


# IUCLID format: update on OHTs amendments

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

OHT n./Name	IUCLID Backlog (#)
<b>29</b> Biodegradation in water and sediment: simulation tests	Updates in line with endpoint summaries harmonization; optimization of the use of the csv upload function (#2309)
<b>30</b> Biodegradation in soil	
<b>39</b> Field studies	
 <b>50-2</b> Toxicity to terrestrial arthropods	Splitting of current OHT 50-2 into 3 new templates OHT 50-3, 50-4 and 50-5 (#2284)
<b>58</b> 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).
<b>80</b> - Epidemiological data	Changes linked to migration of OpenFoodTox data (#2574; #2576)
<b>84</b> - Toxic effects on livestock and pets	
<b>87</b> 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).
<b>89</b> Efficacy data	Minor changes on MO info (#2142)

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

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

## 6 EU\_PPP docs:

Name	IUCLID Backlog (#)
Endpoint_Study_Record_ <b>Magnitude of residues in pollen and bee products</b>	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. <b>ToxRefValues</b>	Changes linked to migration of OpenFoodTox data (#2574; #2576)
FLEXIBLE_SUMMARY. <b>ResiduesInLivestock</b>	Small fixes to report MATRIX, MRL at LOQ and fish studies (#2376; #2465; #2481)
ENDPOINT_SUMMARY. <b>StabilityResiduesCommodities</b>	Small fixes on picklists (#2464)
<b>Dossier header (MO)</b>	New fields to report submission info (requester, type; reason) (#2357; #2359; #2471)
 Flexible summary_ <b>IsomericCompositionRiskAssessment *</b>	#2583

## 4 CORE docs:

Name	IUCLID Backlog (#)
FLEXIBLE_RECORD. <b>AnalyticalInformation</b>	New field to upload study report/documents (#2223)
ENDPOINT_SUMMARY. <b>MetabolismInLivestock</b>	Updates to align with OHT 85-2/MetaPath (#2075)
ENDPOINT_SUMMARY. <b>AnalyticalProfileOfBatches</b>	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. <b>AnalyticalProfileOfBatches *</b>	Addition of "QC data" (#2489)

\* Docs not included in the PSN presentation on 22 Sep.

**Aim:** 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)
- 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.

- 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\_Biodegradation 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	<b>Picklist values:</b> <ul style="list-style-type: none"> <li>- abiotic control measured at end of test</li> <li>- biologically active treatment at end of test</li> <li>- natural water: freshwater</li> <li>- natural water: marine</li> <li>- natural water: brackish</li> <li>- natural water</li> <li>- water</li> <li>- natural water / sediment: freshwater</li> <li>- natural water / sediment: marine</li> <li>- natural water / sediment: brackish</li> <li>- natural water / sediment</li> <li>- natural sediment: freshwater</li> <li>- natural sediment: marine</li> <li>- natural sediment: brackish</li> <li>- natural sediment</li> <li>- artificial sediment</li> <li>- sediment</li> <li>- activated sludge</li> <li>- wastewater</li> <li>- anaerobic sludge</li> <li>- treated effluent: surface water mixing zone</li> <li>- untreated effluent: surface water mixing zone</li> <li>- entire system</li> <li>- other:</li> </ul>
94.	Parameter	List sup. (picklist with remarks)  Display: Basic	<b>Picklist values:</b> <ul style="list-style-type: none"> <li>- DT50</li> <li>- DT50 (normalised)</li> <li>- DT90</li> </ul>



- ✓ **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 LDD<sub>50</sub>; TRT-LDD<sub>50</sub>);
  - *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 to newly developed EU guidance document (SANTE/11956/2016rev.9) (#2147 #2468).



**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.

Line no.	Field name	Field type Display type	Picklist Free-text template	Help text	Remarks Guidance Cross-ref
1.	Administrative data	Header 1			
2.		Confidentiality Display: Basic			
3.	Endpoint	List sup. (picklist with remarks) Display: Basic	<b>Picklist values:</b> <ul style="list-style-type: none"> <li>- residues in honey</li> <li>- residues in pollen</li> <li>- <a href="#">residue in nectar</a></li> <li>- residues in other bee products</li> </ul>	From the picklist select the relevant endpoint addressed by this study summary. In some <a href="#">cases</a> there is only one endpoint title, which may be entered automatically depending on the software application.	

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

<a href="#">42.</a>	<a href="#">Study design</a>	<a href="#">Header 2</a>	
<a href="#">42.4.</a>	<a href="#">Study type</a>	<a href="#">List sup. (picklist with remarks)</a>	<ul style="list-style-type: none"> <li>-Syrup feeding tests</li> <li>-Tunnel trials</li> <li>-Field trials</li> <li>-Others (specify)</li> </ul>

<a href="#">47.</a>	<a href="#">Trial site</a>	<a href="#">Text (2,000 char.)</a>	
<a href="#">44.4.</a>	<a href="#">Duration of trial</a>	<a href="#">Numeric (decimal including unit)</a>	<a href="#">Picklist: value</a> h d m yr
<a href="#">49.</a>	<a href="#">Tunnel size/ Field size</a>	<a href="#">Numeric (decimal including unit)</a>	<a href="#">Picklist: value</a> m <sup>2</sup> 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):

Appendix 1							
Test#	Number	Application Method	Application Rate	Number of Applications	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

109. Treatment groups

Block of fields (repeatable) Start

110. Test no.

Text (255 char.)

Display: Basic

111. Number

Text (255 char.)

Display: Basic

112. PHI / PBI

Text (255 char.)

Display: Basic

113. Method of application

Text (255 char.)

Display: Basic

114. Rate(s) of application

Text (255 char.)

Display: Basic

115. Number of applications

Text (255 char.)

Display: Basic

Appendix 2					
ID	Common Name / Code	Chemical Name	SMILES	Parent(s)	
1	parent				
2	metabolite 1			1	
3	metabolite 2			2	
4	metabolite 3			2,3	

206. Identity of compound

Link to entity (single)

Display: Basic

207. Parent compound(s)

Link to entity (multiple)

Display: Basic

208. Treatment group (Test no.)

Link to repeatable entry

Display: Basic

- 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.

Appendix 3				
	Test #1	Test #2	Test #3	
parent	linked	linked		
metabolite 1	linked	linked		
metabolite 2	linked	linked		
metabolite 3	linked	linked		

# OHTs 85-4 (livestock feeding studies)

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

Endpoint	List sup. ( <a href="#">picklist</a> with remarks)  Display: Basic	<b>Picklist values:</b> - residues in livestock  <del>-residues in fish and fish products</del>
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- Picklist updates:

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

Matrix / tissue sampled	List sup. ( <a href="#">picklist</a> with remarks)  Display: Basic	<b>Picklist values:</b> - eggs - meat - milk - 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  <del>- Fish Fillet + skin</del>  <del>- Fish Liver</del>  <del>- Fish Carcass</del> - other:
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Guideline	List (picklist)  Display: Basic	<b>Picklist values:</b> - OECD Guideline 505 (Residues in 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  <del>- SANTE/10252/2021 (magnitude of residues in fish)</del> - other:
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- 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):

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

70	<u>Identity of compound</u>	<u>Link to entity (single)</u> <u>Display: Basic</u>		<p>Give the identity of the compound, <u>i.e.</u> either the test substance or any metabolite.</p> <p>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.</p> <p>Once stored in the Substances Inventory a reference substance can be re-used in the data set.</p> <p>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.</p>	<u>Cross-reference:</u> <u>REFERENCE. SUBSTAN</u> <u>CE</u>
71	<u>Parent compound(s)</u>	<u>Link to entity (multiple)</u> <u>Display: Basic</u>		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.	<u>Cross-reference:</u> <u>REFERENCE. SUBSTAN</u> <u>CE</u>
72	<u>Test conditions</u>	<u>List sup. (picklist with remarks - 2,000 char.)</u> <u>Display: Basic</u>	<u>Picklist values:</u> - baking, <del>brewing</del> 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.	

✓ 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

	Results and discussion	Header 1										
Recovery	Analyte	Matrix	MRM/ m/z	Fortification level (mg/kg)	Units	Number replicates	Range recovery (%)	Mean recovery (%)	RSDr (%)	Remarks	Recovery	
Data type:	Link to entity	Text	Numeric range	Decimal	Picklist	Integer	Numeric range	Decimal	Decimal	Text		
LOQ/LOD	Analyte	Matrix	Limit of quantification (mg/kg)	Limit of detection (mg/kg)	Units	Remarks	LOQ/LOD					
Data type:	Link to entity	Text	Decimal	Decimal	Picklist	Text						
Calibration	Analyte	Standards	Matrix	MRM/ m/z	Calibration range (mg/kg)	Units	Calibration equation	Correlation coefficient (r)	Calibration coefficient (r2)	Number of replicates	Remarks	Calibration
Data type:	Link to entity	Picklist multiple	Text	Numeric range	Numeric range	Picklist	Text	Decimal	Decimal	Integer	Text	

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

# OECD consultation – have your say!

**Sept – Oct 2022**

Launch of OECD  
consultation



OHTs

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

- At <https://community.oecd.org/docs/DOC-218941>
- **IUCLID team** ([iuclid6@echa.europa.eu](mailto:iuclid6@echa.europa.eu))

**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)

EU\_PPP

Comments to EFSA by **30 Oct**:

- [PSN Teams folder](#)