

12th meeting of the PSN IUCLID sub-group

11 - 12 Mar 2025

IUCLID REPORT GENERATOR USE FOR DOSSIER LIFECYCLE



OUTLINE

- IUCLID PPP Dossiers-Datasets: Terminology and Structure Overview
- Run Reports with Report Generator
 - HOW to run Reports
 - WHO should use them
 - WHEN to run Reports in Dossier lifecycle
 - WHICH Report to choose according to the stage (e.g., dossier admissibility)
 - WHY Reports should be used
- IUCLID Demo (GAP Report)



IUCLID PPP DOSSIERS - DATASETS: TERMINOLOGY AND STRUCTURE OVERVIEW

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DATASET-DOSSIER

- **Dataset*** a collection of documents that relate to a particular chemical substance, or grouping of chemical substances. It can be of type:



Substance



Mixture/Product

- **Dossier*** a read-only snapshot of a dataset. It contains a *Dossier header* that has a structure determined by the *working context*.

Datasets are editable. **Dossiers** are read-only.

In IUCLID EFSA Agency instance, MS have access to **Dossiers**.



GENERALIZED EU PPP DOSSIER STRUCTURE

In **EU PPP** *working contexts* **Dossiers** consist of:*

 One or many Mixture **Datasets**

with

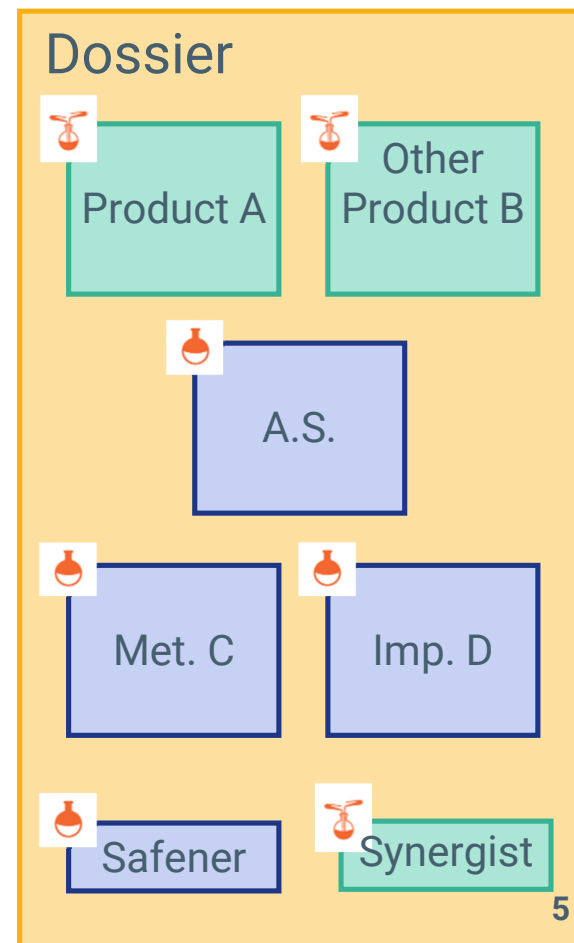
 One and only one Active Substance **Dataset**

plus (where applicable)

 One or many Metabolites and/or Impurities **Datasets**

plus (technically possible but not fully operational)

  One or many Co-Formulants, Safeners and Synergists **Datasets**



PRODUCT AND ACTIVE SUBSTANCE DATASETS

Product Dataset

Product Table of Contents (ToC)*

Representative product BC 1 (LoE/PhysChem)
08da4a8c-0c82-4a63-aca3-93ac951efea3

Type at least 3 characters X

EU PPP Active substance application (product)

Representative product BC 1 (LoE/PhysChem)

- 1 Identity of the plant protection product and applicant 7
 - 1.1 Identity of the plant protection product, trade name or proposed trade name, and applicant 1
 - 1.2 Producer of the plant protection product 2
 - 1.3 Producer's development code number if appropriate
 - 1.4 Detailed quantitative and qualitative information on the composition of the plant protection product 4
- 2023_Detailed quantitative and qualitative information on the composition of the representative plant protection product

Active substance BC (LoE/PhysChem)

UUID: 08da4a8c-0c82-4a63-aca3-93ac951efea3

Other identifiers

Confidential

Contact persons

Mixture/Product name*
Representative product BC 1
Public name

Legal entity owner
EFSA IUCLID demo | Parm
Third party

Representative product BC 200 EC (LoE/PhysChem)

Active substance BC (LoE/PhysChem)

- 1 Identity of the active substance and applicant 21
- 2 Physical and chemical properties of the active substance 38
- 3 Further information on the active substance 8
- 4 Analytical methods 22
- 5 Toxicological and metabolism studies on the active substance 81
- 6 Residues in or on treated products, food and feed 44
- 7 Fate and behaviour in the environment 30
- 8 Ecotoxicological studies on the active substance 49
- 9 Literature data and change log 13
- 10 Classification and labelling of the active substance 3
- 11 Summary and evaluation 7

Inherited templates

Active Substance (A.S.) Dataset

Active Substance ToC*



MAIN ELEMENTS WITHIN A PPP DOSSIER-DATASET

Dossier Header

 EU PPP Active substance application (product)

Metabolite Dataset(s)

1.4.4 Information on metabolites 1

Information on metabolites.001

Active substance BC (LoE/PhysChem)

Metabolite 2 >>

EFSA Tender: Metabolite 1

Impurity Dataset(s)

1.4.6 Impurities 1

Impurities.001

Active substance BC (LoE/PhysChem)

Impurity B >>

Other Product Dataset(s)

1.4.5 Other representative products 1

Other representative products.001

Other representative product (LoE/PhysChem) >>

ToC Sections

7 Toxicological studies on the plant protection product 14

7.1 Acute toxicity 10

2023_Summary_Acute Toxicity

7.1.1 Oral toxicity 1

1989_Oral toxicity_01

Documents*

ENDPOINT_Summary

ENDPOINT_Study_Record

1989_Oral toxicity_01

UUID: cc503573-9200-4da6-8cbd-7731b4078a3e

EU: PPP

Administrative data Data source Material: 2

Results and discussion

Preliminary study
Not applicable.

Effect levels + New item Import file

Key result	Sex	Dose descriptor	Effect level	Based on
1 <input checked="" type="checkbox"/>	male/female	LD50	> 2000 mg/kg bw	test mat.



RUN REPORTS WITH REPORT GENERATOR (RG) - HOW

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RG TOOL – HOW TO ACCESS IT

The screenshot shows the RG Tool interface for a dossier titled "Representative product BC 1 (LoE/PhysChem)" with UUID: 08da4a8c-0c82-4a63-aca3-93ac951efea3. The left sidebar contains a tree view with the following items:

- EU PPP Active substance application (product)
- Representative product BC 1 (LoE/PhysChem) (selected)
- 1 Identity of the plant protection product and applicant (7)
 - 1.1 Identity of the plant protection product, trade name or proposed trade name, and applicant (1)
 - 1.2 Producer of the plant protection product (2)
 - 1.3 Producer's development code number if appropriate
 - 1.4 Detailed quantitative and qualitative information on the composition of the plant protection product (4)
- 2023_Detailed quantitative and qualitative information on the composition of the representative plant protection product
- Active substance BC (LoE/PhysChem) (highlighted with a green box)

The main content area displays the following information:

- UUID: 08da4a8c-0c82-4a63-aca3-93
- Other identifiers
- Contact persons
- Mixture/Product name*
Representative product BC 1
- Public name
- Legal entity owner
EFSA IUCLID demo | Parm
- Third party
- Other identifiers + New
- Confidential
- Contact persons + New

The screenshot shows the RG Tool interface with the "Generate report" dropdown menu open. The menu options are:

- Export to i6z
- Create PDF/RTF
- Generate report (highlighted with a green box)
- Compare
- Clone
- Copy data from ...
- Bulk operations

Below the menu, there is a search bar and a "Please select" dropdown. The "Default IUCLID reports" section shows two RTF files. The "Uploaded IUCLID reports" section shows one RTF file.

A green box highlights the "Generate report" option in the dropdown menu, and a green arrow points from this box to the "RTF" option in the "Please select" dropdown menu.



HOW TO RUN REPORTS FOR OTHER REPR. PRODUCTS

IUCLID USER INTERFACE

EU PPP Active substance application (product)

Representative product BC 200 EC (LoE/PhysChem)

1 Identity of the plant protection product and applicant 7

> 1.1 Identity of the plant protection product, trade name or proposed trade name, and applicant 1

> 1.2 Producer of the plant protection product 2

1.3 Producer's development code number if appropriate

> 1.4 Detailed quantitative and qualitative information on the composition of the plant protection product 4

> 2023_Detailed quantitative and qualitative information on the composition of the representative plant protection product

1.4.1 (Cf. 1.4) Composition of the plant protection product

1.4.2 (Cf. 1.4) Information on the active substances

1.4.3 (Cf. 1.4) Information on safeners, synergists and co-formulants

> 1.4.4 Information on metabolites 1

> 1.4.5 Other representative products 1

> Other representative products.001

Other representative product (LoE/PhysChem)

MIXTURE Document

UUID: 540600f8-15ff-444d-95ce-7dafb89326dc

Other identifiers Contact persons Role in the supply chain

Mixture/Product name*
Other representative product (LoE/PhysChem)
Public name
Legal entity owner
Third party

Other identifiers + New item Import file

Confidential	Name type	Name	Country	Role
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Contact persons + New item Import file

Role in the supply chain

☐ Manufacturer
☐ Importer
☐ Only representative
☐ Downstream user

View Dossiers

Validate

Create dossier



Compare Document



Generate sub entity report

Important Note: sub-entity report generation is required with **Dossiers** and it is needed to generate reports for other representative Products datasets.

RUN REPORTS WITH REPORT GENERATOR (RG) – WHO, WHEN, WHICH, WHY

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RUN REPORTS WITH RG – WHO AND WHEN

Report Generator should be used as much as possible during the entire Dossier lifecycle and in support to the DAR/RAR preparation:

- a) To check if IUCLID Datasets are complete during compilation (**Applicant**).
- b) To check if IUCLID Dossiers information is complete and consistent during admissibility (**RMS**) – a dossier update might be needed before proceeding to the next steps.
- c) Use all available reports in RG to prepare DAR/RAR (**RMS**): this will ensure consistency of information among the Assessment Report and the IUCLID Dossier.



RUN REPORTS WITH RG – WHICH

The below reports (at least) are recommended to be used during the admissibility check and in the preparation of the DAR/RAR:

- **GAP Table** (mandatory) – new GAP mapping file will be published in Zenodo in May 2025 following next IUCLID release. A video demonstration on how to use this report will be presented in the final slide.
- **List of Substances and Metabolites** – fill in the “Remarks” field to populate the column “Compound found in” in the report (see next slides).
- **Table of Analytical Methods** – use the cross-reference function to ensure a method is included in the report (see next slides).

Refer to Agenda item 6_“*IUCLID report generator updates*” to check the status of other reports.



RUN REPORTS WITH RG – LIST OF SUBSTANCES AND METABOLITES

IUCLID METABOLITES DOCUMENT

1.4.4 Information on metabolites 1

> Information on metabolites

1.4.5 Other representative products 1

1.4.6 Impurities

1.5 (Cf. 1.4) Type and code of the plant protection product

1.6 (Cf. 2.2) Function

Metabolites

+ New item

Import file

Link to metabolite dataset

1

EFSA Tender: Metabolite 1 | Metabolite_example 1 | IUPAC name | 147-965

Remarks

Where found: soil

IUCLID

REF.SUBSTANCE

Reference substance name*
Metabolite_example 1

IUPAC name
IUPAC name

Description
Dummy metabolite

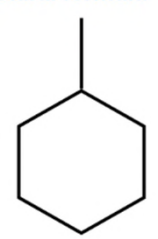
CAS number
147-965

SMILES notation
SMILES

InChI
InChI

InChIKey
InChIKey

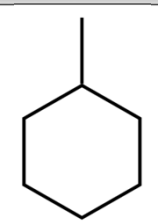
Structural formula



Report

1. Substances and metabolites: structures, codes, synonyms

Table 1.1.

Name and CAS number	IUPAC name, SMILES, InChI	Structural formula	Compound found in
EFSA Tender: Metabolite 1 (ref.: Metabolite_example 1) 147-965	IUPAC name SMILES InChI		Where found: soil



RUN REPORTS WITH RG – TABLE OF ANALYTICAL METHODS

2023_Physical and chemical properties of the active substance

- 2.1 Melting point and boiling point 5
- > 2.1.1 Melting point 2
- > 2.1.2 Boiling point 3
- > 2023_Boiling point
- > 2023_Boiling point
- Boiling point_Waiver
- 2.2 Vapour pressure, volatility 4
- 2.3 Appearance (physical state) 0

2023_Boiling point IUCLID ENDPOINT_STUDY_RECORD

UUID: e2f772eb-9e3c-40a0-8bd5-e3c734b38ad6

EU: PPP

Administrative data
Data source
Materials and met...
Results and discu...
Over

Cross-reference
+ New item
Import file

	Reason / purpose for cross-reference	Related information
1	method used in study *	RA_physchem2 1 (reliable without restriction)
2	method used in study *	RA_physchem

Analytical (primary) method

Instrument / detector

✓ HPLC-DAD

Residue method

multi analyte

Analytical (primary) method

Instrument / detector

✓ GC-MS/MS

1. Table of Analytical Methods (Appendix D)

Report

Table 1.1. Analytical Methods

#	IUCLID section	Author, date	Study title	Analytical method Author, date, No.	Technique, residue method, LOQ of the method, validated working range	Method meets analytical validation criteria	Remarks	Acceptability of the method
1	2.1.2 Boiling point	Author, 2023	Technical BC: physical and chemical characteristics	1. Me M., 2021, Analytical method physchem 2 2. Serafimova R., 2021, Analytical method physchem1	1. Primary: • Instrument: HPLC-DAD • Residue method: multi analyte • LOQ: ISO name active substance BC = 0.07 mg/kg 2. Primary: • Instrument: GC-MS/MS • LOQ: ISO name active substance BC = 0.01 mg/kg	1. not specified 2. yes	1. unclear	1. 1 (reliable without restriction)



RUN REPORTS WITH RG – WHY

- **RMS** is reminded to ensure alignment among the information which will be included in the DAR/RAR and the information contained in the IUCLID dossier. The DAR/RAR preparation should start from all available reports. Therefore, we recommend to make full use of the IUCLID Report Generator functionality.
- **EFSA** will ensure alignment among the DAR/RAR and the IUCLID dossier before entering the peer-view phase.



Missing info in this GAP example

- MS/Country codes (therefore assumed to be all EU)
- Crop location according to EPPO codes (F/G/I)
- Formulation Type
- Re-treatment interval in days (min-max)
- Concentration a.s. in dilution (min-max)
- Pre-Harvest Interval in days

