EFSA IUCLID pilot on Pesticides dossiers

Report generator

ECHA EUROPEAN CHEMICALS AGENCY

OECD

IUCLID 6 is developed by the European Chemicals Agency in association with the OECD

Introduction to the report generator

Report Generator

What is the IUCLID **Report Generator** engine

The report generator engine supports the extraction and conversion of IUCLID data into a standalone format:

- RTF
- PDF
- **CSV***
- **XML***
- HTML

***(also) used as machine-readable formats

Report Generator

Visualising the generated formats

RTF/PDF

XML

HTML

CSV

Table of Contents

PART A .....
1. SUMMARY OF RISK MANAGEM
2. DECLARATION THAT RISK MA
3. DECLARATION THAT RISK MA
PART B .....
1. IDENTITY OF THE SUBSTANCE
1.1. Name and other identifiers o
1.2. Composition of the substanc
1.3. Physicochemical properties ..
2. MANUFACTURE AND USES .....
2.1. Manufacture .....
2.2. Identified uses .....
3. CLASSIFICATION AND LABELL
3.1. Classification and labelling according to CLP / GHS 21
4. ENVIRONMENTAL FATE PROPERTIES 24
4.1. Degradation 24
4.1.1. Abiotic degradation 24
4.1.1.1. Hydrolysis 24
4.1.1.2. Phototransformation/photolysis 24
4.1.1.2.1. Phototransformation in air 24
4.1.1.2.2. Phototransformation in water 24
4.1.1.2.3. Phototransformation in soil 25
4.1.2. Biodegradation .....
4.1.2.1. Biodegradation in water .....
4.1.2.1.1. Screening tests .....
4.1.2.1.2. Simulation tests (water and sedime
4.1.2.1.3. Summary and discussion of biodegradation in water and sediment. 26
4.1.2.2. Biodegr
4.1.3. Summary and dis
4.2. Environmental distributio
4.2.1. Adsorption/deson
4.2.2. Volatilisation .....
4.2.3. Distribution mod
4.2.4. Summary and dis
4.3. Bioaccumulation.....
4.3.1. Aquatic bioaccun
4.3.2. Terrestrial bioacc

<?xml version="1.0" encoding="UTF-8" standalone="true"?>
<!-- SPC main template file -->
<ns4:SPC xml:lang="en" xmlns:ns4="http://echa.europa.eu/schema/spc/1.0/" xmlns:ns3="http://www.w3.org/1999/xhtml" xmlns:ns2="
<!-- Macros -->
<!-- Functions -->
<ns4:lang>
<representation>en</representation>
</ns4:lang>
<!-- ProductInfo -->
<ns4:ProductInfo>
<ns4:FormulationType code="[illegible]">[illegible]</ns4:FormulationType>
<ns4:Composition xsi:type="ns4:ProductCompositionType" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
<ns4:ActiveSubstance>
<ns4:Concentration>
<ns4:Value>95</ns4:Value>
</ns4:Concentration>
</ns4:ActiveSubstance>
<ns4:OtherSubstance>
<ns4:CommonName>coumarin</ns4:CommonName>
<ns4:C[illegible]
<ns4:I[illegible]/ns4:IUPACName>
<ns4:EC>[illegible]/ns4:EC>
<ns4:Con[illegible]
<ns4:[illegible]s4:Value>
</ns4:Concentration>
</ns4:OtherSubstance>
</ns4:Composition>
</ns4:ProductInfo>
<!-- CNLInfo -->

Study information: My Substance YuP

Search..

FILTER AND SEARCH ANY TEXT HERE

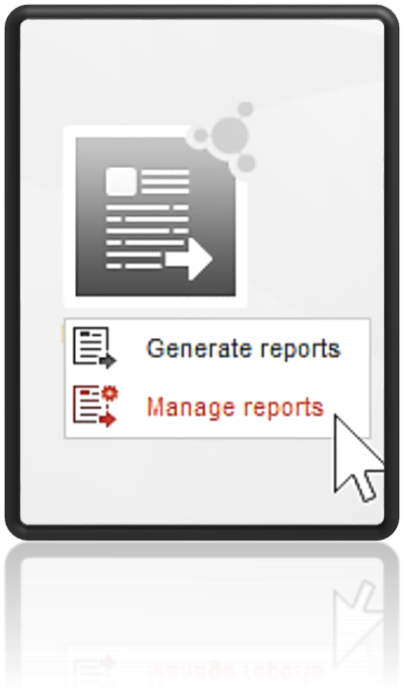
Type of Entity and name	Document name and UUID	Confidentiality claim on endpoint	Robust s
Substance Appearance/physical state/colour	arance / physical state / colour.001 c7260[illegible]-04a4-4403-81e0-191a53610e79	endpoint is not flagged confidential	yes
Substance Appearance/physical state/colour	Appearance / physical state / colour.001 c7260a75-04a4-4403-81e0-191a53610e79	endpoint is not flagged confidential	yes

HIDE IRRELEVANT COLUMNS BY CLICKING ON THE EYE (TO RESTORE HIDDEN COLUMNS, JUST REFRESH THE WEBPAGE)

	A	B	C	D	E	F	G	H	I	J	K	L	M
1	Annex II ar	Section number	Section name	Document name	Link to doc	Document UUID	Name of bi	Function o	Attachmen	Attachmen	Attachmen	Attachment size	
2	Trade nam	2.1	Trade name or	Test mixture for repo	http://local	f24f0b26-cbe4-4e76-87ae-b128e1f2	Test mixtur	Biocidal Pr	java_certificates.txt		text/plain	142500	
3	Trade nam	2.1	Trade name or	Test mixture for repo	http://local	f24f0b26-cbe4-4e76-87ae-b128e1f2	Test mixtur	Biocidal Pr	Untitled.epio		application	8536	
4	Biocidal pr	1.3	Biocidal produc	Biocidal product man	http://local	890a5cdc-1b18-4a4e-9a84-e88618f(	Test mixtur	Biocidal Pr	Untitled.ep	untitled	application	8536	
5	Biocidal pr	1.3	Biocidal produc	Biocidal product man	http://local	890a5cdc-1b18-4a4e-9a84-e88618f(	Test mixtur	Biocidal Pr	java_certifi	remarks att	text/plain	142500	
6	Location of	1.3.1	Sites	Location of manufact	http://local	03ec4cdb-c170-41ac-87f9-5b2957e8	Test mixtur	Biocidal Pr	Untitled.epio	p	application	8536	
7	Location of	1.3.1	Sites	Location of manufact	http://local	03ec4cdb-c170-41ac-87f9-5b2957e8	Test mixtur	Biocidal Pr	java_certifi	iop	text/plain	142500	
8	Location of	1.3.1	Sites	Location of manufact	http://local	de3fcfce-b836-480b-af3d-d45e9042	Test mixtur	Biocidal Pr	Untitled.epgz		application	8536	
9	Manufactu	2.2	Manufacturer's	Manufacturer's devel	http://local	57d5b0ef-7478-4b9b-b187-33ff623(	Test mixtur	Biocidal Pr	java_certificates.txt		text/plain	142500	
10	Biocidal pr	2.3	Biocidal produc	Biocidal product com	http://local	db19887a-bd63-4dbf-a699-6a91021	Test mixtur	Biocidal Pr	java_certifi	yjkdsue	text/plain	142500	
11	No BPR ani	No section number	Biocidal produc	Biocidal product fami	http://local	5d264838-2cf8-488e-a674-c99e0ed	Test mixtur	Biocidal Pr	6.2-to-6.3_migration_(		text/plain	330	
12	No BPR ani	No section number	Biocidal produc	Biocidal product fami	http://local	8a84444d-20d4-4afe-b166-c0a44d8	Test mixtur	Biocidal Pr	6.2-to-6.3_migration_(		text/plain	330	
13	PHYSICAL C	3	Physical chemic	Physical and chemica	http://local	6b7970c4-faad-4d18-aafb-828e647	Test mixtur	Biocidal Pr	Untitled.epgz		application	8536	
14	Appearanc	3.1	Appearance (at	Appearance (at 20Â°(	http://local	5aaaebef-6f9e-4f59-a63c-b2e8a7d5	Test mixtur	Biocidal Pr	java_certifi	rgebebehrh	text/plain	142500	

Report Generator

What is the **Report Generator**



Out-of-the-box feature

- Contains a number of pre-built-in report templates made and added for REACH/Biocides/PCN users

IUCLID users can re-use any existing reports

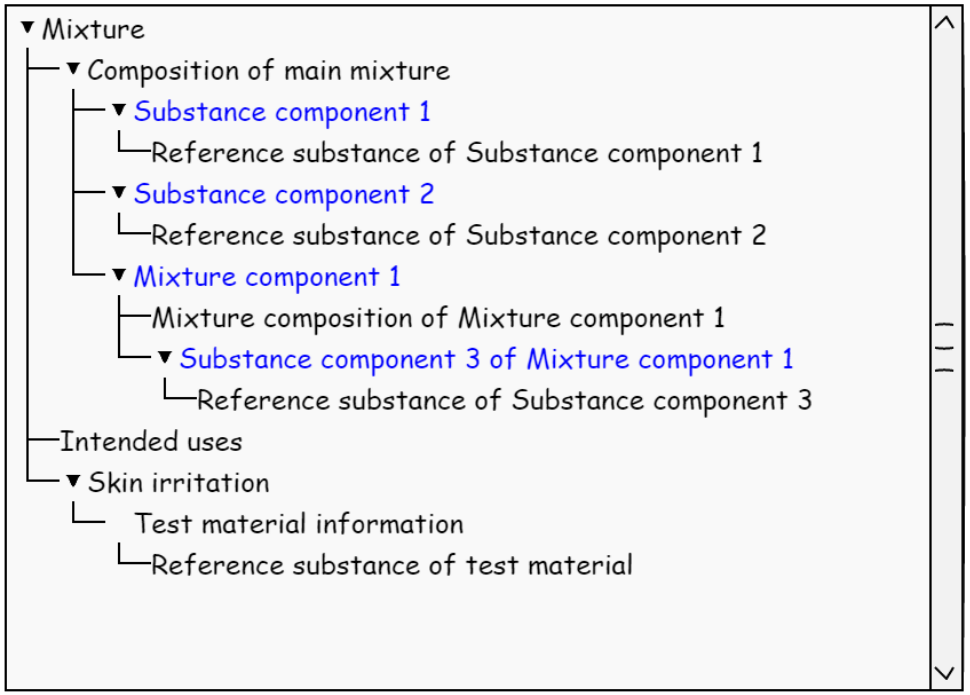
As a configurable extension

- IUCLID allows you to write and upload your own report templates. More info on the IUCLID website: https://iuclid6.echa.europa.eu/reports

IUCLID users can customise their own reports

Report Generator

Data extraction in the IUCLID data model



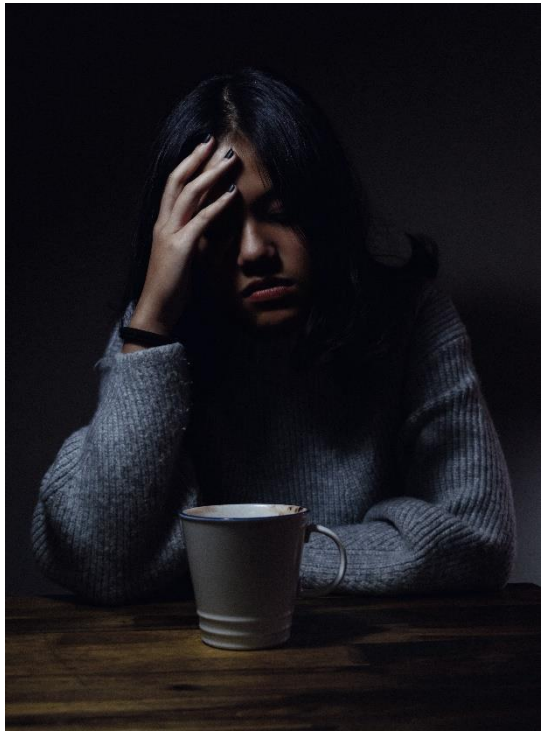
What can be extracted using a report template?

- Root entity (mixture/substance)
  - All IUCLID documents under the root entity
  - All linked complex entities referenced in a IUCLID document (e.g. substance referenced in a mixture composition document)
  - All linked entities referenced in a IUCLID document (e.g. reference substances / test materials / contacts etc)

Report Generator

Report template writing

Non-IT professionals may need help, but they get there in the end



https://iuclid6.echa.europa.eu/reports

Report Generator

Freemarker is at the core of report template writing

- **PDF/RTF** Generation
  - Use **Freemarker** + Docbook langauges
- **CSV** Generation
  - Use **Freemarker** language (plus comma-separation)
- **HTML** Generation
  - Use **Freemarker** + HTML/CSS languages
- **XML** Generation
  - Use **Freemarker** + xml namespaces

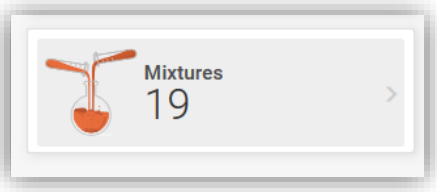
```
<book version="5.0" xmlns="http://docbook.org/ns/docbook" xmlns:xi="http://www.w3.org/2001/XInclude">

    <#assign substance = _subject />
    <#assign mixture = _subject />

    <info>
        <title>Annotations Report</title>
        <cover>
            <para>
            <para><@com.emptyLine/></para>
                <#if com.getReportSubject(rootDocument).documentType=="MIXTURE">
                    <para>
                        <emphasis role="bold"><phrase role="green">Product name: </phrase></emphasis>
                        <#assign docUrl=iuclid.webUrl.entityView(mixture.documentKey)/>
                        <#if docUrl?has_content>
                            <ulink url="${docUrl}"><@com.text mixture.MixtureName/></ulink>
                                <#else>
                            <@com.text mixture.MixtureName/>
                        </#if>
                    </para>
                </#if>
```

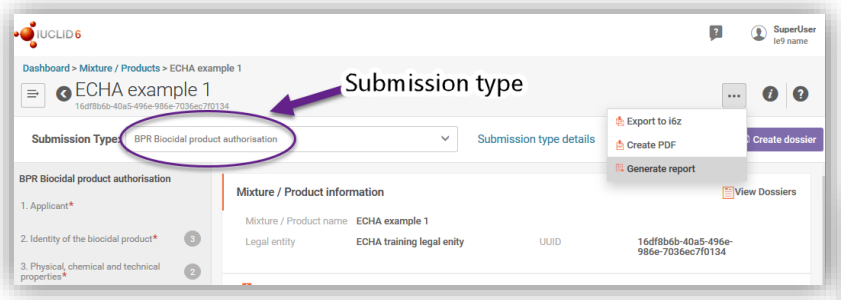
Freemarker:
https://freemarker.apache.org/

Report Generator

How to generate a report in the web interface

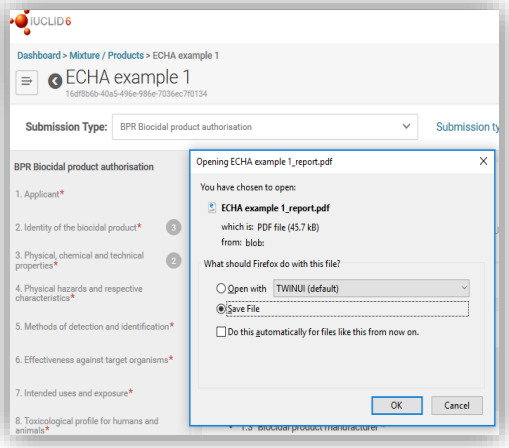
Go into your mixture or substance dataset or dossier





Select ‘Generate report’ from the menu

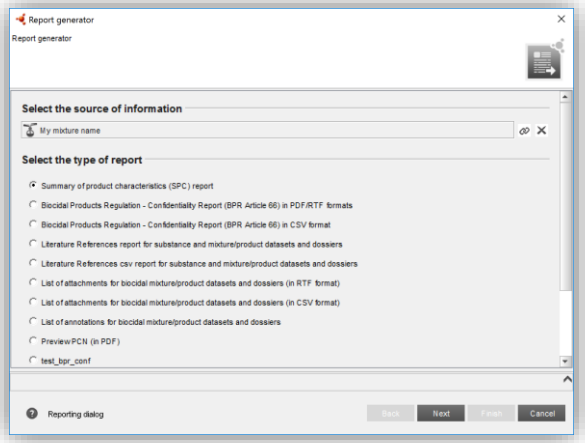
Save or open the file directly (*Note that different web browsers have different ways of saving/opening files)



Report Generator

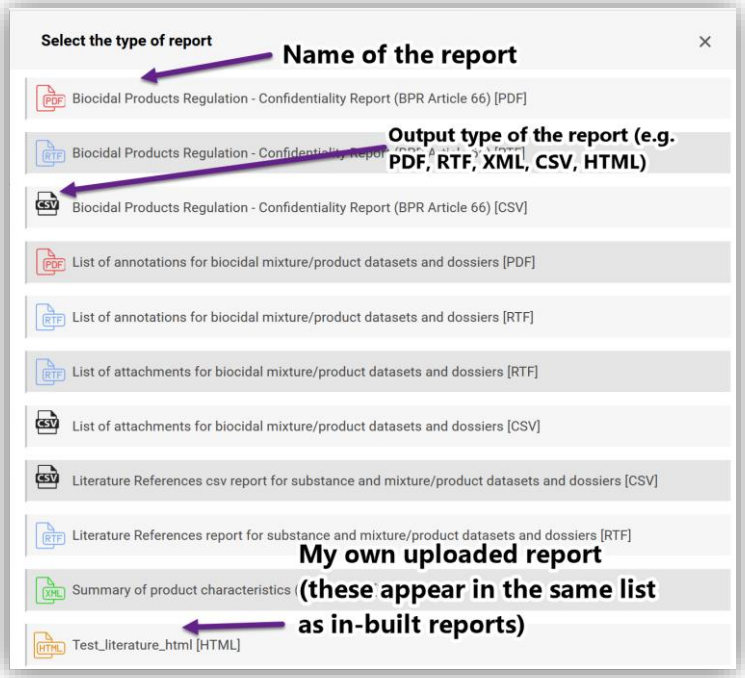
List of pre-built-in reports

Classic interface



Reports are progressively added to the list, and updated to the latest format

Web interface (April 2019 release)



What reports are seen by the user depend on the:

root entity or entities which they are valid for and …

the submission type(s) they are associated to

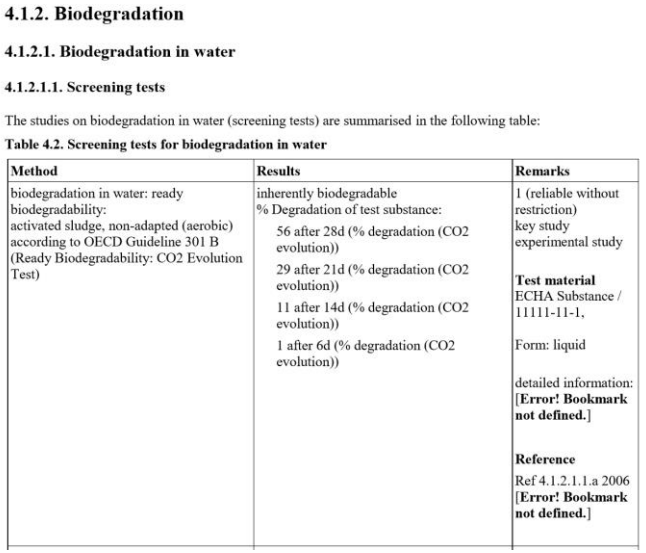
Report Generator

Substance-based reports

- Chemical safety report* (RTF/PDF/XML)
- Attachments report (RTF)
- Literature references report (RTF)
- Uses report (Dow Chemicals) (CSV, to automate population of use data in SAP system)
- C&L report for lead registrations under REACH (PDF)

*A chemical safety report (**CSR**) is required for all substances subject to registration in quantities of 10 tonnes a year

The CSR documents the chemical safety assessment performed as part of the REACH registration process.



4.1.2. Biodegradation

4.1.2.1. Biodegradation in water

4.1.2.1.1. Screening tests

The studies on biodegradation in water (screening tests) are summarised in the following table:

Table 4.2. Screening tests for biodegradation in water

Method	Results	Remarks
biodegradation in water: ready biodegradability: activated sludge, non-adapted (aerobic) according to OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test)	inherently biodegradable % Degradation of test substance: 56 after 28d (% degradation (CO2 evolution)) 29 after 21d (% degradation (CO2 evolution)) 11 after 14d (% degradation (CO2 evolution)) 1 after 6d (% degradation (CO2 evolution))	1 (reliable without restriction) key study experimental study **Test material** ECHA Substance / 11111-11-1, Form: liquid detailed information: **[Error! Bookmark not defined.]** **Reference** Ref 4.1.2.1.1.a 2006 **[Error! Bookmark not defined.]**

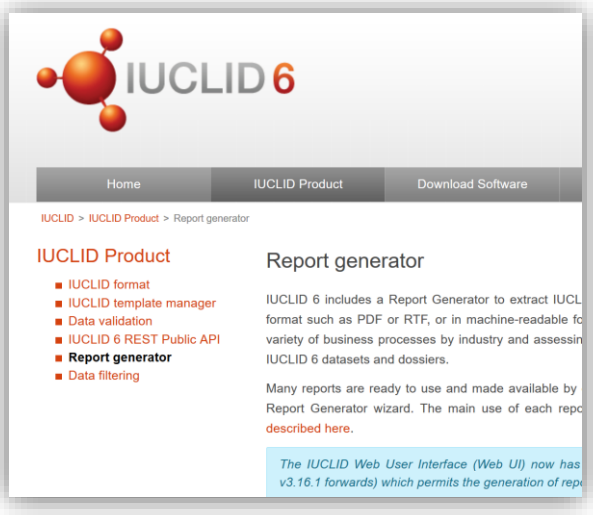
Report Generator

Reports relevant to Biocides' users

For Biocides users, the key reports are:

- *EU Biocidal Products Regulation (BPR)* ***Confidentiality Report***
- ***Literature References report*** *for substance and mixture/product datasets and dossiers*
- *EU Biocidal Products Regulation (BPR)* ***List of Attachments*** *for mixture/product datasets and dossiers*
- *EU Biocidal Products Regulation (BPR)* ***Table of Annotations***
- *EU Biocidal Products Regulation (BPR)* ***Cross References report***
- EU Biocidal Products Regulation (BPR) ***Summary of Product Characteristics*** (SPC)

Go to the Report generator webpage for a description of the main uses of the reports

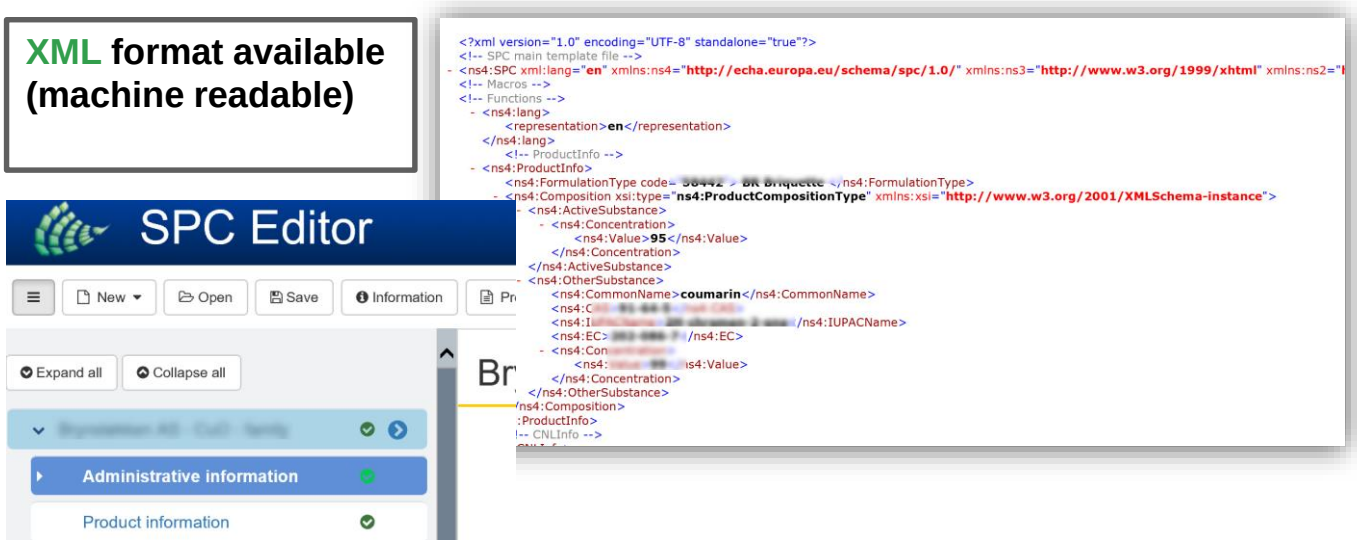


Report Generator

Reports for Biocides users'

The report extracts SPC-related information for single products from IUCLID, which can then be imported and transferred directly into the SPC Editor.

XML format available (machine readable)

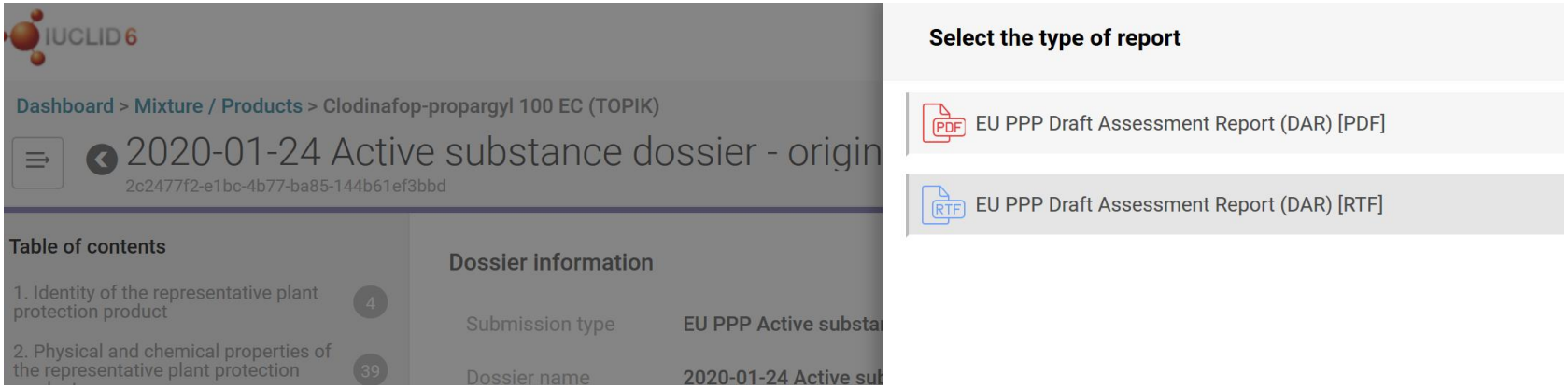


Report generator applied to the Proof of Concept pesticide dossier

Reports relevant to pesticides

Draft Assessment Report prototype

- Prototype built for pesticides
- Can be triggered from the web interface



Reports relevant to pesticides

Draft Assessment Report (DAR) prototype

- The DAR prototype was created as a combination of the DAR template and sections of information previously extracted for the Chemical Safety Report under REACH

European Commission

Draft Assessment Report prepared according to the Commission Regulation (EU) N° 1107/2009

CLODINAFOP-PROPARGYL

1.3. Identity of the active substance

Table 1.1. Active substance identity

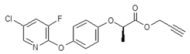
CAS number	105512-06-9
IUPAC name	(R)-2-[4-(5-chloro-3-fluoro-pyridin-2-yloxy)-phenoxy]-p prop-2-ynyl ester
Synonyms	common name: clodinafop-propargyl
Molecular formula	C17H13ClFNO4
Molecular weight range	349.8
Structural formula	**Figure 1.1. a.s.png** 
Remarks on molecular structure	SMILES notation and InChi newly created - the original include this information

Table 1.2. Composition of the Active Substance (DUMMY example: General specification

2.5.8.1.1. Carcinogenicity: oral

The results of studies on carcinogenicity after oral administration are summarised in the following table:

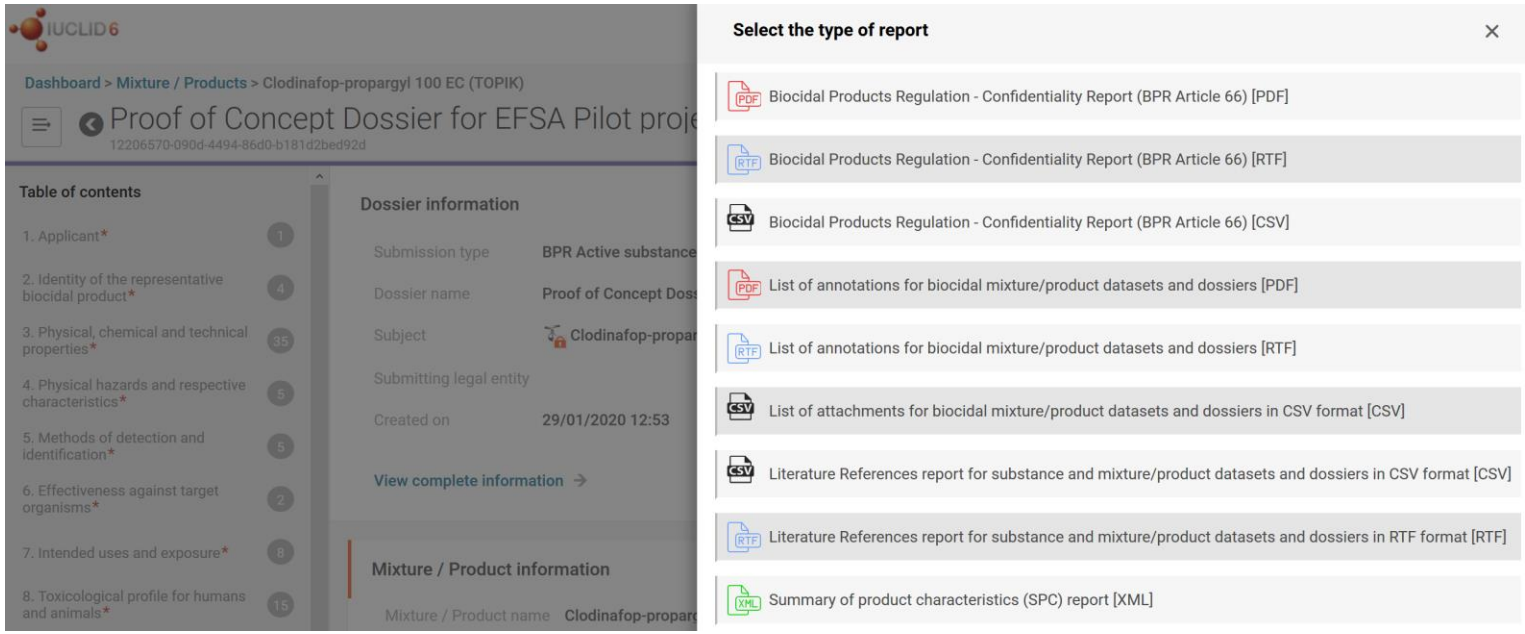
Table 2.13. Studies on carcinogenicity after oral administration

Method	Results	Remarks
mouse (Tif:MAGf [mouse]) male/female (oral: feed) 1ppm nominal: m: 0.115 mg/kg bw/day f: 0.132 mg/kg bw/day actual: m: 0.113 mg/kg bw/day f: 0.129 mg/kg bw/day 10ppm nominal: m: 1.141 mg/kg bw/day f: 1.291 mg/kg bw/day actual: m: 1.101 mg/kg bw/day f: 1.246 mg/kg bw/day 100ppm nominal: m: 11.15 mg/kg bw/day f: 12.84 mg/kg bw/day actual: m: 10.97 mg/kg bw/day f: 12.63 mg/kg bw/day 250ppm nominal: m: 29.32 mg/kg bw/day f: 32.72 mg/kg bw/day actual: m: 29.61 mg/kg bw/day f: 33.05 mg/kg bw/day	NOAEL: 10 ppm (male) based on: (test mat.) based on liver findings (1.1 mg/kg bw/day) NOAEL: 10 ppm (female) based on: (test mat.) based on liver findings (1.25 mg/lg bw/day) LEL: 100 ppm (male) based on: (test mat.) liver (11 mg/kg bw/day)	1 (reliable without restriction) key study experimental study **Test material** clodinafop_3, Form: solid: particulate/powder (full information in **Annex II**). **Reference** **Fankhauser, H. (1992a) (summary)**

Reports relevant to pesticides

Other reports available

- For the purpose of this pilot exercise, we have identified other potentially relevant reports built for Biocides
- The Pesticides PoC dossier has been converted into a Biocide active substance dossier, and uploaded in the Cloud instance
- Reports developed for biocides can then be experimented



Reports relevant to pesticides

List of attachments

- Available in .csv format
- Information covered
  - Annex II and Annex III requirements
  - Section number
  - Section name
  - Document name
  - Document UUID
  - Name of biocidal product or component
  - Function of component
  - Attachment filename
  - Attachment remarks
  - Attachment media type
  - Attachment size

Annex II and Annex III requiremen	Sectio	Section name	Document name	Document UUID	Nam
Measures to protect humans animals a	11	Measures to prot	4.1 Safety intervals	e9ad6502-4802-42	Clo
Measures to protect humans animals a	11	Measures to prot	4.1 Safety intervals	e9ad6502-4802-42	Clo
Measures to protect humans animals a	11	Measures to prot	4.1 Safety intervals	e9ad6502-4802-42	Clo
Measures to protect humans animals a	11	Measures to prot	4.1 Safety intervals	e9ad6502-4802-42	Clo
Appearance (at 20Â°C and 101.3 kPa)	3.1	Appearance / phy	Gerhardt P. (1999)	ff7b78e9-4015-414	Clo
Acidity alkalinity	3.2	pH	Gerhardt P. (1999)	aff5cda0-cd17-490	Clo
Relative density (liquids) and bulk tap	3.3	Density	Schneider B.(1999)	243eb4fb-bb27-4e	Clo
Relative density (liquids) and bulk tap	3.3	Density	Schneider B. (1999)	f1b6fa3f-920e-49b	Clo
Relative density (liquids) and bulk tap	3.3	Density	Vaille C.(1997)	c7b98014-9eeb-4a	Clo
Storage stability tests	3.4.1	Storage stability a	Vaille C. (1997)_acc	70a4ca58-5ac5-46	Clo
Storage stability tests	3.4.1	Storage stability a	Gerhardt P. (2000)_	97d5c02a-3d32-4c	Clo
Storage stability tests	3.4.1	Storage stability a	Wochner F. (2001a)	f3271b6b-8e6c-4c	Clo
Storage stability tests	3.4.1	Storage stability a	Wochner F.(2001b)	8ad27560-9294-44	Clo
Storage stability tests	3.4.1	Storage stability a	Wochner F. (2001c)	433f4f13-546b-4b	Clo

Reports relevant to pesticides

List of studies (and references)

- Available as .CSV and .RTF
- More fields covered in the .CSV report

Table 1.1. Literature References generated from a Mixture/Product (including Literature References in any linked Substance)

Author(s)	Year and Report date	Annex II/III requirements and IUCLID section	IUCLID document name	Title and Report number	Type of publication	Source (where different from company) and Study sponsor	GLP	Data Protection Claimed (Yes/No)
Author: Gerhardt P.	Year: 1999	**Annex II/III requirement:** Appearance (at 20°C and 101.3 kPa) **IUCLID Section No.** 3.1	IUCLID Document name: Gerhardt P. (1999) (summary)	Title: Technical characteristics of A7957C Report no. 78861	Type of publication: study report	Company Owner: Novartis Crop Protection AG	yes	No
Author: Gerhardt P.	Year: 1999	**Annex II/III requirement:** Acidity, alkalinity **IUCLID Section No.** 3.2	IUCLID Document name: Gerhardt P. (1999) (summary)	Title: Physico-chemical characteristicsof A7957C Report no. 78860	Type of publication: study report	Company Owner: Novartis Crop Protection AG	yes	No
Author: Schneider B.	Year: 1999	**Annex II/III requirement:** Relative density (liquids) and bulk, tap density (solids) **IUCLID Section No.** 3.3	IUCLID Document name: Schneider B.(1999) (summary)	Title: Chemical Composition of A7959C Report no. 78122	Type of publication: study report	Company Owner: Novartis Crop Protection AG	yes	No
Author: Vaille C.	Year: 1997	**Annex II/III requirement:** Storage stability	IUCLID Document name: Vaille C.	Title: A-7957 C: Report on physico-chemical	Type of publication: study report	Company Owner: Novartis Agro S.A.	yes	No

Reports relevant to pesticides

List of studies (and references)

- More fields covered in the .CSV report

Type
Section number
Section name
Document name
Document UUID
Robust study summary
Adequacy of study
Study period
Data waiving
Data waiving justification
Type of information
Reliability
Data access
Guideline (materials and methods)
GLP compliant
Test material information
name (and CAS number of test material)
Species / test organism
Strain / cell type
Route of application / dose method
Exposure duration
Metabolic activation
Metabolic activation system
Study outcome (dose descriptor)
Study outcome (value/result)
Reference type
Title
Author
Bibliographic source
Year
Testing Laboratory
Report number
Company owner
Company study number
Report date
Remarks
Confidentiality claim on endpoint
Regulatory programme(s)

Reports relevant to pesticides

List of annotations

- Currently available in .PDF and .RTF format

1. Annotations in substances

Table 1.1. Annotations in attached substance(s)

Document details	Annotation details	Annex
Last updated: Jan 28, 2020 1:37:28 PM Document **Hartmann, H.R. (1991)** **Document UUID of the Active substance:** 1599221c-9c40-45aa-b418-68b2cafa909d **Annex II/III requirement:** Acute toxicity: oral **Section Number:** 8.7.1 **Section Name:** Acute toxicity: oral	Annotation **Annotation on Hartmann, H.R. (1991)** **UUID of the annotation:**1e144dc7-c41e-4b72-8a95-67bd8b0a29b1 **Last updated:** Jan 28, 2020 1:37:28 PM	**More information in annex**
Last updated: Jan 28, 2020 1:37:28 PM Document **Hassler, S. (2001b)** **Document UUID of the Active substance:** 982826cd-3f8f-4f02-b222-c29648ee1744 **Annex II/III requirement:** Further toxicokinetic and r studies in mammals **Section Number:** 8.8.1 **Section Name:** Basic toxicokinetics	Annotation **Annotation on Hassler, S., 2001a** **UUID of the annotation:**6fb2a50b-615b-4300-9de9-c14d14f3f0c4	**More information in**
Last updated: Jan 28, 2020 1:37:28 PM Document **Hassler, S. (2001b)** **Document UUID of the Active substance:**		

Basic data

Additional annotation information for Annotation on Hartmann, H.R. (1991)

Annotation UUID: 1e144dc7-c41e-4b72-8a95-67bd8b0a29b1
Annotation status: Sent to applicant
Annotation basic remarks:

Please complete the Materials and Methods section, including a link to the test material, information on the test species and the enviromental conditions

Dataset data

Report Generator

Reports for Biocides users'

A **list of Confidentiality claims** made on biocidal products and active substances in accordance with Article 66(4) of the BPR regulation. MSCAs assess the confidentiality requests, whilst ECHA provides the required functionality to permit applicants to make a CFD claim, as well as collect and record the claims

RTF / CSV / PDF formats available

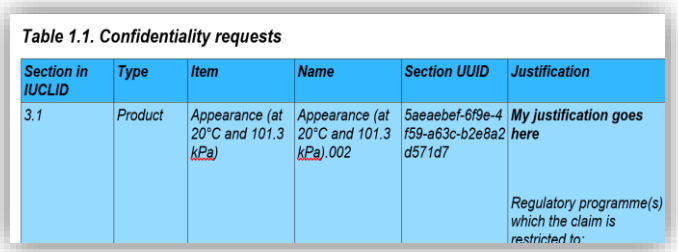
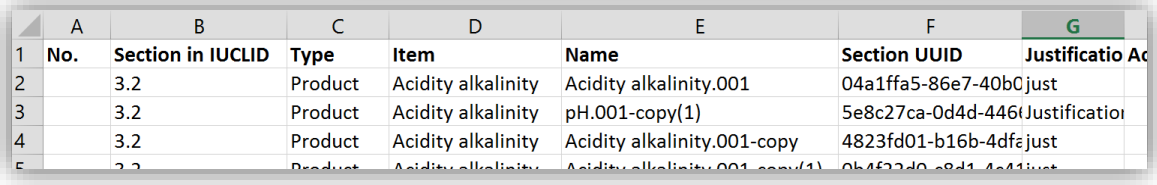


Table 1.1. Confidentiality requests

Section in IUCLID	Type	Item	Name	Section UUID	Justification
3.1	Product	Appearance (at 20°C and 101.3 kPa)	Appearance (at 20°C and 101.3 kPa).002	5aeaebef-6f9e-4f59-a63c-b2e8a2d571d7	**My justification goes here** Regulatory programme(s) which the claim is restricted to:



	A	B	C	D	E	F	G
1	**No.**	**Section in IUCLID**	**Type**	**Item**	**Name**	**Section UUID**	**Justificatio Ac**
2		3.2	Product	Acidity alkalinity	Acidity alkalinity.001	04a1ffa5-86e7-40b0	just
3		3.2	Product	Acidity alkalinity	pH.001-copy(1)	5e8c27ca-0d4d-446(	Justificatio
4		3.2	Product	Acidity alkalinity	Acidity alkalinity.001-copy	4823fd01-b16b-4df	just

Thank you!

ECHA
EUROPEAN CHEMICALS AGENCY

OECD

IUCLID 6 is developed by the European Chemicals Agency in association with the OECD