7th meeting of the PSN IUCLID sub-group

19-20 June 2023

PSN IUCLID VERSION 6.7

Jane Richardson (MESE unit)

EUROPEAN FOOD SAFETY AUTHORITY

NEW EFSA WORKING CONTEXT

"***EFSA Chemicals Database***" available in IUCLID 6.7 (May 2022 release)

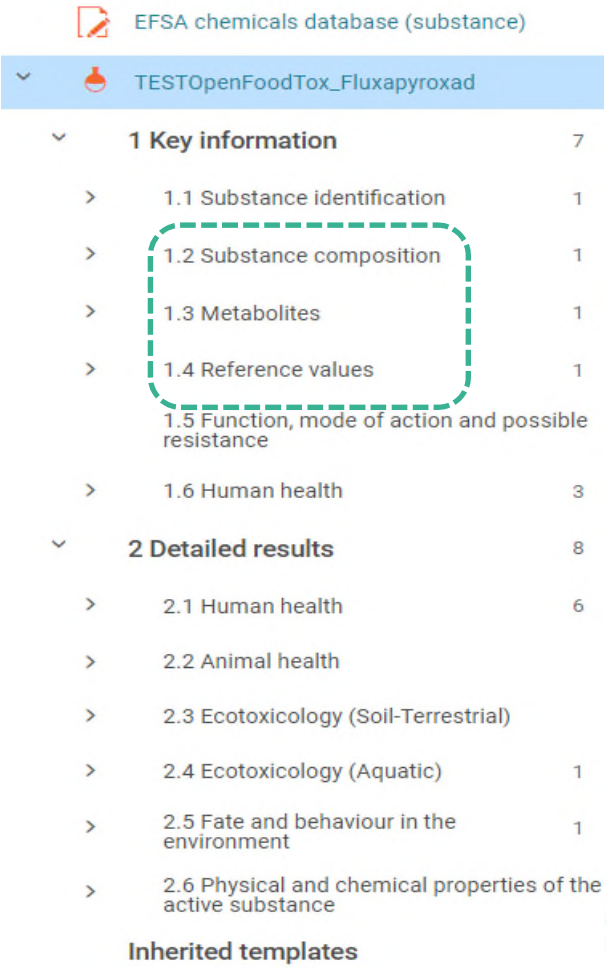
Substance and **Mixture datasets** available in *EFSA Chemicals database* Working Context

Key information (*Flexible/Endpoint Summaries*) and **Detailed results** (*EndpointStudyRecords*)

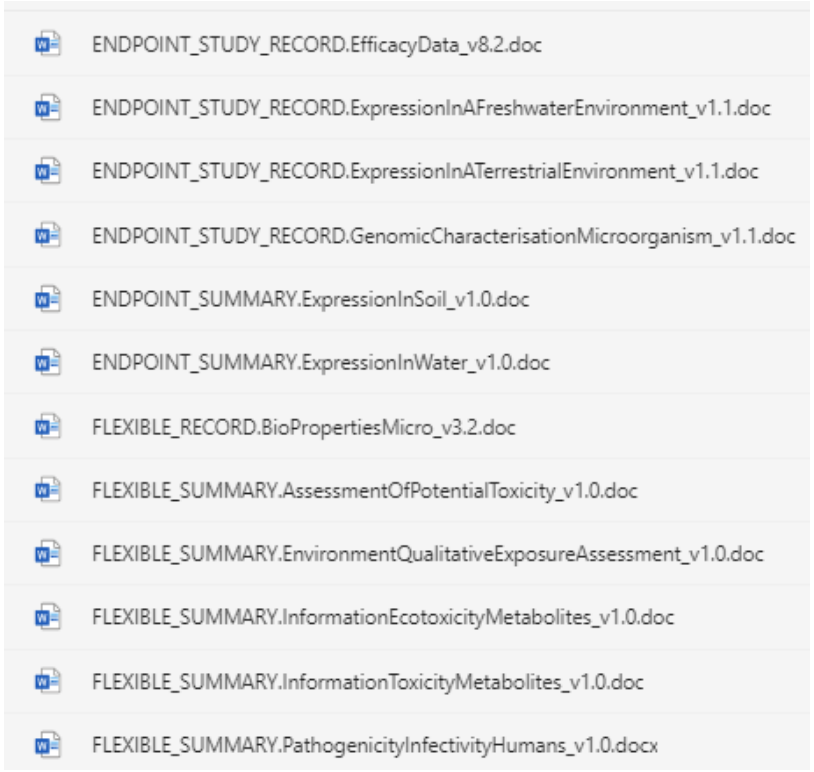
PURPOSE: Format suitable for migration of historical datasets into IUCLID format

E.g. OpenFoodTox, genotoxicity data, additives & flavouring, botanicals

https://www.efsa.europa.eu/it/data-report/chemical-hazards-database-openfoodtox
https://www.efsa.europa.eu/en/data-report/compendium-botanicals
https://data.europa.eu/data/datasets/database-pesticide-genotoxicity-endpoints?locale=en



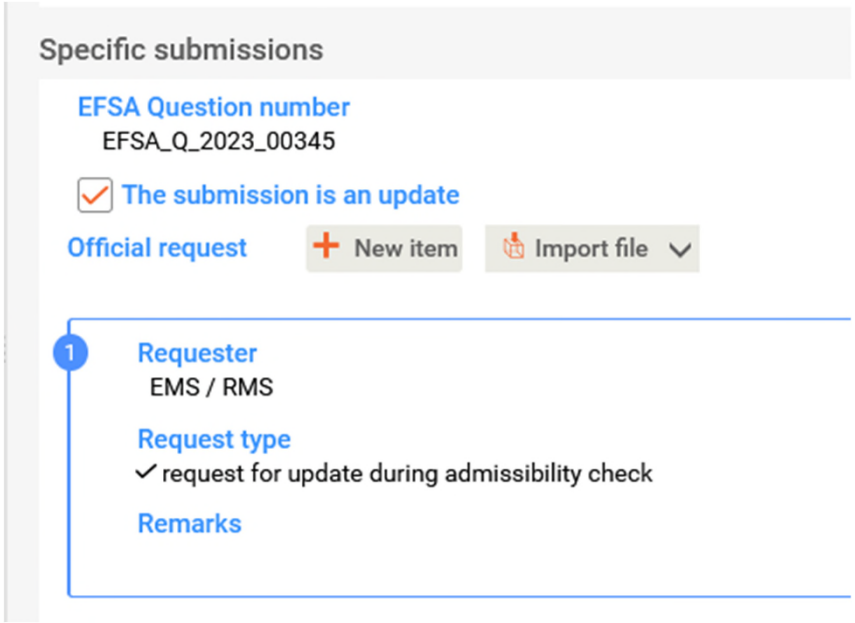
MICROORGANSIM NEW DATA REQUIREMENTS



Specific instructions for these documents have been prepared and will be circulated shortly with the Introduction section of the Microorganism manual

Further information will be provided based on the input from the reformed **Working Party on Microorganism**

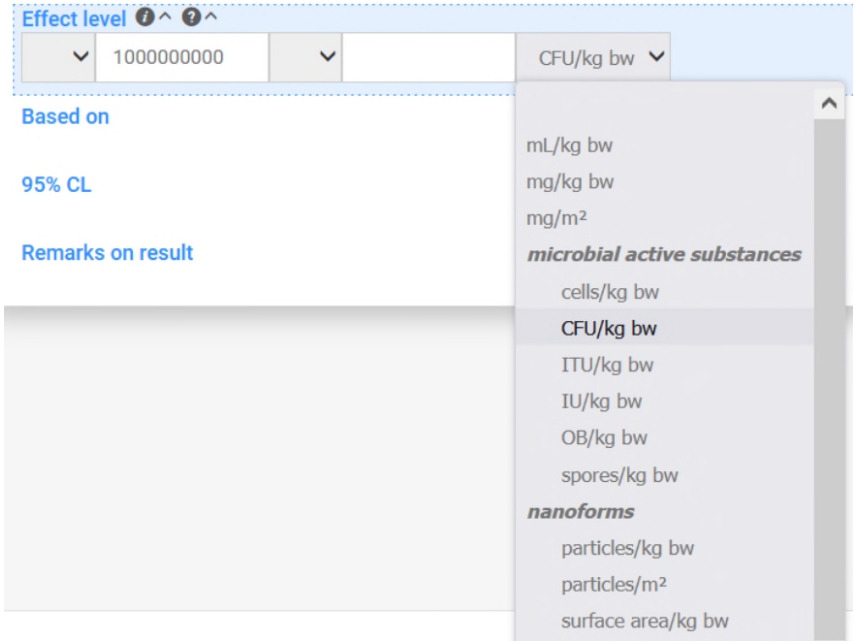
REASON FOR RESUBMISSION



- Location: At the bottom of the dossier header
- Check submission is an update if it is not the first submission
- Indicate which organisation/s have requested the update and under which circumstances
- Further information can be provided as remarks

CHANGES MADE TO SEVERAL OECD HARMONISED TEMPLATES:

- Harmonisation of units for microorganisms in relevant OHTs
- Change ‘Study period’ field in OHTs from text field to date fields for ‘start’, ‘end’ + remark
- Field ‘Illustration’ moved to the ‘Attachments’ fields in all OHTs
- Identification of metabolites extended, added in relevant endpoints



REPEATABLE BLOCK TO REPLACE TEMPLATE 5.1

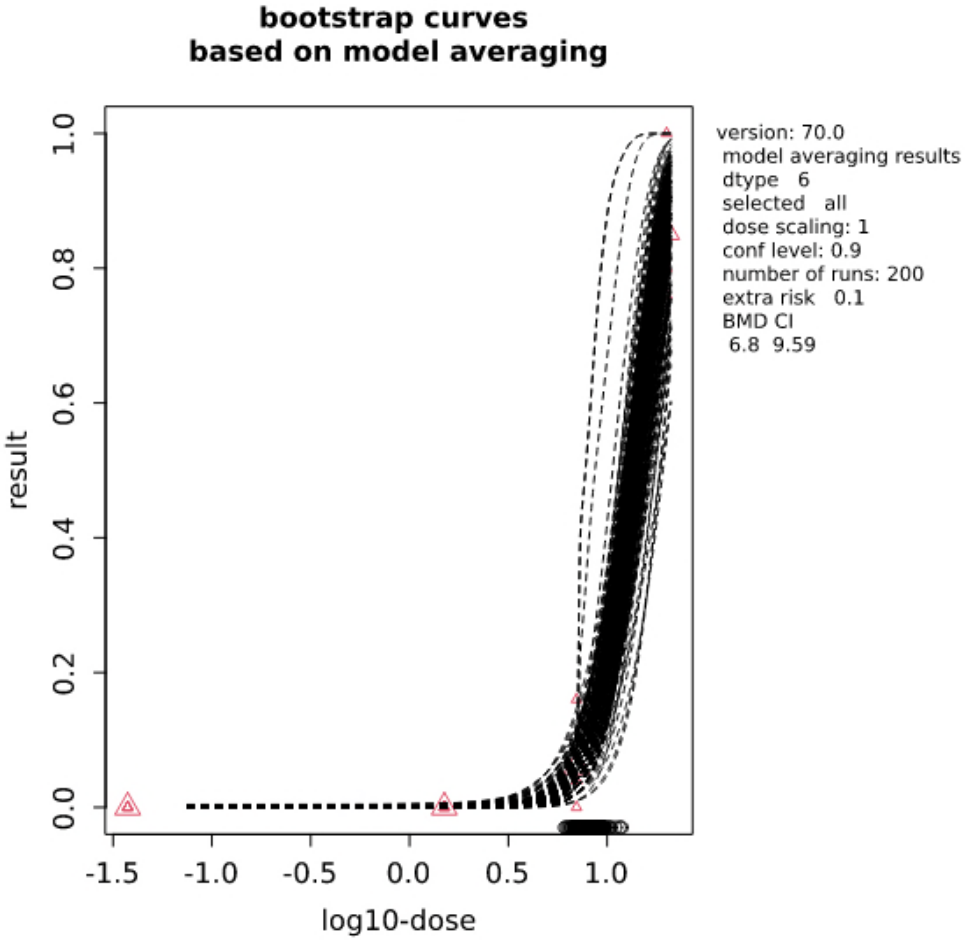
Trial of new table in Repeated dose toxicity to support Bench Mark Dose calculations in R4EU to replace Template 5.1 results in tabular format for mammalian toxicology studies

Detailed toxicology results

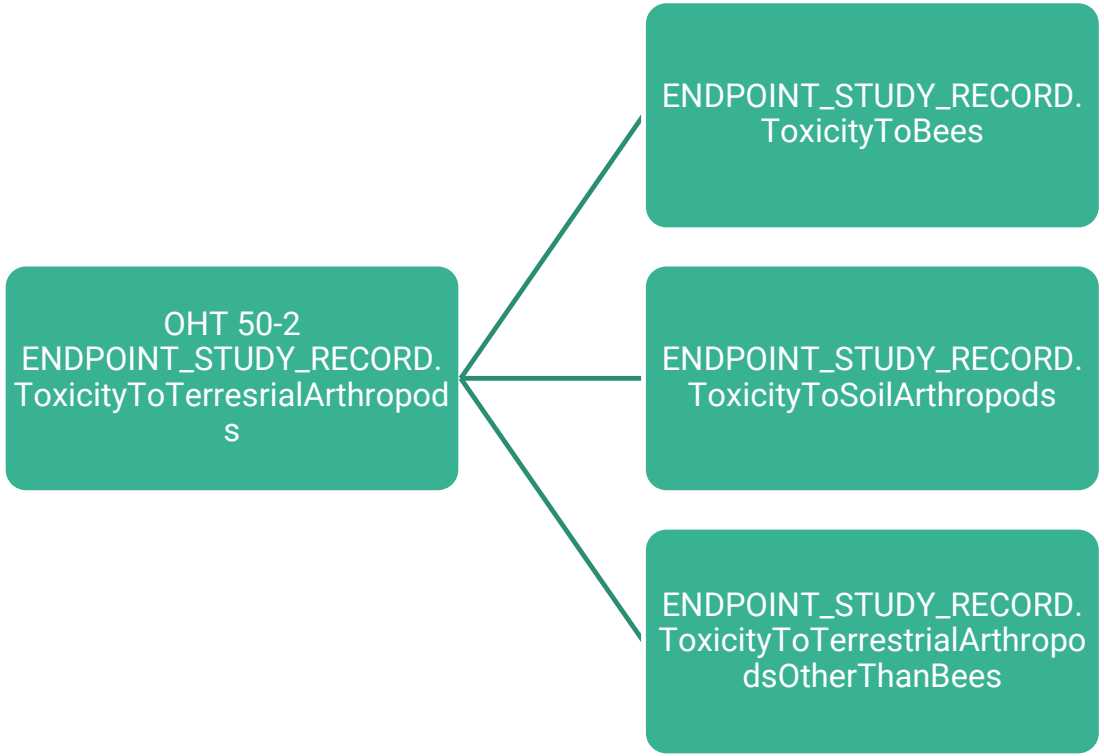
Detailed toxicology results + New item Import file

#	Sex	Additional cov...	Dose / conc.	No. of animals...	Examination	Experimental
1	male	other: F0	0	25	granuloma	0
2	male	other: F0	1.5	25	granuloma	0
3	male	other: F0	7	25	granuloma	1
4	male	other: F0	20	25	granuloma	20

https://sar4euaks.z6.web.core.windows.net/R4EU/unified.html?ui_locales=en

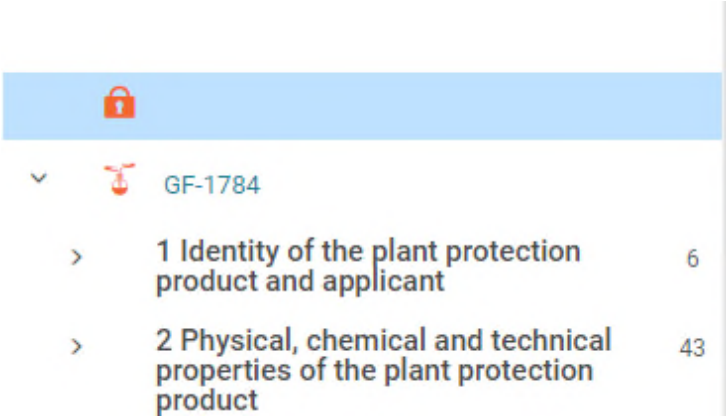


3 OHTS FOR ARTHROPODS



- Note: The (obsolete) EU PPP Endpoint summary for toxicity to terrestrial arthropods did not allow referencing the newly created OECD Harmonised Templates for terrestrial arthropods. This created impossibility to import IUCLID files in some specific case (Ref. 874188)
- FIXED IN VERSION 7.0.2

ISSUE WITH WORKING PPP WORKING CONTEXTS



An issue has been identified in EFSA Agency. It affects AIR, NAS and MO dossiers. The working context was not migrated in the dossier header. This issue is causing problems with validation assistant, report generator and the automatic message if a new dossier exists.
The issue is under investigation and we will update you as soon as we have more information.

FIX Working context for specific dossier types not fully migrated to IUCLID 6 v7. This impacts IUCLID 6 v6 dossiers of the following types, migrated to IUCLID 6 v7:
- EU PPP Active substance application (product)
- EU PPP Microorganisms - active substance application (product)

The fix applies to all cases (data not yet migrated to IUCLID 6 v7 or data already migrated to IUCLID 6 v7) during upgrade to this version. The issue does not impact newly created dossiers in IUCLID 6 v7 and is mainly relevant to Authorities accessing these dossiers (Ref.874098)

FIXED IN VERSION 7.0.2

Q106 ISSUE WITH DESCRIPTION OF KEY INFORMATION

A106. The content of the fields 'Description of key information' (KeyInformation) has been identified to be lost during the migration to IUCLID 6 v7 for the following endpoint summaries:

- Acute Toxicity
- Repeated dose toxicity
- Carcinogenicity
- Neurotoxicity
- Immunotoxicity

- We recommend the following actions:
- In case you have not been using the fields or the IUCLID documents mentioned above, there is no action required.
- If you have not updated yet to IUCLID 6 v7, wait for the new updater to be made available before upgrading your installations. – **EFSA Agency IUCLID will be updated in the next window for system updates**

FIXED IN VERSION 7.0.4

ISSUE WITH REPORT GENERATOR LINKS

Clicking on a link in the report results in page not found.

Year	Title Reference type Report and/or Study No. Source or Testing facility, if different from Sponsor
2020	Determination of Magnitude of Residue of Boscalid in/on Winter Wheat at fixed Intervals and harvest Following two applications of Boscalid 50% WG fungicide Study report

The link is pointing to localhost and not to ECHA cloud services

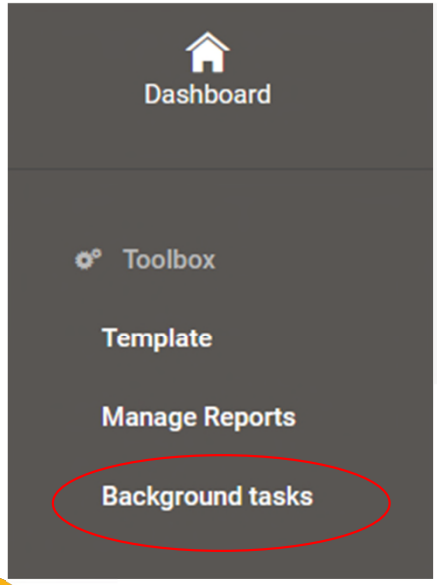
https://localhost/iuclid6-web/?key=071d4512-fb96-4994-bb1d-12e0ac933ed5/da09d407-adca-4b8a-9f75-ac05fa8ac8e5

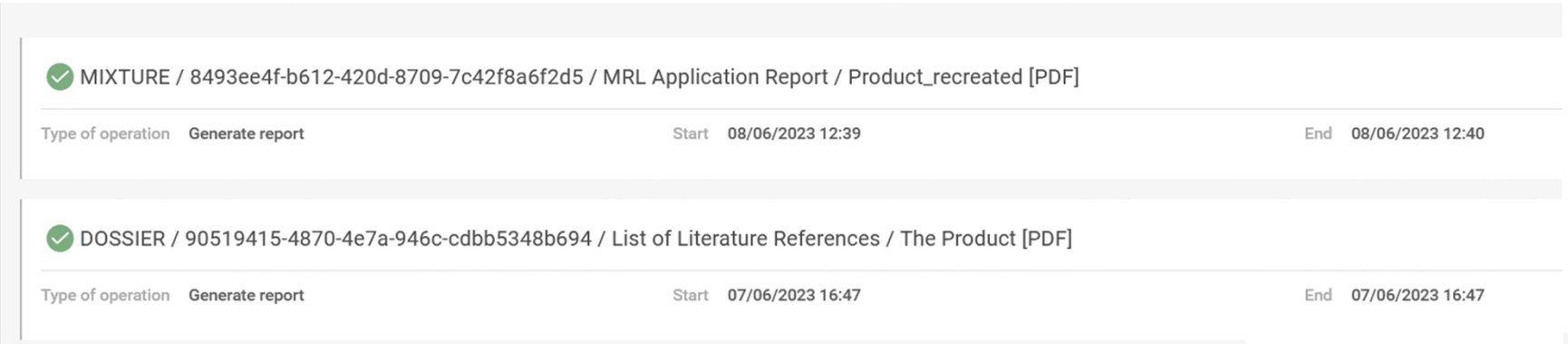
Copy the uuid between the key= and / and the UUID can be pasted into the IUCLID dashboard search box – we appreciate this is not convenient

The problem is only seen EFSA Agency IUCLID – ECHA is investigating

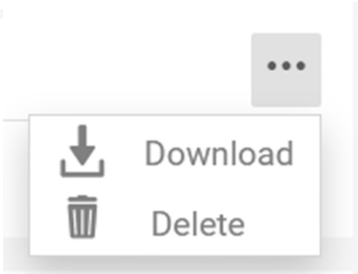
BACKGROUND TASKS

Tasks such as running reports or exporting a dossier now run as background jobs





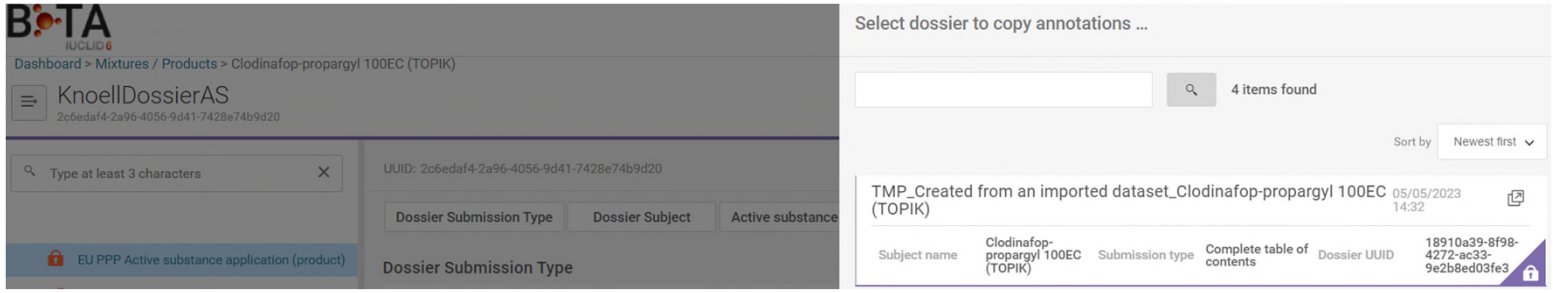
View the status of background jobs in the table – once completed there are options to download and/or delete



More details in the IUCLID user manual page 189
IUCLID Manual

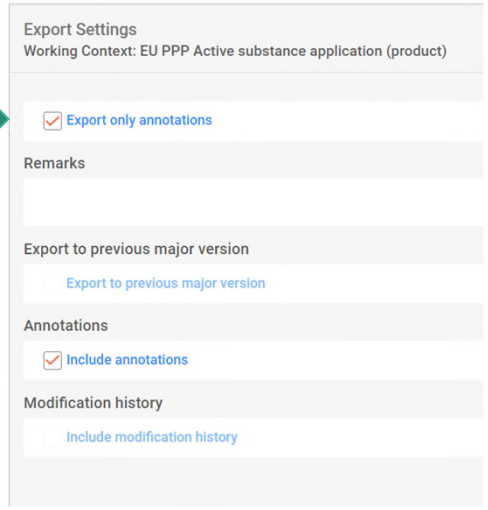
NEW TRANSFER ANNOTATIONS (REF. 265678)

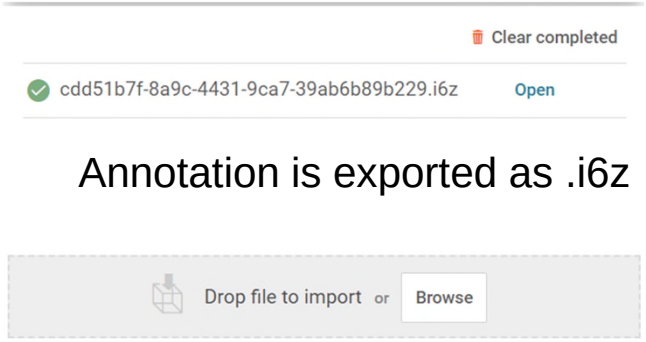
Within an IUCLID instance you can copy annotations



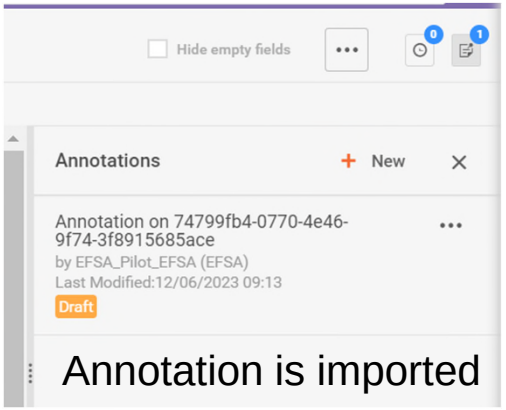
For more information on annotations see page 92
IUCLID Manual

Between IUCLID instances you can include annotations or export only annotations





Annotation is exported as .i6z



Annotation is imported

WEB INTERFACE PERFORMANCE

- In IUCLID 6 v7, performance improvements have been made to specific parts of the application
  - Report generation is now a background task and background tasks can be accessed
  - The navigation tree loading has been optimised (to avoid unnecessary reloading)
- Still improvements are required for
  - Dossier creation and export
  - Extract to dataset
  - …
- A survey will be shared to collect your feedback on performance and identify the next improvement areas

REPORT GENERATOR WORKSHOP

IUCLID Reporting Workshop

IUCLID Reporting Workshop

Based on last year's successful IUCLID Reporting Workshop, in which a new report was developed (The List of Study Summaries) the European Chemicals Agency (ECHA) and the European Food Safety Authority (EFSA) intend to host a IUCLID Reporting Workshop in early November 2023.

The Workshop would be a **hybrid** meeting to support both existing and new IUCLID users:

- to increase understanding of the projects being undertaken to develop reusable IUCLID Reports which represent the intrinsic and hazardous properties of chemicals
- to coordinate and maximise the use of the IUCLID Report Generator across the various Stakeholder communities using IUCLID.

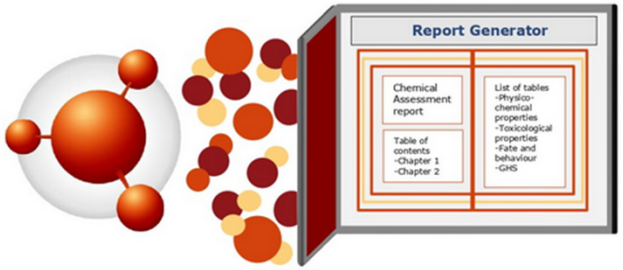
We would be grateful if you could answer a few questions below so that we can:

- get your requests and wishes for the Workshop
- estimate who would attend in person or remotely

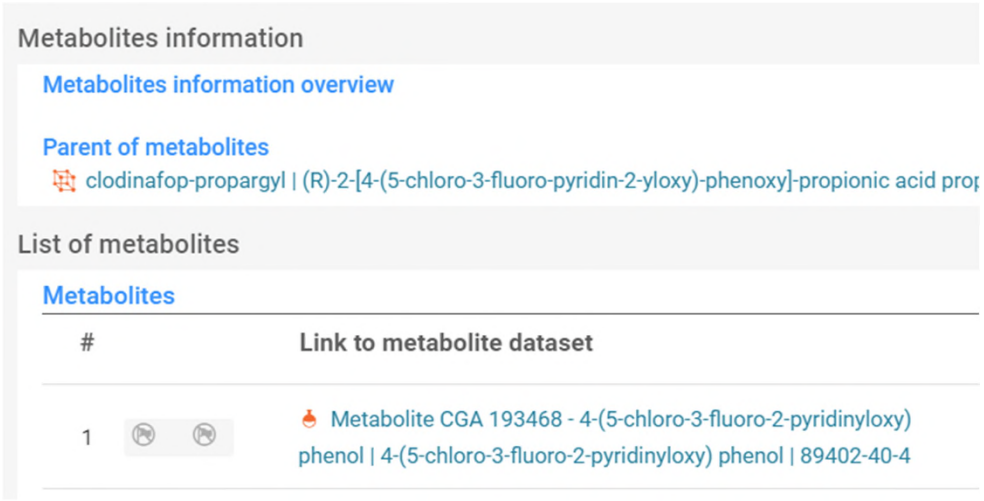
We look forward to your response.

(ECHA and EFSA IUCLID teams)

https://ec.europa.eu/eusurvey/runner/fdd802ca-b872-7914-d6f7-6892bf791385



ADVANCED SEARCH METABOLITES #2488



Extend the Advanced search function to retrieve information about metabolites included in dossiers or datasets. Input parameters could be Substance name or substance UUID

23/05/2023, EVJ: During the MSCA User Group meeting several countries found this feature quite useful. Tobias Opialla (BfR) indicated that: This would be helpful, but especially a structure similarity search and a search by drawing a (sub)structure would be even more helpful, especially when this would be combineable with the QSAR-Toolbox from OECD.
On top of that, Christian Erdmann (Baua) also indicated that: It could be useful to be able to limit the search to substance datasets or dossiers created by the legal entity of the user performing the search.
31/05/2023, EVJ: BfR additional comment: Structure and Substructure search within the data would be helpful. Currently this feature will be passed to the OECD QSAR Toolbox using the TEDRA Plugin. This is useful for model creating but cumbersome the plain search. In addition: different fingerprint algorithms should be considered for similarity search depending on the user needs

The IUCLID format includes a document where all metabolites in the dossier can be listed

Slido question: Is the requirement for?

- https://app.sli.do/event/ujVVv9QDQdmH2UmHjHAF5i

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