



7th meeting of the PSN IUCLID sub-group

19-20 June 2023

PSN IUCLID VERSION 6.7

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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>

EFSA chemicals database (substance)

TESTOpenFoodTox_Fluxapyroxad	
1 Key information	7
> 1.1 Substance identification	1
> 1.2 Substance composition	1
> 1.3 Metabolites	1
> 1.4 Reference values	1
> 1.5 Function, mode of action and possible resistance	
> 1.6 Human health	3
2 Detailed results	8
> 2.1 Human health	6
> 2.2 Animal health	
> 2.3 Ecotoxicology (Soil-Terrestrial)	
> 2.4 Ecotoxicology (Aquatic)	1
> 2.5 Fate and behaviour in the environment	1
> 2.6 Physical and chemical properties of the active substance	
Inherited templates	

MICROORGANSIM NEW DATA REQUIREMENTS

	ENDPOINT_STUDY_RECORD.EfficacyData_v8.2.doc
	ENDPOINT_STUDY_RECORD.ExpressionInAFreshwaterEnvironment_v1.1.doc
	ENDPOINT_STUDY_RECORD.ExpressionInATerrestrialEnvironment_v1.1.doc
	ENDPOINT_STUDY_RECORD.GenomicCharacterisationMicroorganism_v1.1.doc
	ENDPOINT_SUMMARY.ExpressionInSoil_v1.0.doc
	ENDPOINT_SUMMARY.ExpressionInWater_v1.0.doc
	FLEXIBLE_RECORD.BioPropertiesMicro_v3.2.doc
	FLEXIBLE_SUMMARY.AssessmentOfPotentialToxicity_v1.0.doc
	FLEXIBLE_SUMMARY.EnvironmentQualitativeExposureAssessment_v1.0.doc
	FLEXIBLE_SUMMARY.InformationEcotoxicityMetabolites_v1.0.doc
	FLEXIBLE_SUMMARY.InformationToxicityMetabolites_v1.0.doc
	FLEXIBLE_SUMMARY.Pathogenicity/InfectivityHumans_v1.0.docx

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

Specific submissions

EFSA Question number

EFSA_Q_2023_00345

☒ The submission is an update

Official request

+ New item

Import file ▼

1

Requester

EMS / RMS

Request type

✓ request for update during admissibility check

Remarks

- 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

The screenshot shows a form interface with a dropdown menu open. The dropdown is titled 'Effect level' and contains a list of units. The units are grouped into three categories: 'Based on', '95% CL', and 'Remarks on result'. The units listed are: mL/kg bw, mg/kg bw, mg/m², **microbial active substances**, cells/kg bw, **CFU/kg bw**, ITU/kg bw, IU/kg bw, OB/kg bw, spores/kg bw, **nanoforms**, particles/kg bw, particles/m², and surface area/kg bw. The unit 'CFU/kg bw' is currently selected.

Effect level	1000000000	CFU/kg bw
Based on		
95% CL		
Remarks on result		



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](#)

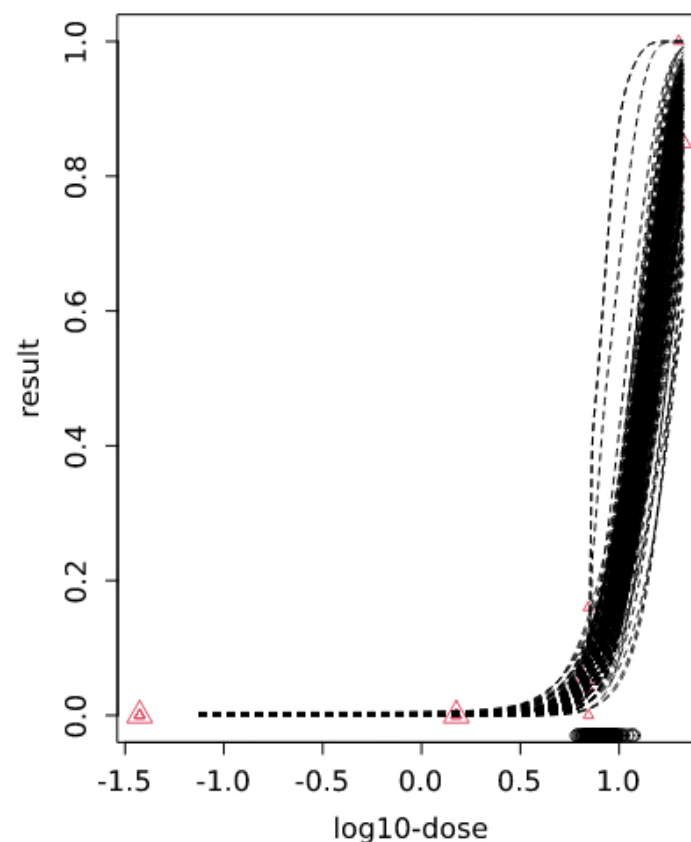
+ New item

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

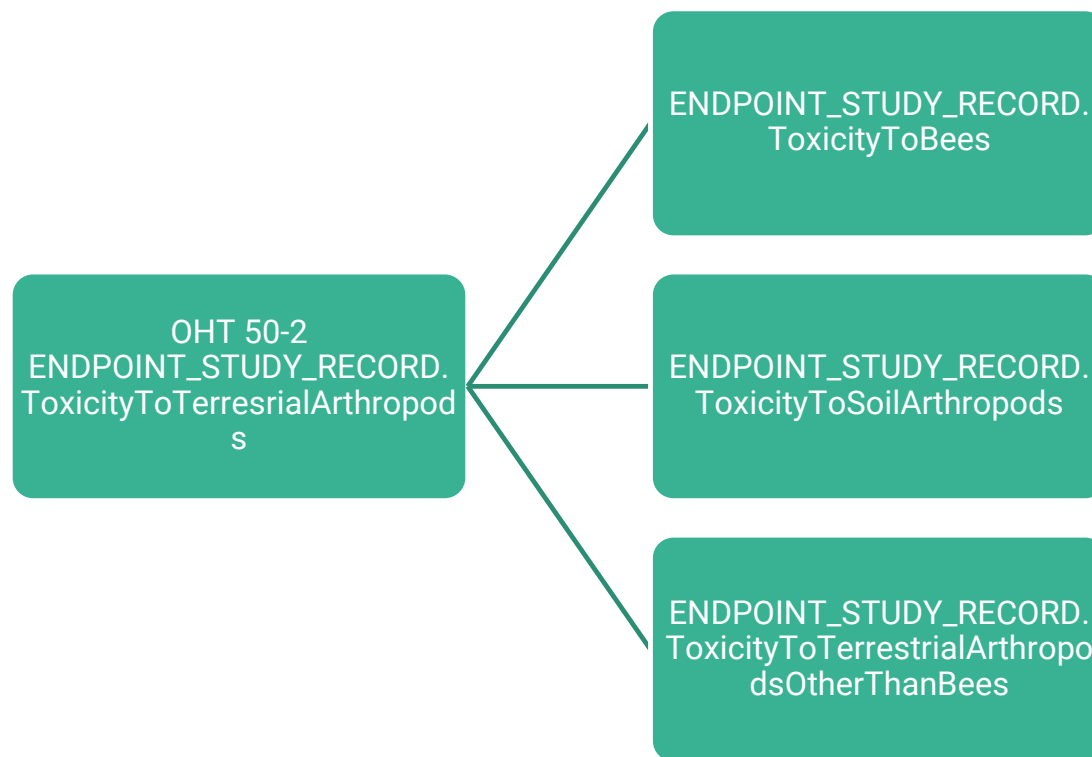
https://sar4euaks.z6.web.core.windows.net/R4EU/unified.html?ui_locales=en

bootstrap curves
based on model averaging



version: 70.0
model averaging results
dtype 6
selected all
dose scaling: 1
conf level: 0.9
number of runs: 200
extra risk 0.1
BMD CI
6.8 9.59



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

		
▼	 GF-1784	
>	1 Identity of the plant protection product and applicant	6
>	2 Physical, chemical and technical properties of the plant protection product	43

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>

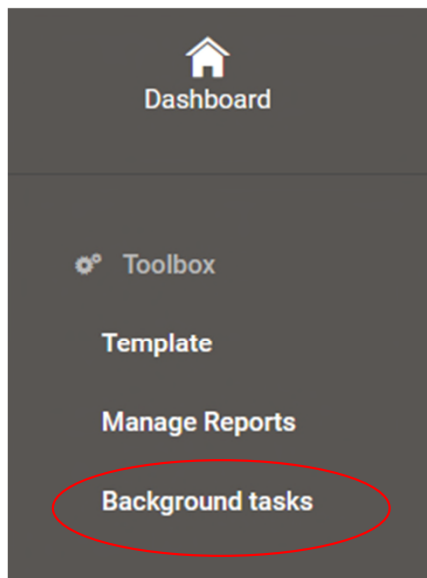
Copy the uuid between the key= and / and the UUID can be pasted into the IUCLID dashboard search box – we appreciate this is not convenient

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



✓ MIXTURE / 8493ee4f-b612-420d-8709-7c42f8a6f2d5 / MRL Application Report / Product_recreated [PDF]

Type of operation Generate report

Start 08/06/2023 12:39

End 08/06/2023 12:40

✓ DOSSIER / 90519415-4870-4e7a-946c-cdbb5348b694 / List of Literature References / The Product [PDF]

Type of operation Generate report

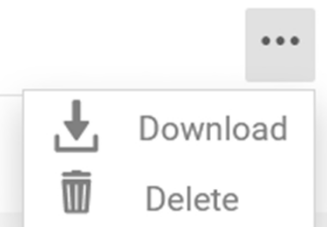
Start 07/06/2023 16:47

End 07/06/2023 16:47

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

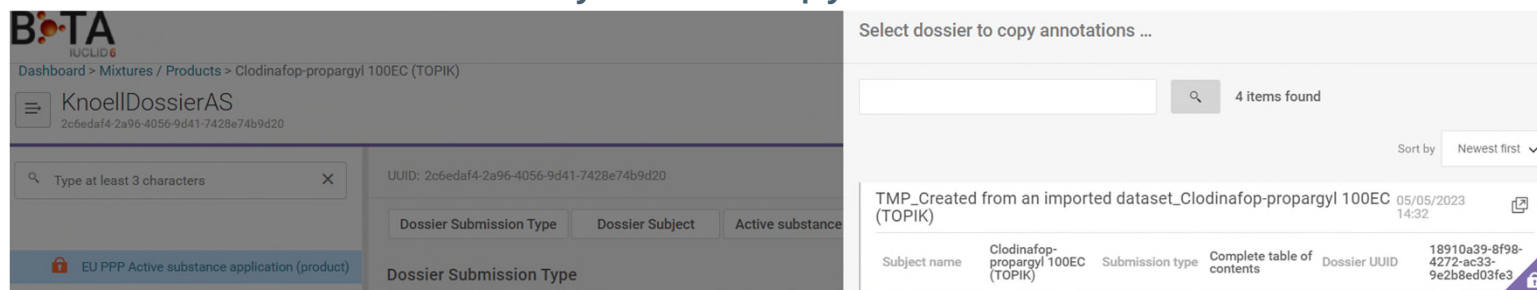
More details in the IUCLID user manual page 189

[IUCLID Manual](#)



NEW TRANSFER ANNOTATIONS (REF. 265678)

Within an IUCLID instance you can copy annotations

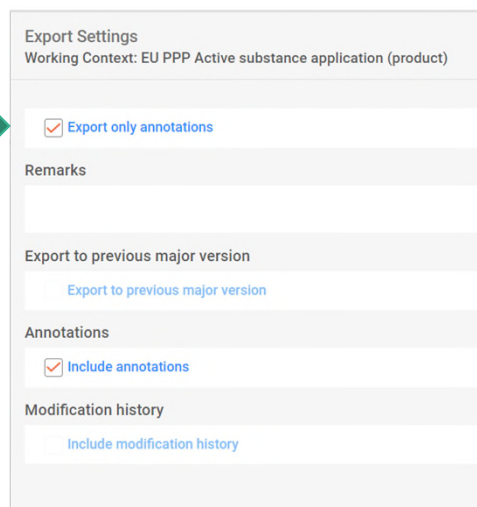


The screenshot shows the IUCLID 6 interface. On the left, the 'KnoellDossierAS' dossier is selected. The main area displays a dialog titled 'Select dossier to copy annotations ...'. It shows a search bar with '4 items found' and a table of results. The table has columns for 'Subject name', 'Submission type', 'Complete table of contents', and 'Dossier UUID'. The first row is 'TMP_Created from an imported dataset_Clodinafop-propargyl 100EC (TOPIK)' with a 'Dossier UUID' of '18910a39-8f98-4272-ac33-9e2b8ed03fe3'.

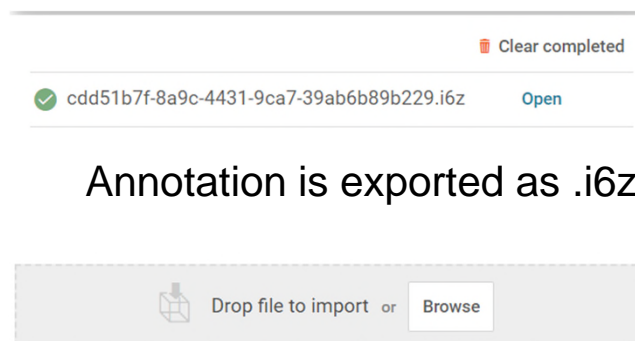
For more information on annotations see page 92

[IUCLID Manual](#)

Between IUCLID instances you can include annotations or export only annotations

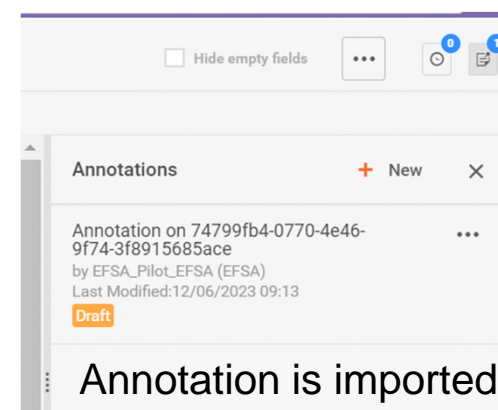


The screenshot shows the 'Export Settings' dialog. It has a 'Working Context: EU PPP Active substance application (product)'. There are three sections: 'Remarks', 'Export to previous major version', and 'Annotations'. The 'Annotations' section has a checkbox 'Include annotations' which is checked. There is also a link 'Export to previous major version'.



The screenshot shows the 'Exported annotations' dialog. It has a 'Clear completed' button. Below it, there is a green checkmark and the text 'cdd51b7f-8a9c-4431-9ca7-39ab6b89b229.i6z' with an 'Open' button. At the bottom, there is a dashed box with a file icon and the text 'Drop file to import or Browse'.

Annotation is exported as .i6z



The screenshot shows the 'Imported annotations' dialog. It has a 'Hide empty fields' checkbox and a 'New' button. Below it, there is a list of annotations. The first annotation is 'Annotation on 74799fb4-0770-4e46-9f74-3f8915685ace by EFSA_Pilot_EFSA (EFSA)' with a 'Last Modified' date of '12/06/2023 09:13' and a 'Draft' status. At the bottom, there is a large text box with the text '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.

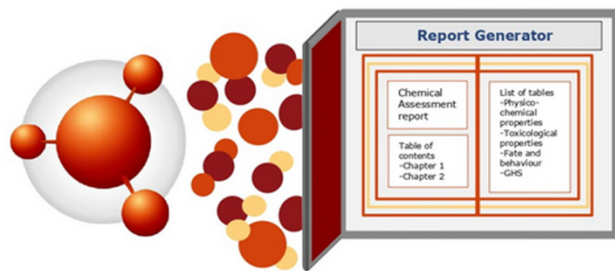
We would be grateful if you could answer a few questions below so that we can:

- 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/fd802ca-b872-7914-d6f7-6892bf791385>



ADVANCED SEARCH METABOLITES #2488

Metabolites information

Metabolites information overview

Parent of metabolites

 clodinafop-propargyl | (R)-2-[4-(5-chloro-3-fluoro-pyridin-2-yloxy)-phenoxy]-propionic acid prop

List of metabolites

Metabolites

#	Link to metabolite dataset
1	 Metabolite CGA 193468 - 4-(5-chloro-3-fluoro-2-pyridinyloxy) phenol 4-(5-chloro-3-fluoro-2-pyridinyloxy) phenol 89402-40-4

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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