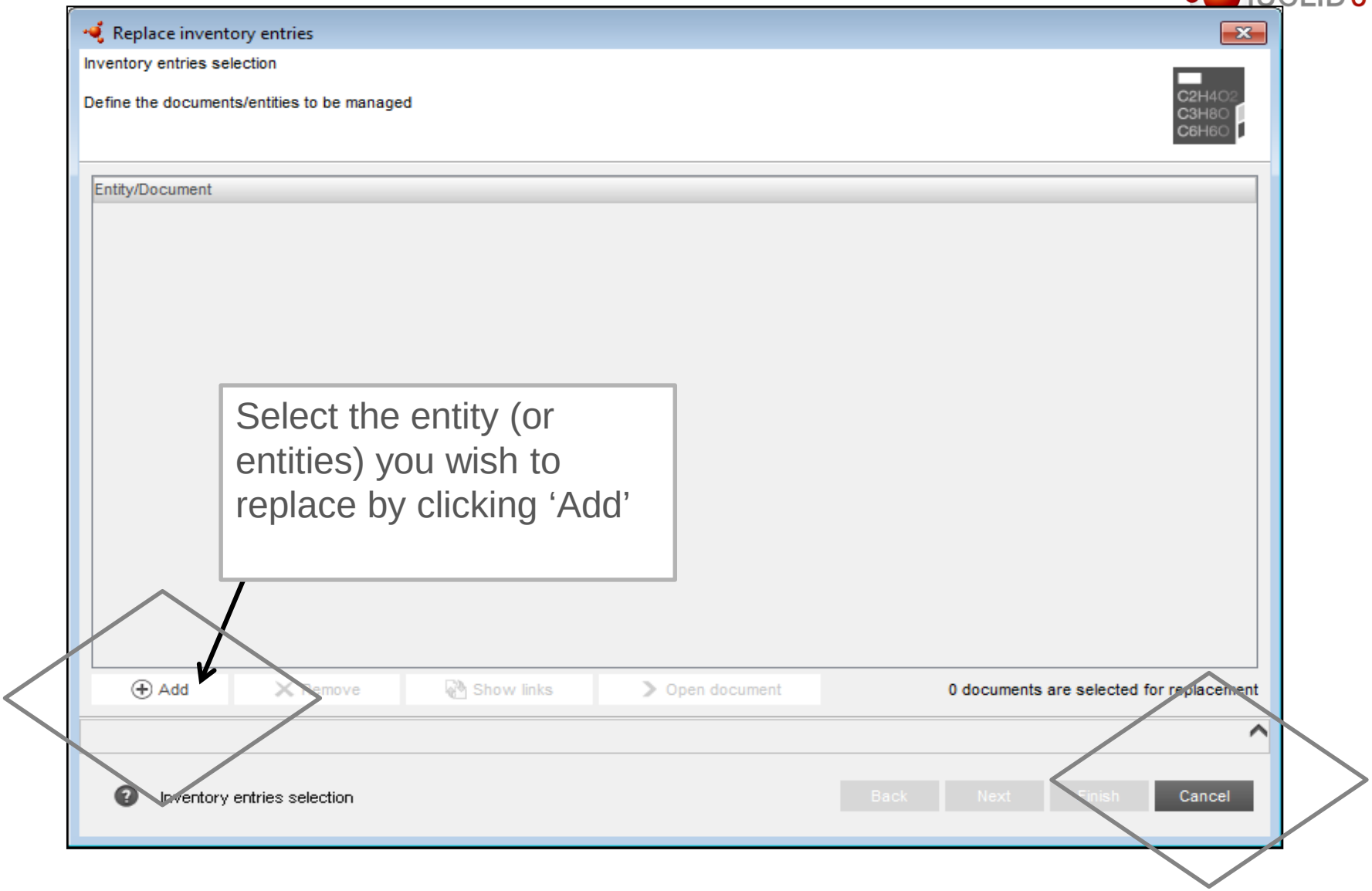
- Substance
  - Section 1.7
  - Section 1.8
- Template
- Mixture-Product
  - Section 1.3

Legal Entity 3

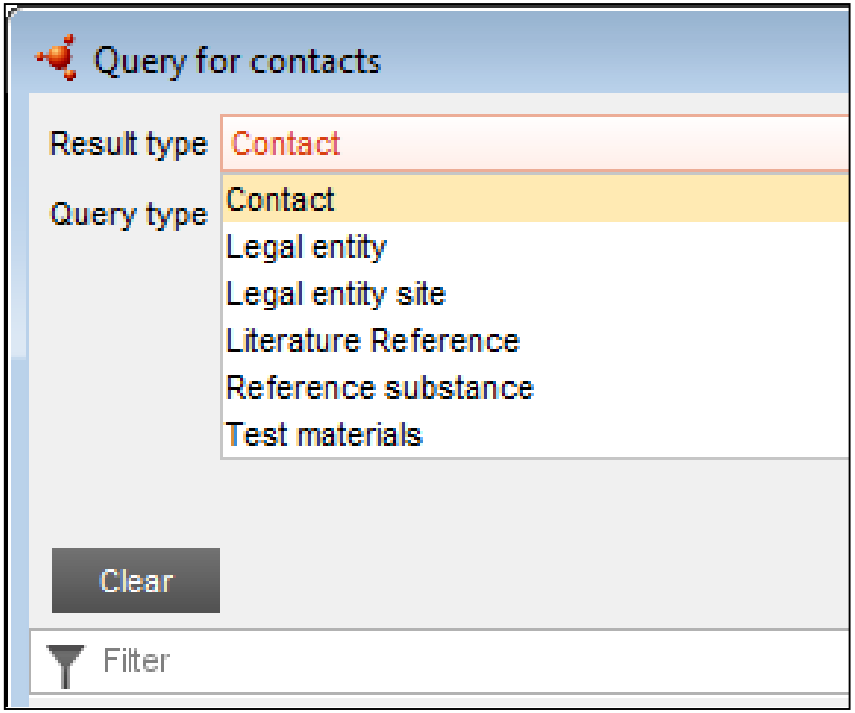
- Substance
  - Section 1.5
  - Section 1.7
  - Section 1.8
- Template
- Mixture-Product
  - Section 1.3
- Category
- Legal Entity Site

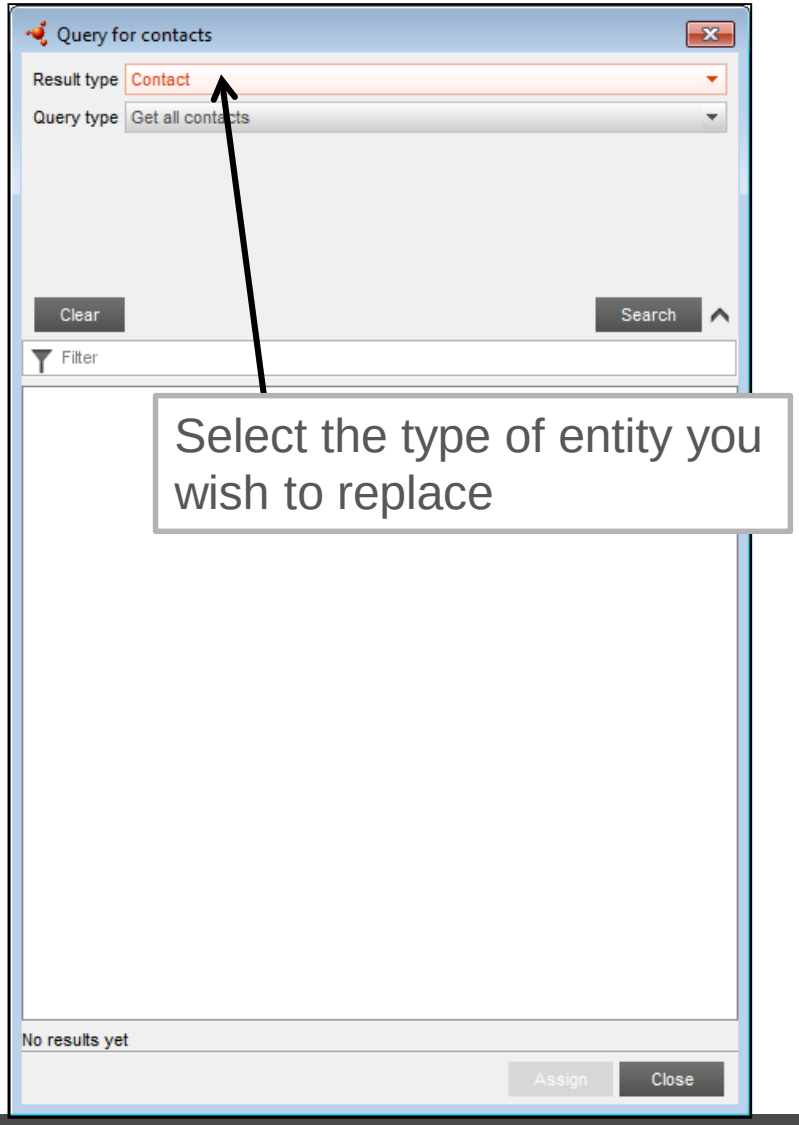
- Legal Entity 1 and 2, are also removed from the list of Legal Entities
- When replacing an entity in an Inherited Template, that entity will be replaced in All datasets where that template is used

Inventory Management



Inventory Management





Inventory Management

Refine your search using the ‘Query Type’

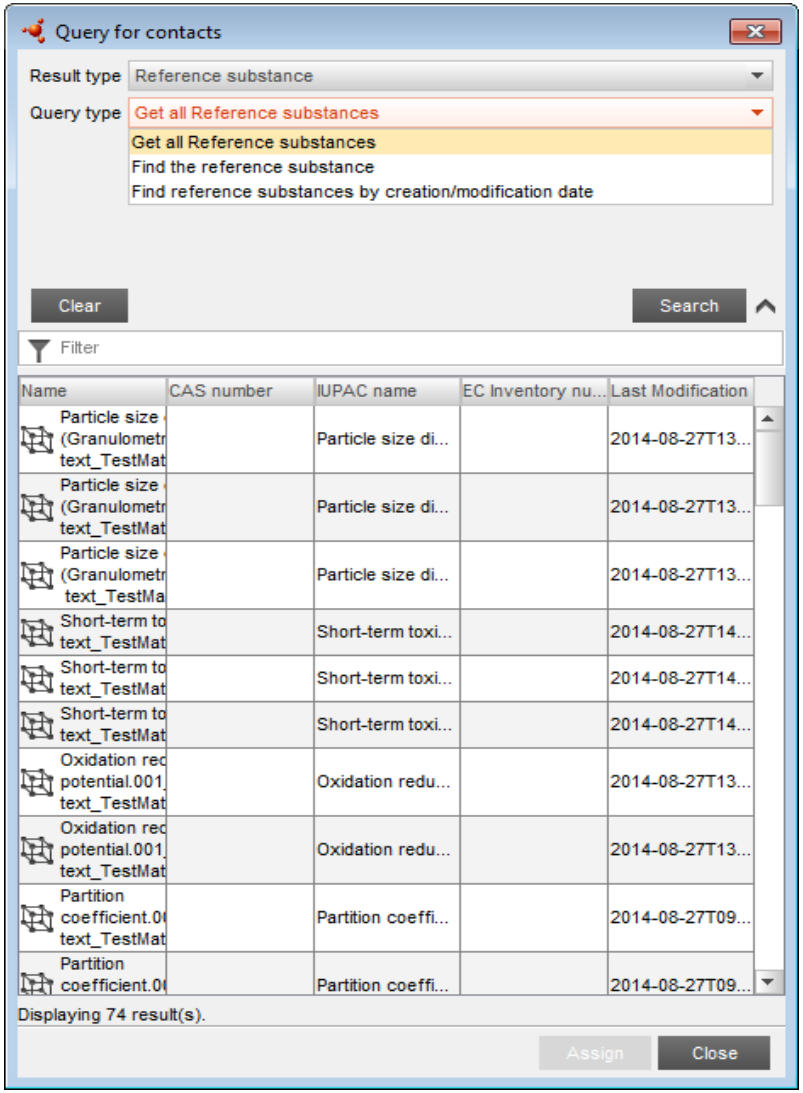
Get all

- Contacts, Legal Entities, Test Materials ….

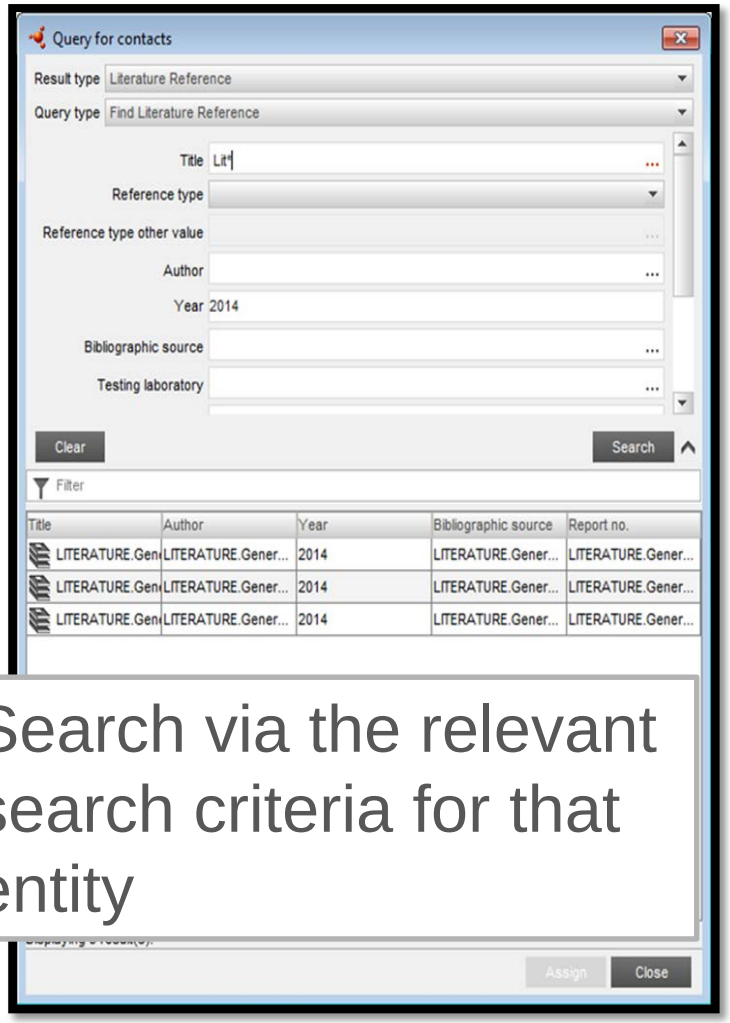
Find an entity

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

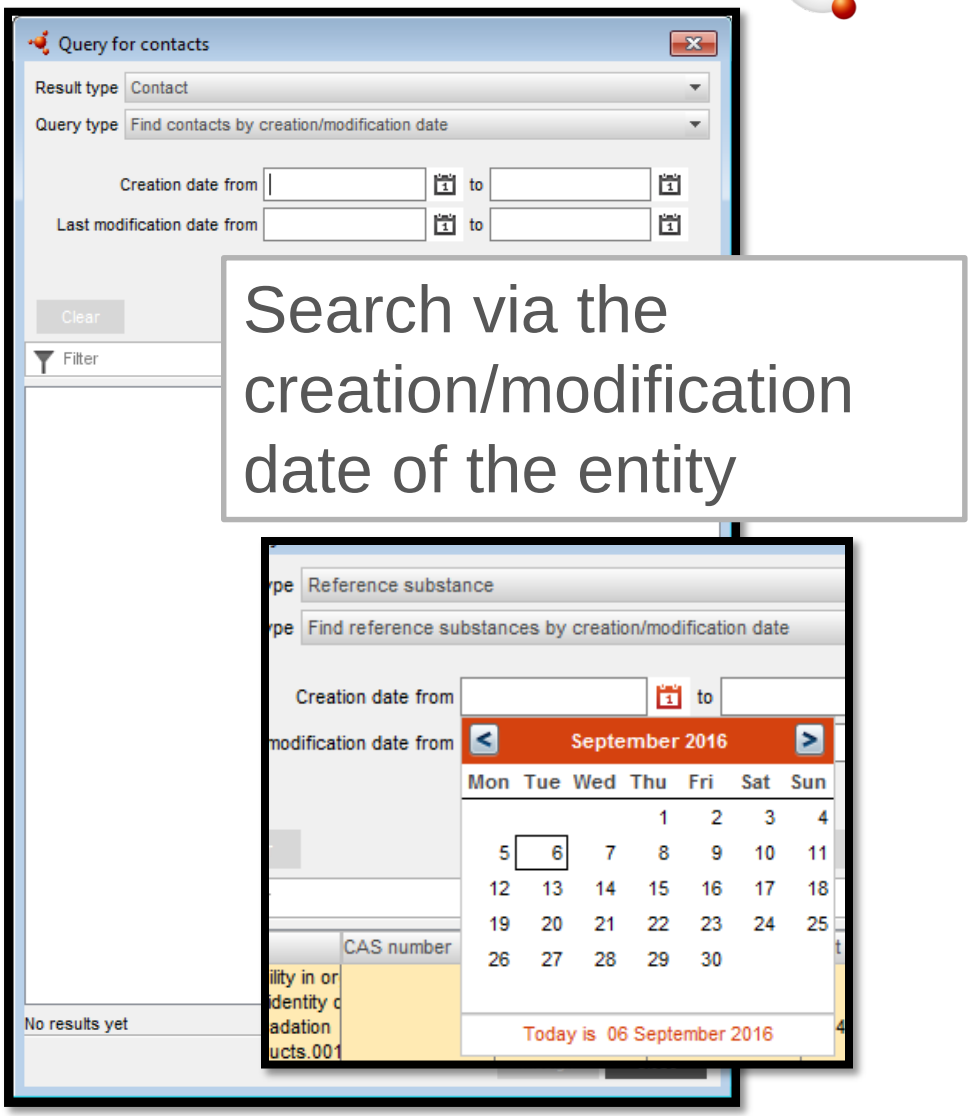
Search by creation/modification date



Inventory Management

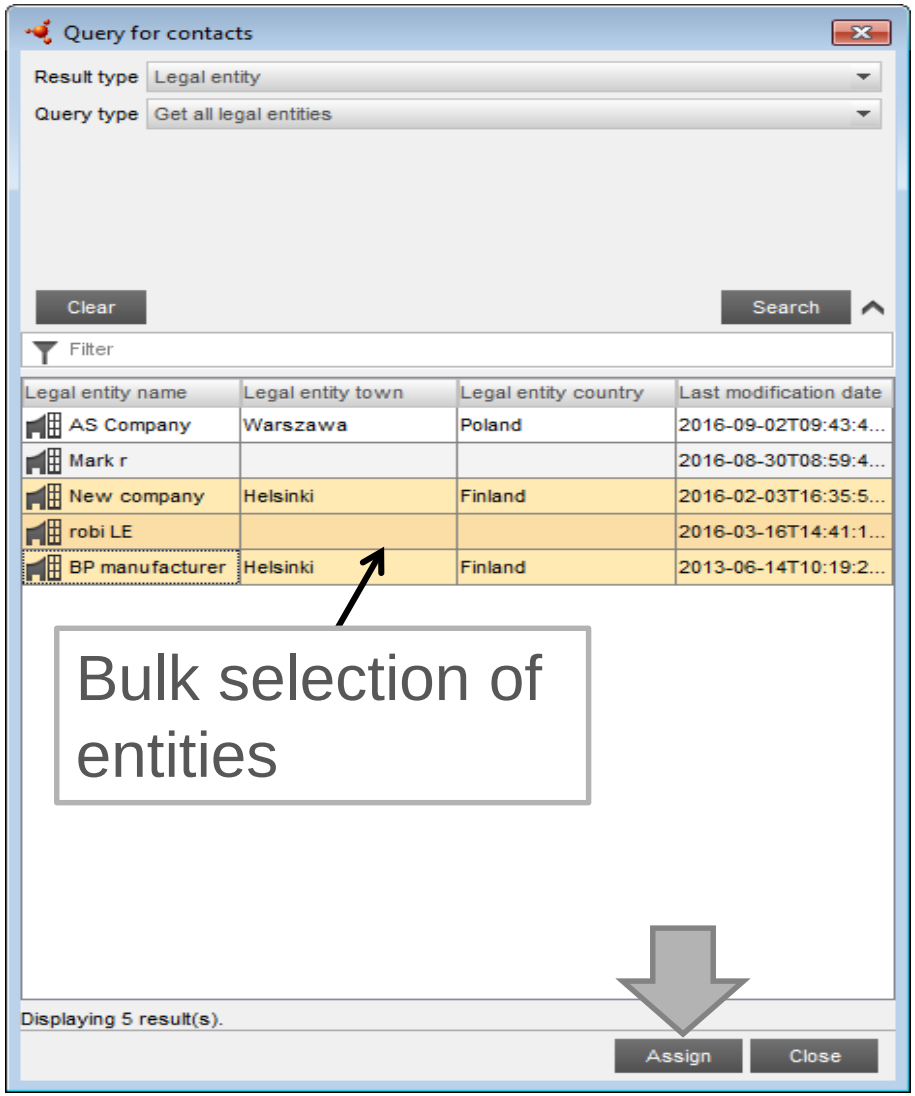


Search via the relevant search criteria for that entity

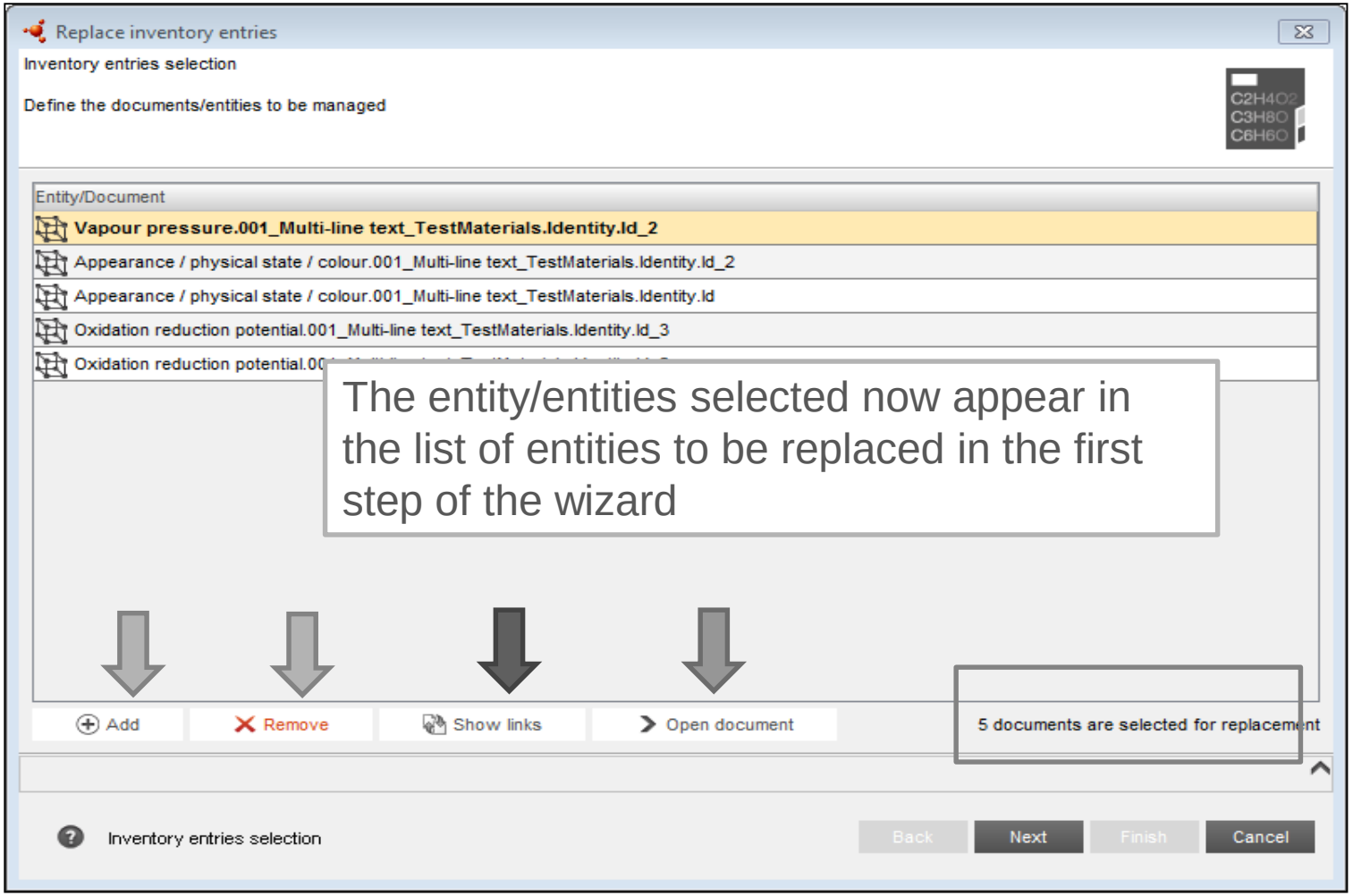


Search via the creation/modification date of the entity

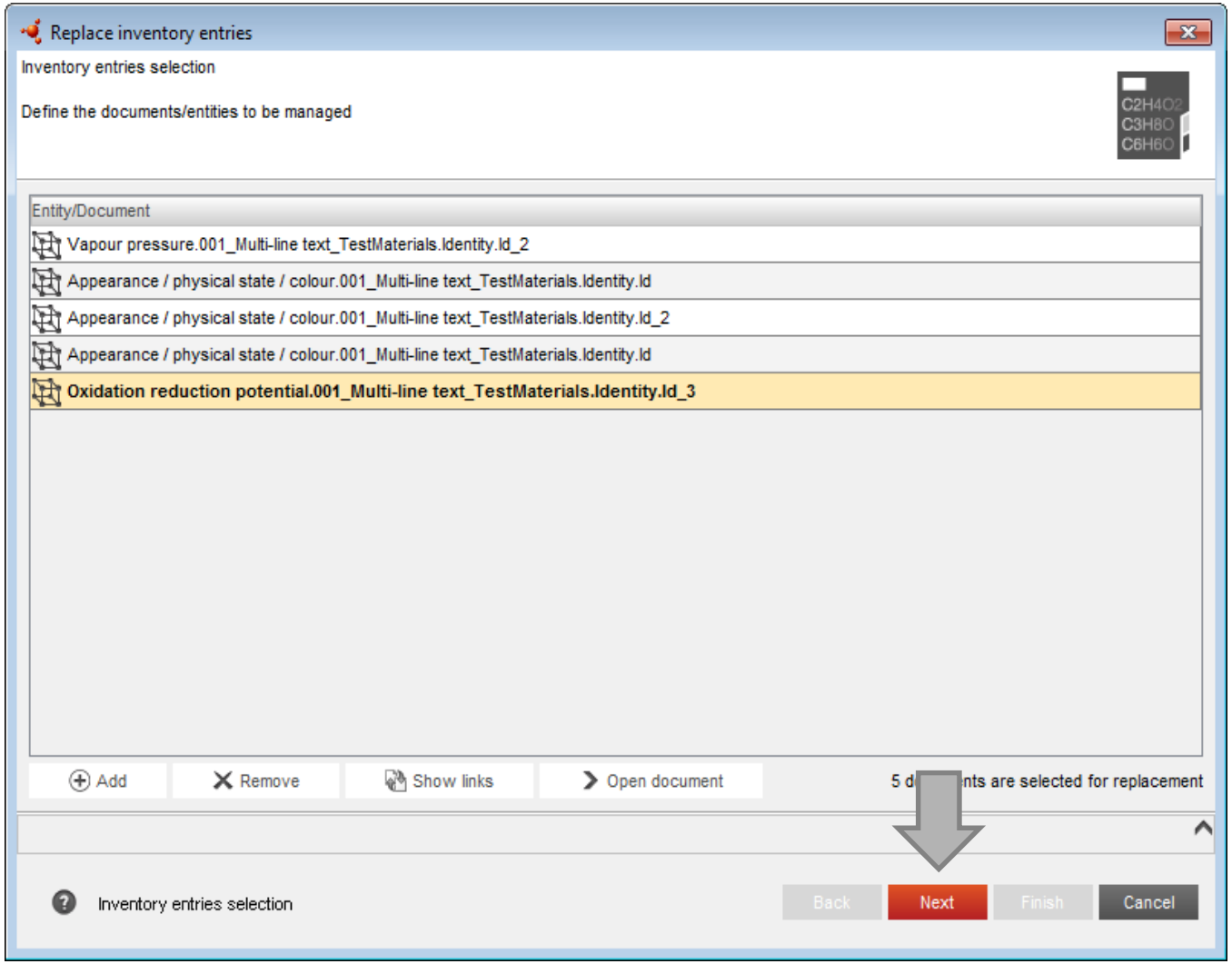
Inventory Management



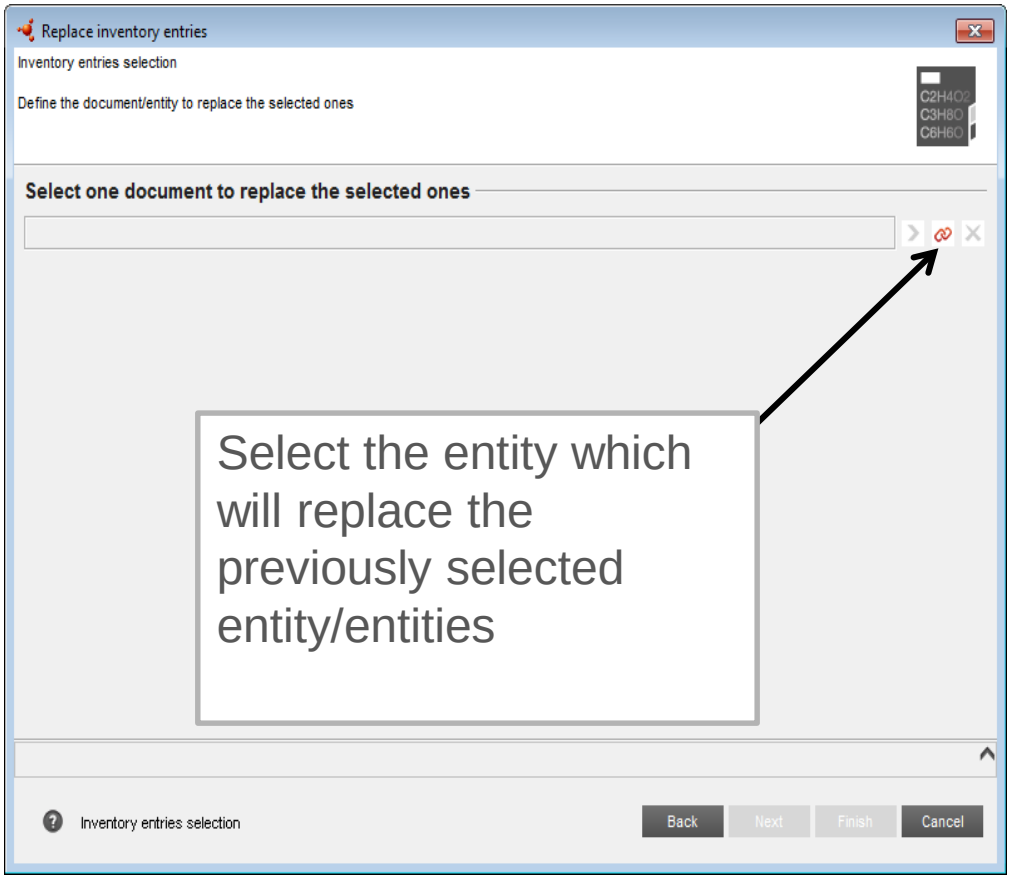
Inventory Management

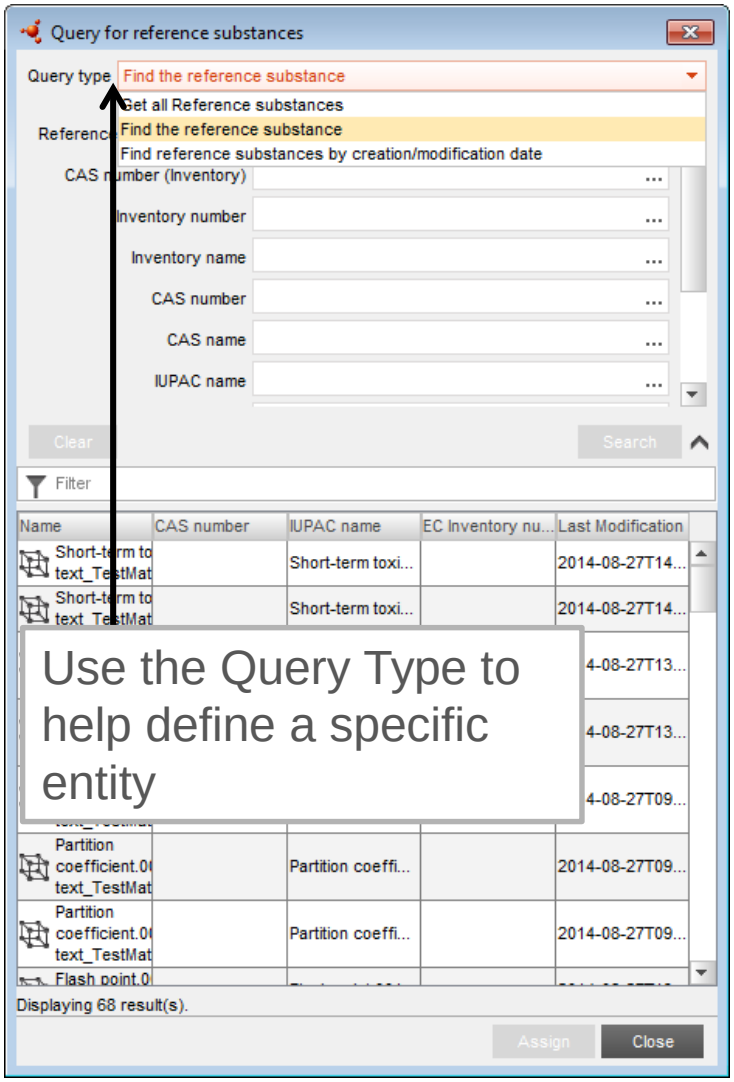


Inventory Management

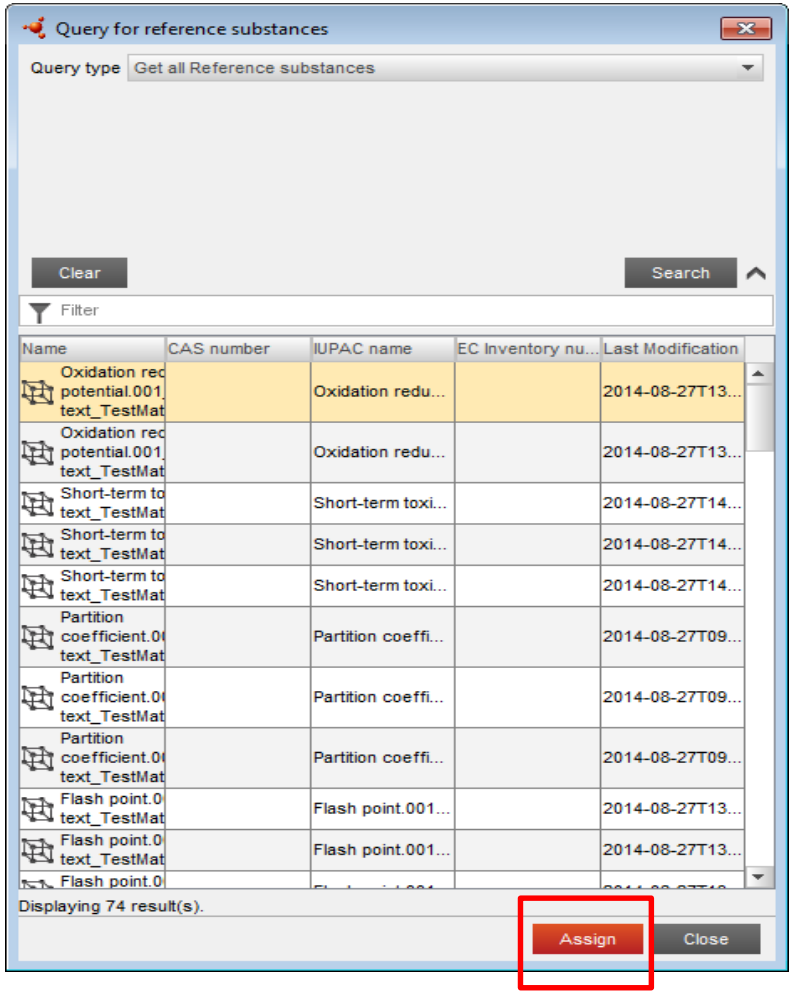


Inventory Management

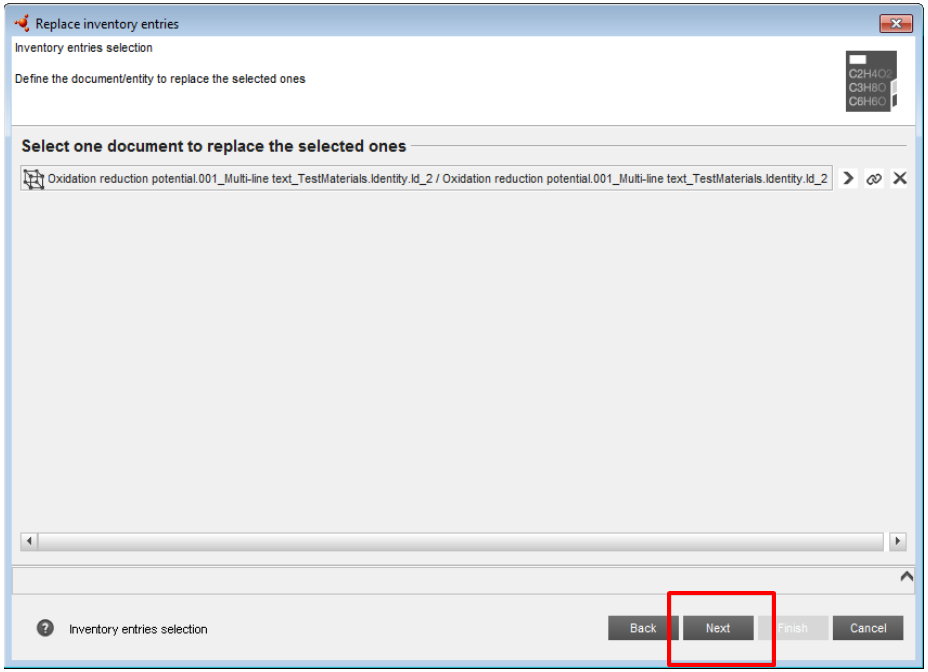




Inventory Management



Assign and move to the Next step



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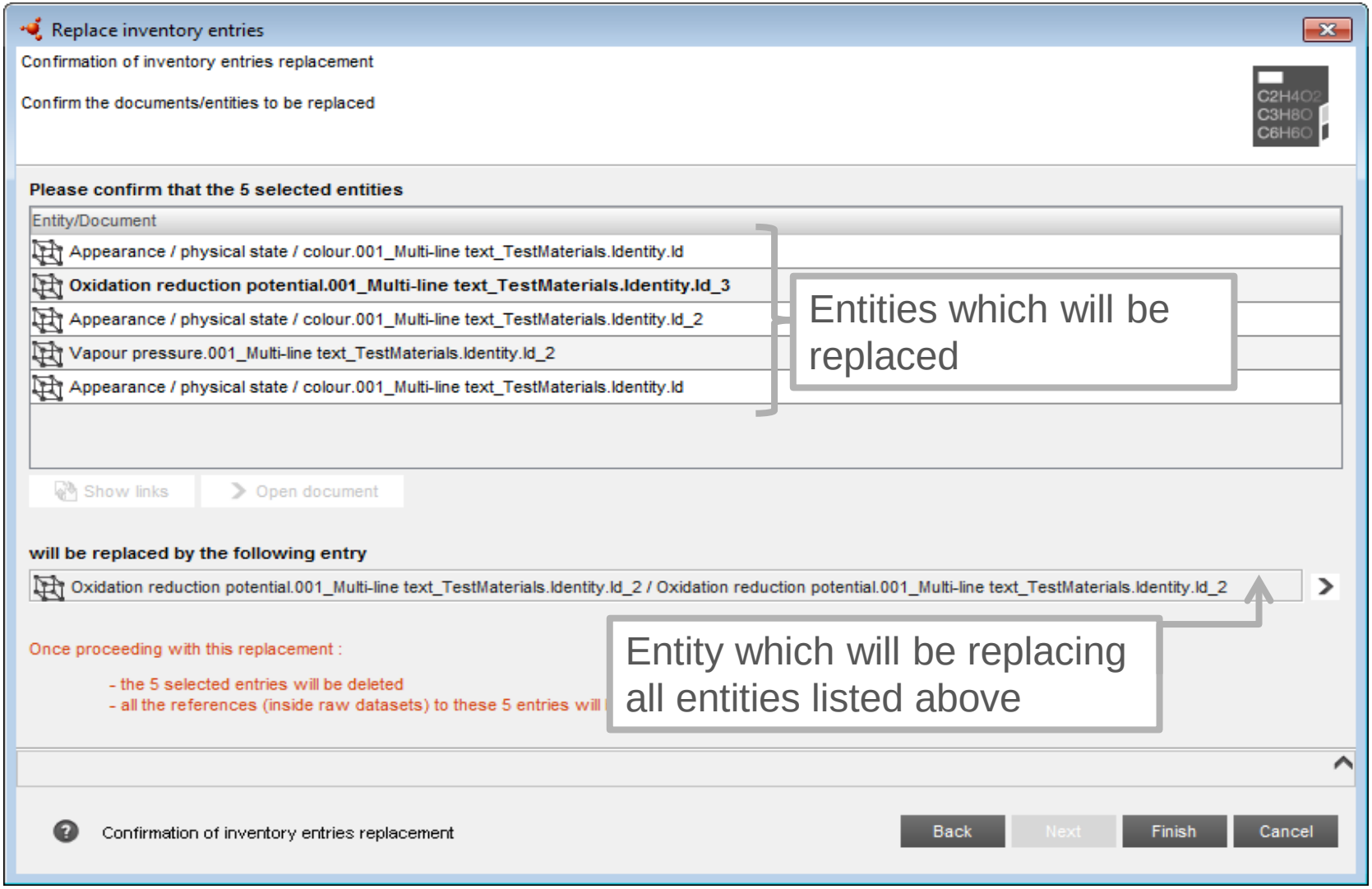
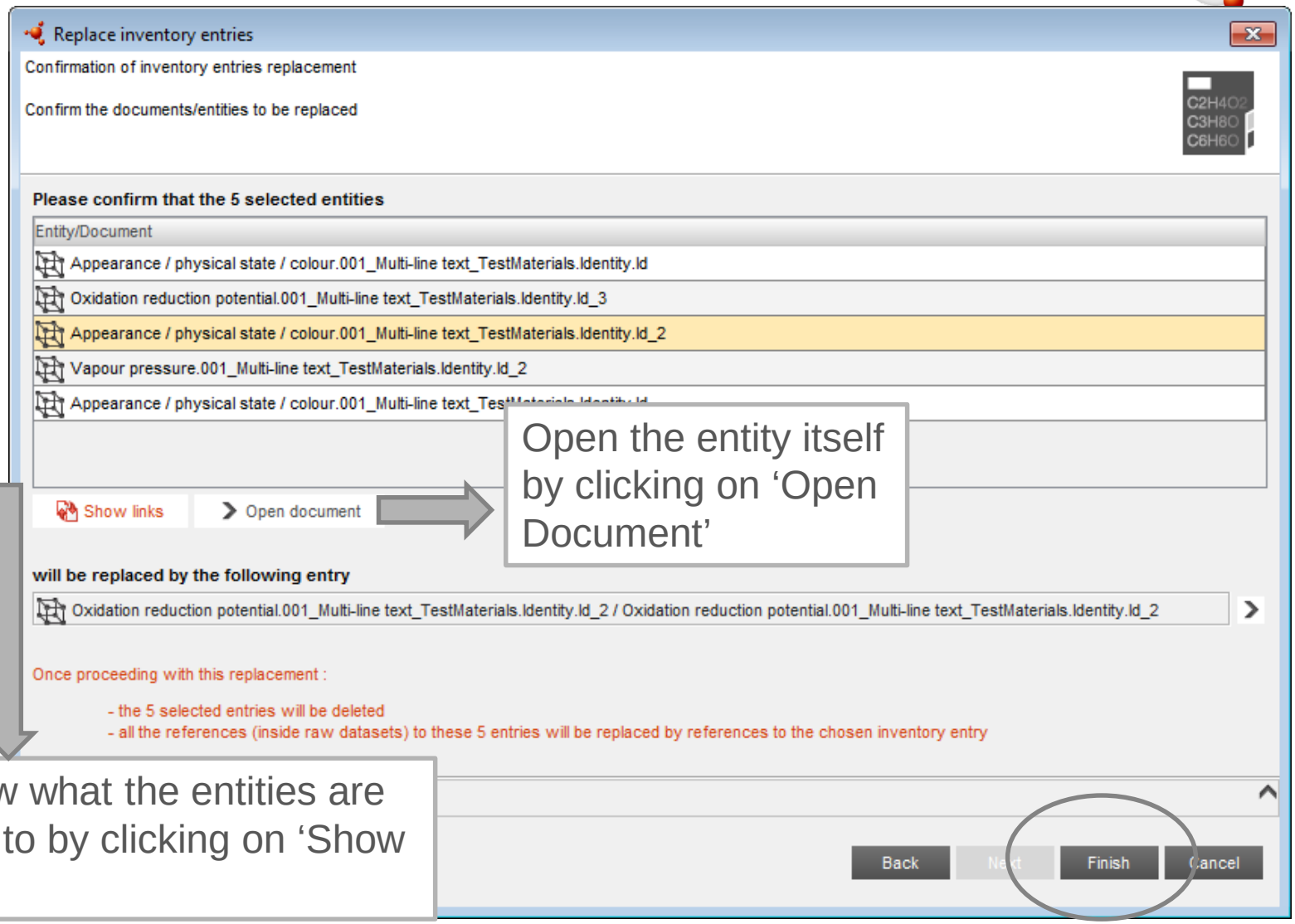


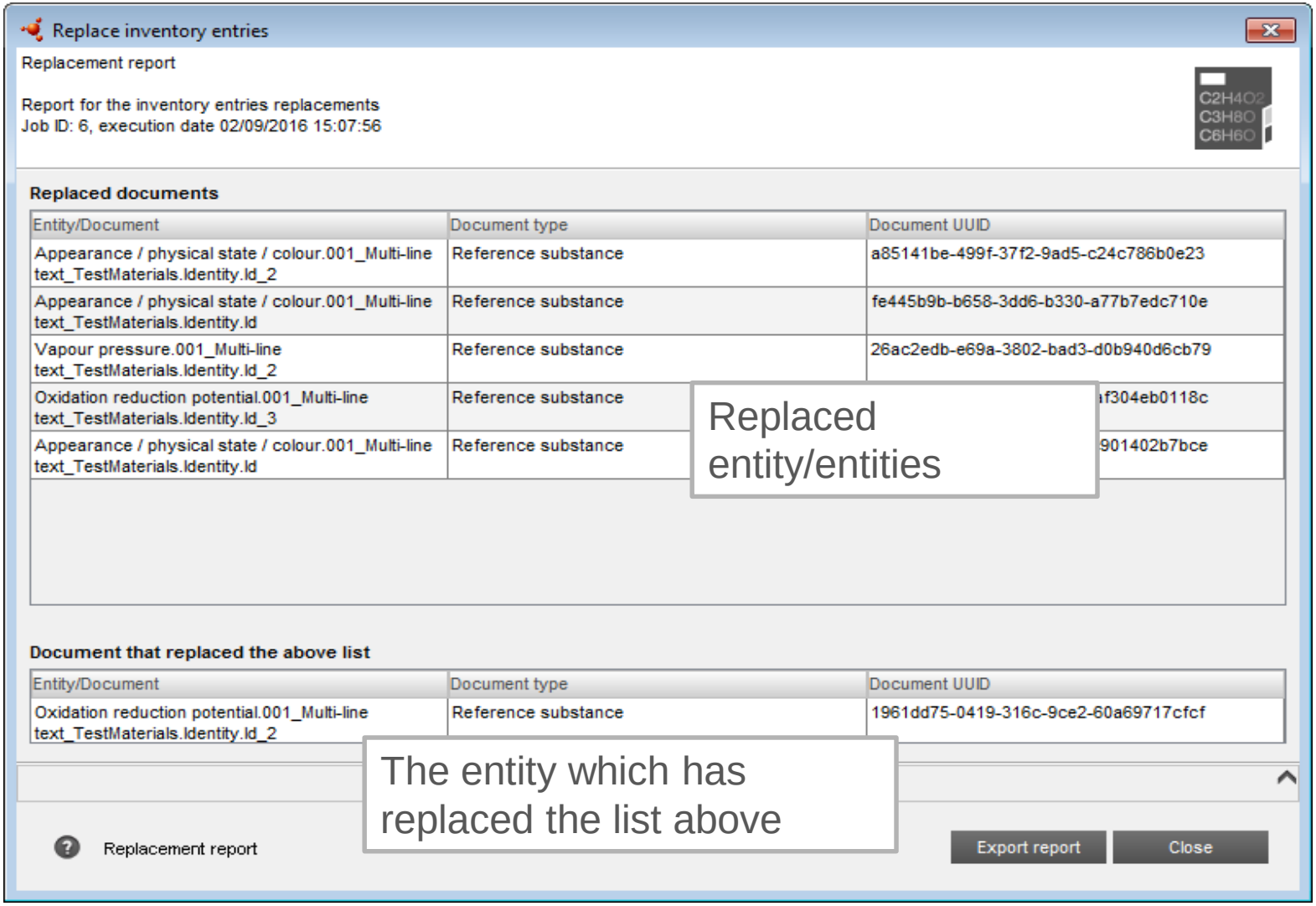
Inventory Management



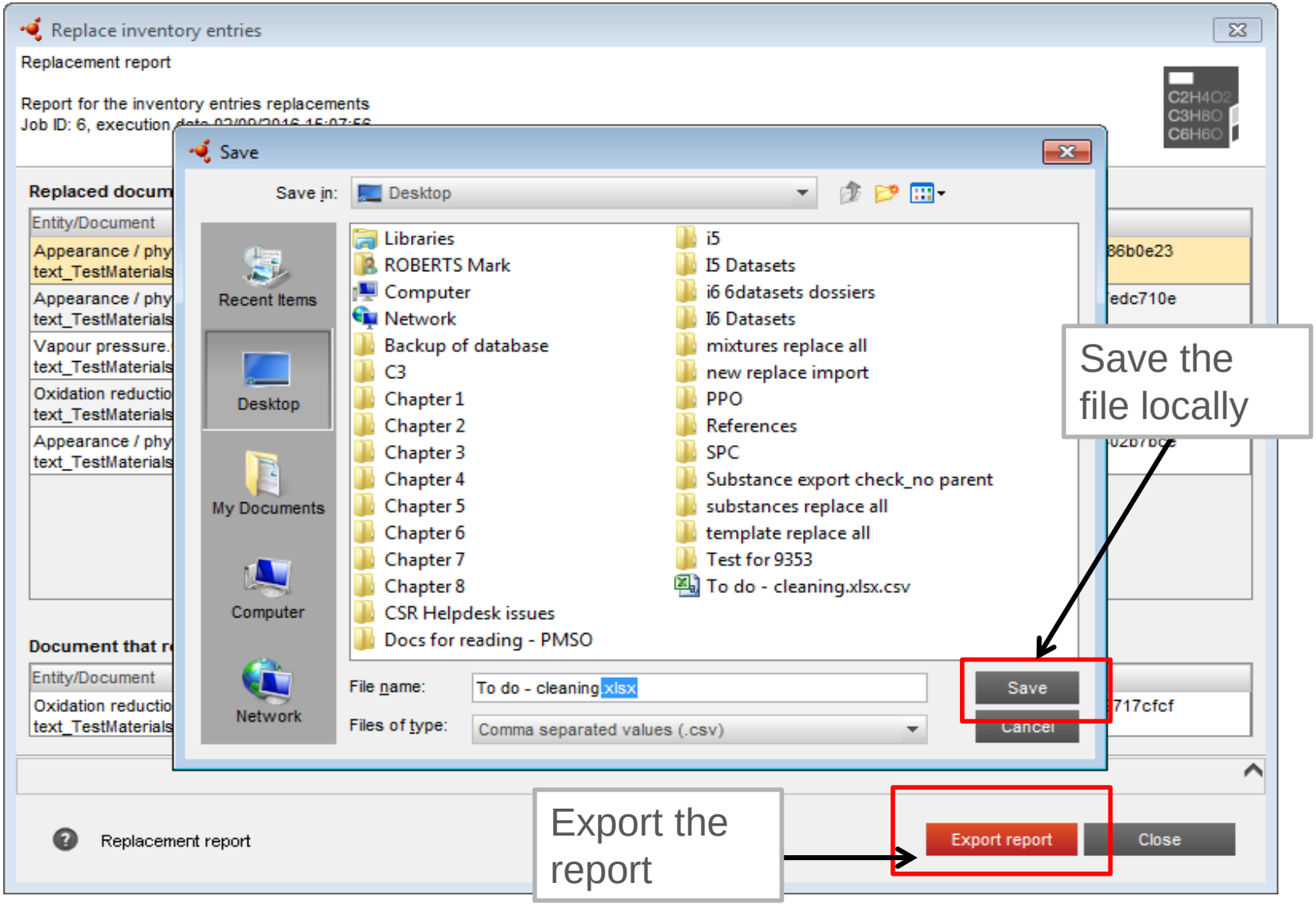
Open the entity itself by clicking on ‘Open Document’

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

Inventory Management



Inventory Management



Compatibility between IUCLID versions

IUCLID 6 2.0.0

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.

IUCLID 6 version 2.0.0

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

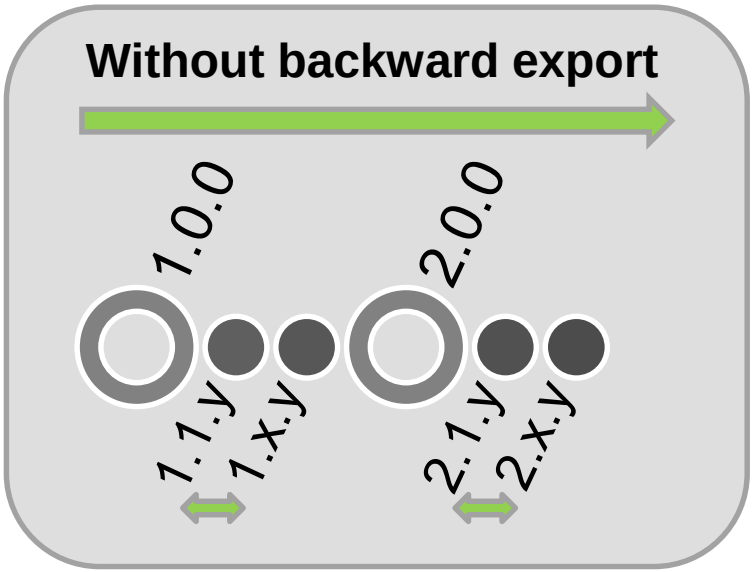
- At the same time improvements have been made, for example
  - Implemented new quality rules (QLT) for hazard endpoints (sections 7.3.1, 7.3.2, 7.4.1, 7.6.1, 7.8.1, 7.8.2)
  - Improved completeness check rule TCC_0102_20 which checks that UVCB substances contain a composition or a justification for deviations
  - A new validation scenario for the new submission type ‘Exchange of experimental data’ (outside the REACH or CLP regulatory context)

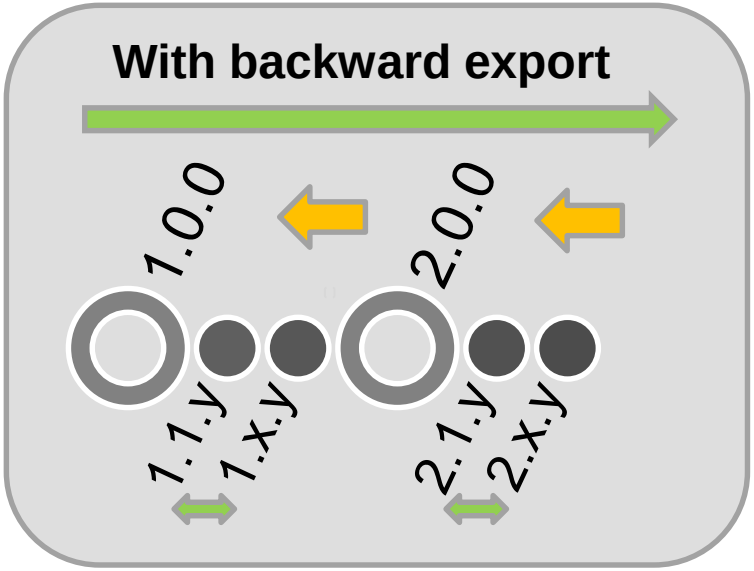
- Full details are available in the release notes

IUCLID 6 version 2.0.0

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

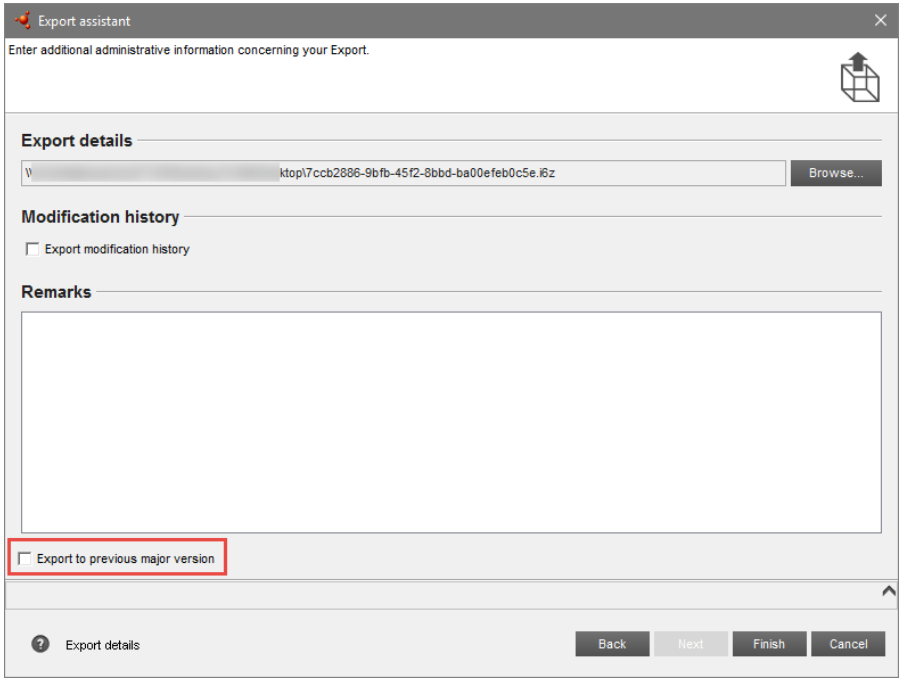




IUCLID 6 version 2.0.0

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



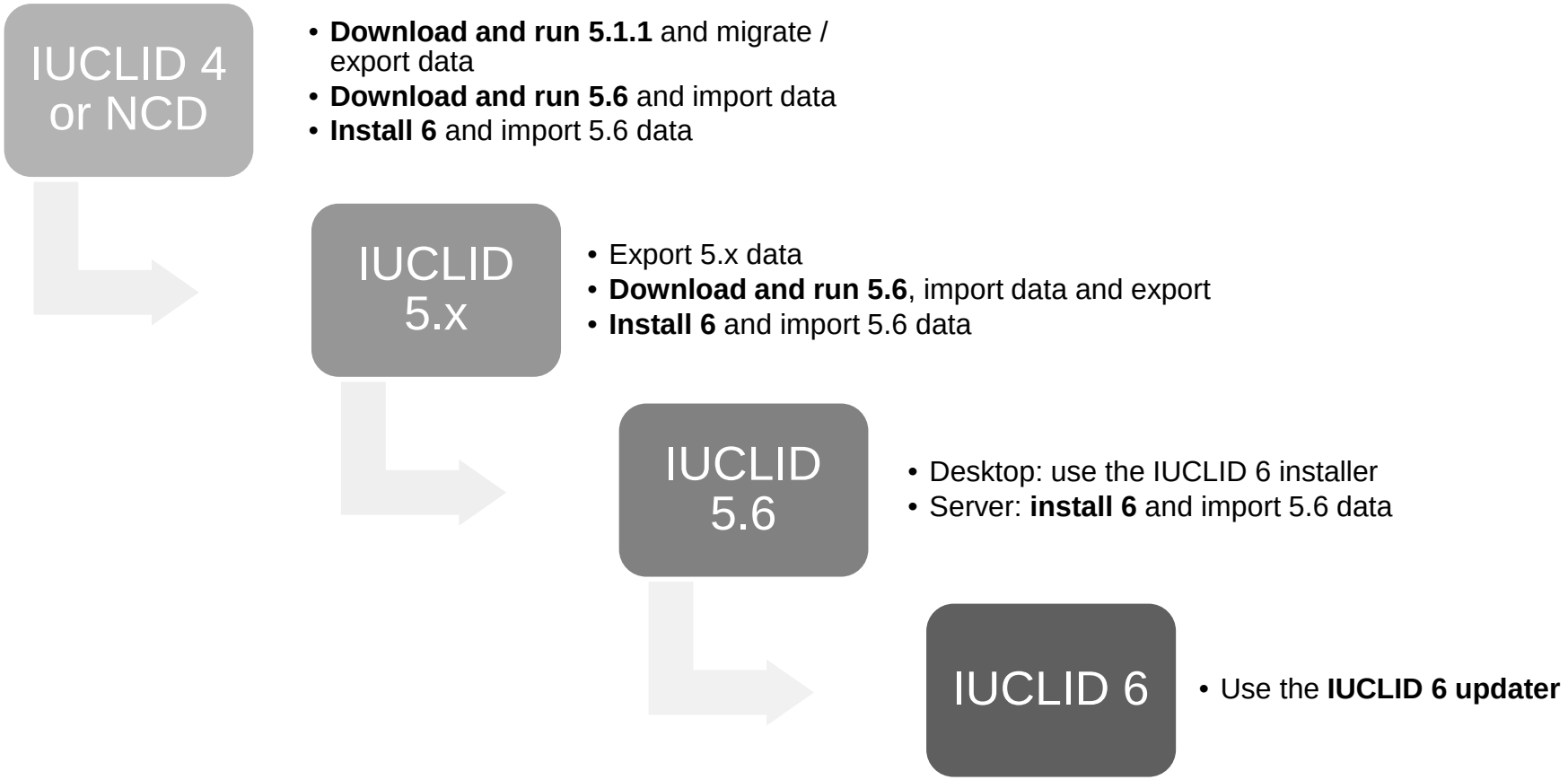
IUCLID 6 version 2.0.0

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)

Update

Different processes depending on your starting point

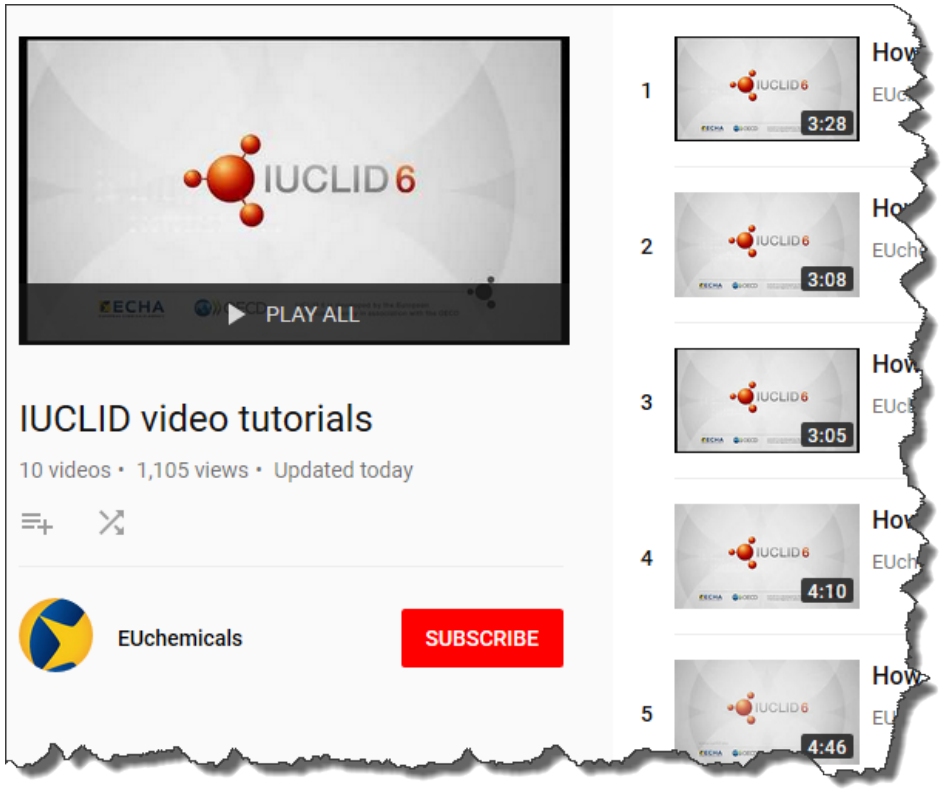


More information

IUCLID 6

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



https://www.youtube.com/playlist?list=PLOPGDACSd6qyDkdXwPua1Fjb5bJksY75k

IUCLID 6

News and next events

- **LinkedIn** group

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

- Platform to exchange, discuss and provide feedback on the use of IUCLID and on future evolutions of the product

- Join now to be involved in the development of our database

Thank you for your participation

echa.eu | iuclid6.echa.europa.eu | oecd.org/ehs/templates

ECHA EUROPEAN CHEMICALS AGENCY

OECD

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