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IUCLID format updates (OECD): April 2023 release



• 9 revised Endpoint Study Record (OHTs) – Series on Environmental Fate and Behaviour; Health effect; Effects on biotic systems; Efficacy.

OHT n./Name	IUCLID Backlog (#)
29 Biodegradation in water and sediment: simulation tests	Updates in line with endpoint summaries harmonization; optimization of the use of the csv upload function (#2309)
30 Biodegradation in soil	the use of the esv apload function (#2505)
39 Field studies	
50-2 Toxicity to terrestrial arthropods	Splitting of current OHT 50-2 into 3 new templates OHT 50-3, 50-4 and 50-5 (#2284)
58 Basic toxicokinetics	Update to support integration with METAPATH (alignment with other OHT on metabolism by addition of the appendix: metabolites and their parent treatment groups).
80 - Epidemiological data	Changes linked to migration of OpenFoodTox data (#2574; #2576)
84 - Toxic effects on livestock and pets	
87 Analytical methods	Full revision including comments from the OHT Expert Group (July 2021) and SANTE/2020/12830 rev. 1. (Residues methods) (#1855, #2144, #2354; #2228).
89 Efficacy data	Minor changes on MO info (#2142)

IUCLID format updates (OECD): April 2023 release



• 7 revised Endpoint Study Record (OHTs) – Series on Pesticides Residue Chemistry

OHT n./Name	IUCLID Backlog (#)
85-2 Metabolism of residues in livestock	Update to support integration with METAPATH (#2482 possibility to report studies on metabolism in fish)
85-3 Metabolism of residues in crops and in rotational crops	Update to support integration with METAPATH (#2089,#1787, #1790)
85-4 Residues in livestock	Minor updates - animal number (#2375); Possibility to report fish feeding studies
85-5 Residues in crops (field trials)/rotational crops	Changes by OECD Secretariat & BfR (inclusion of revised OECD TG 509) and EFSA (EU PPP commodities picklist) (#2079; #2089). Full revision in 2023 to support integration with RUEDIS considering simplified/user-friendly structure
85-8 Nature of residues in processed commodities	Update to support integration with METAPATH (alignment with OHT 85-2/3); Addition of the appendix: "metabolites and their parent treatment groups"
85-9 Magnitude of residues in processed commodities	Update of RAC and processed commodities picklist (#2073; #1786). Full revision in 2023 to support integration with RUEDIS considering simplified/user-friendly structure.
85-10 Stability of residues in stored commodities	Small fixes on the picklists (#2463, #2464)

IUCLID format updates (EU_PPP/CORE): April 2023 release



• 6 EU_PPP docs:

Name	IUCLID Backlog (#)
Endpoint_Study_Record_Magnitude of residues in pollen and bee products	Update to report studies on residue levels in pollen and bee products (according to the newly developed EU guidance document SANTE/11956/2016rev.9) and to identify key values for risk assessment (#2147 #2468)
FLEXIBLE_SUMMARY. ToxRefValues	Changes linked to migration of OpenFoodTox data (#2574; #2576)
FLEXIBLE_SUMMARY. Residues In Livestock	Small fixes to report MATRIX, MRL at LOQ and fish studies (#2376; #2465; #2481)
ENDPOINT_SUMMARY. StabilityResiduesCommodities	Small fixes on picklists (#2464)
Dossier header (MO)	New fields to report submission info (requester, type; reason) (#2357; #2359; #2471)
Flexible summary_IsomericCompositionRiskAassessment *	#2583

4 CORE docs:

Name	IUCLID Backlog (#)
FLEXIBLE_RECORD. Analytical Information	New field to upload study report/documents (#2223)
ENDPOINT_SUMMARY. MetabolismInLivestock	Updates to align with OHT 85-2/MetaPath (#2075)
ENDPOINT_SUMMARY. Analytical Profile Of Batches	New section under "Administrative Data" for "Quality Control data" to report info on (number of batches analysed, max/min conc of each component, manufacturing plant, remarks, etc.); table for CSV uploader (#2489)
FLEXIBLE_RECORD.AnalyticalProfileOfBatches *	Addition of "QC data" (#2489)

Endpoint Summary harmonisation (ECHA-EFSA)



<u>Aim</u>: to fuse parallel/overlapping Endpoint Summaries (ES) under **EU PPP**, **NZ HSNO** and **CORE** into one single format per endpoint, to be used by all the relevant contexts;



- ✓ Review of other ESs against principles set in the project (structural consistency);
- ✓ Including **ESs** as OECD Harmonised Templates (OHTs): **105** ESs submitted to the OECD consultation in September 2022:
 - Newly created endpoint summary formats;
 - 20 harmonisation proposals (i.e., **20 EU PPP**, 2 NZ HSNO, 18 CORE formats).
 - Bioaccumulation: aquatic / sediment EU PPP
 - Biodegradation in soil (EU PPP)
 - Route of degradation in soil (EU PPP)
 - Biodegradation in water and sediment: simulation tests (EU PPP)
 - o Route of degradation in water and sediment (EU PPP)
 - Carcinogenicity (EU PPP)
 - Effects on biological methods for sewage treatment
 - Long-term toxicity to aquatic invertebrates EU_PPP
 - Long-term toxicity to fish EU PPP
 - Short-term toxicity to aquatic invertebrates EU_PPP
 - Short-term toxicity to fish EU PPP
 - Sediment toxicity EU_PPP
 - Toxicity to aquatic algae and cyanobacteria EU_PPP
 - Toxicity to birds EU_PPP
 - Toxicity to other above-ground organisms (wild mammals) EU_PPP
 - Toxicity to plants EU PPP
 - Toxicity to terrestrial plants EU PPP
 - Toxicity to soil macroorganisms except arthropods EU PPP
 - Toxicity to soil microorganisms (EU PPP)
 - Toxicity to terrestrial arthropods EU_PPP (cf. project on splitting OHT 50-2)

- ✓ Unique key values (i.e., fixed fields; removal of repeatable blocks);
- ✓ Datatype of the key values (only half-bounded numerical values, qualifier + value);
- ✓ **Linking to relevant Endpoint Study Records** (per relevant key section; generating the list of endpoints report);
- ✓ Streamlined, structured information for assessment purposes;
- Microbial pesticide units added
- ✓ **Long-term toxicity** key values in "Repeated dose toxicity" (including short-term, sub chronic and chronic); "Carcinogenicity" remains.

OHTs #29, #30, #39 - final draft proposal



- New fields to report half-life of parent compound/DT50 values (structured table):
 - OHT 29_Biodegradation in water and sediment: simulation tests (including compartments)
 - OHT 30_Biodegration in soil
 - OHT 39_Field studies

111.	Half-life of parent compound / 50% disappearance time (DT50)	Block of fields (repeatable) Start		For each soil type, include value (or range if reported so) of DT50 and indicate the type of the DT50 (For first order kinetics DT50 = half-life).If relevant, also indicate the DT90 value (or range if reported so) and the DT50 value as normalised to reference conditions.
112.	Key result	Check box Display: Basic		Set this flag for identifying the key information which is of potential relevance for hazard/risk assessment or classification purpose. Consult any programme-specific guidance (e.g. OECD Programme, Pesticides NAFTA or EU REACH) on how to use this field.
113.	Soil No.	List (picklist)	Picklist values: - #1	Select a consecutive soil number from drop-

93.	Compartment	List (picklist) Display: Basic	Picklist values: - abiotic control measured at end of test - biologically active treatment at end of test - natural water: freshwater - natural water: marine - natural water: brackish - natural water - water - natural water / sediment: freshwater - natural water / sediment: brackish - natural water / sediment: brackish - natural water / sediment - natural sediment: freshwater - natural sediment: freshwater - natural sediment: marine - natural sediment: brackish - natural sediment - artificial sediment - sediment - sediment - activated sludge - wastewater - anaerobic sludge - treated effluent: surface water mixing zone - untreated effluent: surface water mixing zone - entire system - other:
94.	Parameter	List sup. (picklist with remarks) Display: Basic	Picklist values: - DT50 - DT50 (normalised) - DT90

New OHTs #50-3; #50-4; #50-5 - final draft proposal



- ✓ **Three NEW Templates** to replace OHT 50-2 *Toxicity to terrestrial arthropods*:
 - i. OHT 50-3 Toxicity to bees
 - ii. OHT 50-4 Toxicity to terrestrial arthropods other than bees
 - iii. OHT 50-5 Toxicity to soil arthropods



- ✓ Addition of **new** fields to report different type of studies:
 - laboratory studies, semi-field studies and field;
 - Text field "Slope of the curve" (per dose descriptor).
- ✓ Inclusion of ECHA/EFSA Guidance Documents on pollinators and EU PPP data requirements for microorganisms (EC, 2020):
 - Dose descriptor (10-d LDD₅₀; TRT-LDD₅₀);
 - Pathogenicity/infectivity (effect conc. units "cells", "ITU").
- ✓ Three **NEW Endpoint Summaries** created together with NZ EPA (harmonisation exercise by ECHA)

NEW ESR Magnitude of residues in pollen and bee products

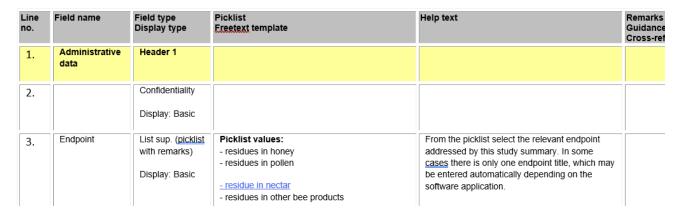


✓ Possibility to report studies on residue levels in pollen and bee products performed according

LEGISLATION_NAME Template #N/A: Magnitude of residues in pollen and bee products (Version [2.3]-[August 2021])

The following table gives a detailed description of the type of information prompted for by the data entry fields.

to newly developed EU guidance document (SANTE/11956/2016rev.9) (#2147 #2468).



✓ Reporting key values for risk assessment (e.g., study type characteristics; trials parameters)

42.	Study design	Header 2	
42. <u>43</u>	Study type	List sup. (picklist with remarks)	-Syrup feeding tests
			- <u>Tunnel trials</u>
			- <u>Field trials</u>
			-Others (specify)

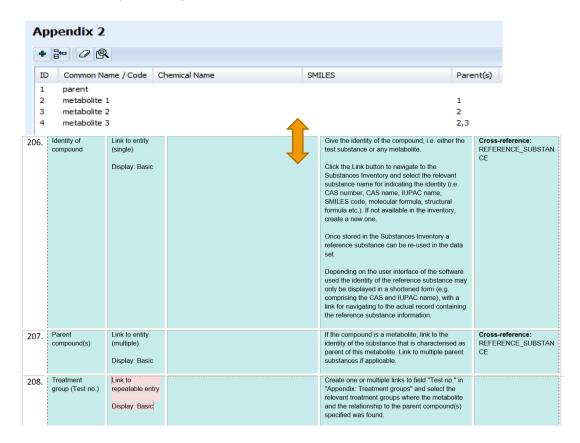
<u>47.</u>	<u>Trial site</u>	Text (2,000 char.)	
44.48	Duration of trial	Numeric (decimal including unit)	Picklist value h d m yr
49.	Tunnel size/ Field size	Numeric (decimal including unit)	Picklist value m² ha

OHTs 85-2; 85-3: metabolism livestock and plants

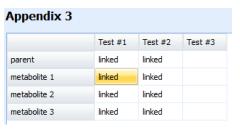


85-2 and 85-3 were checked for compatibility with MetaPath (i.e., MSS composers):

+ =	- 0 Q						
Test#	Number	Application Method	Application Rate	Number of Application	ns Timing of Applications	PHI	Matrix
Test #	‡1 1	Foliar	20 g as/ha	2		21 d	Fruit
Test #	‡2 2	Foliar	20 g as/ha	2		60 d	Fruit
Test #	‡3 3	Foliar	20 g as/ha	2		60 d	leaves
108.	Appendix: Treatment groups	Header 2		1			
109.	Treatment groups	Block of fields (repeatable) Start			Provide information on the treatme used. Copy this block of fields for multiple groups.		
110.	Test no.	Text (255 char.) Display: Basic			Enter a test number (e.g. #1 or alp combination).	hanumeri	С
111.	Number	Text (255 char.) Display: Basic			Enter a number (e.g. #1 or alphan combination) for identifying the su test run.		f a
112.	PHI / PBI	Text (255 char.) Display: Basic		:	Specify the preharvest intervals (F study or plant-back intervals (PBI) crop study.		
113.	Method of application	Text (255 char.) Display: Basic			Describe the method of application	n.	
114.	Rate(s) of application	Text (255 char.) Display: Basic			Specify the rate of application.		
115.	Number of applications	Text (255 char.) Display: Basic			Specify the number of applications	6.	



- Good match was observed!
- Appendix 3 should be automatically derived from appendix 1 and 2 (no need for further manual entries);
- Next steps: more picklist (less free text) and migration.



OHTs 85-4 (livestock feeding studies)



Small fixes + possibility to report fish feeding studies (based on SANTE/10252/2021);

List sup.	Picklist values:
(<u>picklist</u> with	- residues in livestock
remarks)	
	residues in fish and fish products
Display: Basic	
	(<u>picklist</u> with remarks)

• Picklist updates:

Test animals	Header 2	
Species	List multi. (multi-select list) Display: Basic	Picklist values: - cow - fish (rainbow trout) - Fish (Atlantic salmon) - Fish (common carp) - goat - hen - sheep - swine - other:

Matrix / tissue	List sup.	Picklist values:
sampled	(picklist with	- eggs
	remarks)	- meat
		- milk
	Display: Basic	- edible meat by-products: skeletal
		muscle
		- edible meat by-products: perirenal fat
		- edible meat by-products: subcutaneous
		fat / backfat
		- edible meat by-products: liver
		- edible meat by-products: kidney
		- edible meat by-products: other
		- skin
		- skin with fat
		- Fish Fillet + skin
		- Fish Liver
		Figh Carages
		- Fish Carcass
		- other:

Guideline	List (picklist)	Picklist values: - OECD Guideline 505 (Residues in
	Display: Basic	Livestock)
		- EPA OPPTS 860.1480 (Residue
		Chemistry Test Guidelines: Meat / Milk /
		Poultry / Eggs)
		- PMRA Regulatory Directive DIR 98-02 -
		Residue Chemistry Guidelines, Section 8
		- Meat/Milk/Poultry/Eggs
		- SANCO 7031/VI/95 rev.4
		- SANTE/10252/2021 (magnitude of
		residues in fish)
		- other:

• A similar customisation was also done in OHT 85-2 to report studies on metabolism performed in fish.

85-8 (metabolism in process commodities)



- Not yet in MetaPath (no MSS composers);
- Compatibility with MetaPath is anticipated by adding the appendix "Metabolites and their parents in treatment groups" in OHT 85-8 (like in OHT 85-2 and 85-3):

<u>67</u>	Appendix: Metabolites and their parents in treatment groups	Header 2	
<u>68</u>	Metabolites in treatment groups	Block of fields (repeatable) Start	
<u>69</u>	ID no.	List (picklist) Display: Basic	Picklist values: -#1 -#2 -#3 -#4 -#5

<u>70</u>	Identity of compound	Link to entity (single)		Give the identity of the compound, i.e. either the test substance or any metabolite.	Cross-reference: REFERENCE SUBSTAN CE
		<u>Display: Basic</u>		Click the Link button to navigate to the Substances Inventory and select the relevant substance name for indicating the identity (i.e. CAS number, CAS name, IUPAC name, SMILES code, molecular formula, structural formula etc.). If not available in the inventory, create a new one. Once stored in the Substances Inventory a reference substance can be re-used in the data set. Depending on the user interface of the software used the identity of the reference substance may only be displayed in a shortened form (e.g. comprising the CAS and IUPAC name), with a link for navigating to the actual record containing the reference substance information.	<u>VE</u>
<u>71</u>	Parent compound(s)	Link to entity (multiple) Display: Basic		If the compound is a metabolite, link to the identity of the substance that is characterised as parent of this metabolite. Link to multiple parent substances if applicable.	Cross-reference: REFERENCE SUBSTAN CE
<u>72</u>	Test conditions	List sup. (picklist with remarks - 2,000 char.) Display: Basic	Picklist values: - baking, brawing and boiling (60 min, 100°C, pH 5) - pasteurisation (20 min, 90°C, pH 4) - sterilisation (20 min, 120°C, pH 6) - other:	Specify the test condition(s) under which the metabolite is retrieved.	

OHT 87 - final draft proposal



- ✓ Structure improved including **4 sections** (Materials&Methods; Results):
 - Principles of analytical methods (i.e., primary method)
 - Enforcement
 - Confirmatory
 - Independent Laboratory Validation

Method class	List multi. (multi- select list)	Picklist values: - Primary - Enforcement - Independent Laboratory Validation - Confirmatory
Materials and methods	Header 1	

- ✓ **Structured table** for reporting values on:
 - Recovery
 - LOQ/LOD
 - Calibration

✓ Improving the use of **CSV uploader**.

		ults and ussion		Hea	ider 1												
Recover	Recovery Analyte Matrix			RM/ n/z	Fortification level (mg/kg)	Units		Numb replica	er	Range Mea recovery recov (%) (%		ery	RSDr (%)	Remarks	Recovery		
Data type	e:	Link to entity	Te	ext		neric nge	Decimal	Picklis	st	Integ	er	Nume range	I I)acı	mal	Decima	I Text	
LOQ/LOD		Anal	yte Matrix			Limit of detection (mg/kg)		Units	Remarks		LOQ/LOD						
Data type: 1		Link entity		Text		Dec	cimal Decimal		Pickl	Picklist Text							
Calibration	n A	Analyte	Standa	rds I	Matrix	MRM/ m/z	Calibration range (mg/kg)	Units		libration uation	Correlation coefficient (r)		Calibratio coefficien (r2)	t o	lumber f eplicates	Remarks	Calibration
Data type:		ink to entity	Picklist multiple		Text	Numeric range	Numeric range	Picklist	Tex	d .	Decimal		Decimal	Ir	nteger	Text	

OECD consultation – have your say!



Sept - Oct 2022

Launch of OECD consultation

Nov - Dec 2022

Final modifications to the Templates

Feb - March 2023

IUCLID adaptations – Beta testing of the new format

26 April 2023

Publication of IUCLID (+ OECD website)

OHTs

Comments to **OECD** by **24 Oct**:

- At https://community.oecd.org/docs/DOC-218941

- **IUCLID team** (<u>iuclid6@echa.europa.eu</u>)

EU_PPP

Comments to EFSA by **30 Oct**:

- PSN Teams folder