IUCLID 5
Guidance and Support

SNIF Migration Tool
User Manual

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Migration tool from SNIF to IUCLID 5

SNIF is the file format that was used to exchange the data stored in summary notification dossiers that were prepared using the Data Entry Screen (DES) application for the notification of new chemical substances under the former legislation (Directive 67/548/EEC). The exchange occurred between Notifiers, Member State Competent Authorities and the central New Chemical Database (NCD) maintained by the European Commission.

This manual instructs how to use the SNIF migration tool to transfer data from the Structured Notification Interchange Format (SNIF) to the IUCLID 5 format. In addition, it describes the data processing that might be required both before and after using the migration tool.

1. Principles of the migration tool and related processes

The purpose of the SNIF migration tool is to make it as easy as possible to reuse data entered in the DES or the NCD applications in the IUCLID 5 database. This tool is provided as a plug-in for both the stand-alone and the distributed versions of the IUCLID 5 application.

The tool is designed in such a way that the data contained in the SNIF export files are transformed to the new IUCLID 5 format without any user intervention. The migrated data can then be imported - completely or partially - into any IUCLID 5 installation. The import can also be done in a "batch mode", i.e. without any user intervention.

The SNIF migration plug-in allows the user to choose between transferring the SNIF data into IUCLID 5 Substance datasets ("raw data") or into IUCLID 5 Dossiers. The main difference between the two formats is that a Substance dataset is modifiable, whereas a dossier is read-only and therefore cannot be modified.

Care has been taken to map the information present in the SNIF file to the corresponding fields in IUCLID 5. There are many thousands of rules specifying the exact mapping to preserve every possible field and make the information available in IUCLID 5. However, due to the different data structure in IUCLID 5, not all the source fields have direct target fields. In any case, all information present in the SNIF file is preserved during the migration process and transferred in IUCLID 5 either in a "Remarks" field with an appropriate explanatory text or in an annotation attached to the resulting dataset.

In cases where the information cannot be migrated into any field in IUCLID 5, an entry in the Migration report is created where the exact place of the problem is specified and the non-migrated data are deposited.

2. Before starting data migration

Before starting the data migration process you should ensure that:

- you have imported the EC inventory from the [IUCLID 5 download site](#) into your IUCLID 5 application.

- you have imported the recommended reduced list of Reference Substances from the [IUCLID 5 download site](#) into your IUCLID 5 application.

- you have created the three following folders on your computer (for example on your desktop):
  - Input folder (POLL) in which a copy of the SNIF file(s) you want to migrate should be stored (= source file(s))
  - Output folder (OUT) in which the outcome of the migration process is available
  - Error log folder (BAD) in which the eventually incorrect migration result is stored as an error migration report.

- you have valid and complete notification dossier SNIF export file(s) (i.e. exported from DES or NCD). Please note that the summary notification dossier SNIF file consists (or might be consisting) of the following separate files, distinguishable from the last digit of the export file name:

  - the full notification file (with the extension *.***s**)
  - the follow-up classification and labelling (*.***l**)
  - the Conformity Control information (*.***c**)

  The main file that the migration tool checks is the ***.*s** one. If *.***l** and/or *.***c** files are also part of the same dossier, and copied in the POLL folder together with the main one, these data are then included into the final IUCLID 5 dataset. No data related to them are migrated into IUCLID 5 if they are not incorporated in the input folder. It is therefore strongly recommended to copy at the same time all files related to the same dossier into your POLL folder. Refer to the respective DES/NCD user manuals for further information on how to create SNIF export files.

3. Executing data migration

This chapter gives instructions on how to execute the migration of SNIF files into IUCLID 5.

Although the migration tool transforms the SNIF export files into IUCLID 5 datasets, it does not automatically load the newly created files into your IUCLID 5 application. At the end of the process, the tool generates and stores the resulting **.i5z** files in the OUT folder. From there you can easily import one or several files (bulk import functionality) into IUCLID 5 following the instructions provided in the IUCLID 5 End User Manual ("[D. 14.2 Importing a Substance, Template, Mixture or Category](#)", "D.14.8. Importing Dossiers" and "D.14.10 Bulk import feature") and here below summarised.

A prerequisite before you can start using the migration tool is that you have created SNIF export file(s) of the notification dossier(s) you wish to migrate to IUCLID 5.

Caution

Be aware of the hardware system requirements for IUCLID 5. Both the migration and import process would slow down considerably if the memory (RAM) of your PC is not sufficient. A minimum RAM of 1 GB is recommended.

3.1. Step-by-step guide

To migrate a SNIF export file to IUCLID 5, either select the command **Migrate** from the **Plugins** menu on the menu bar or Go Home 🏠 to the Task panel, if you are not already there, and click the **Run** button under the **Migrate data** task.
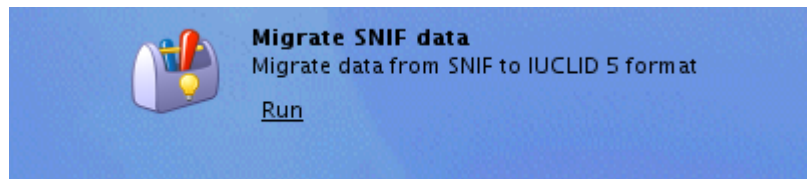
Functions related to the SNIF migration process can be identified by the following symbol in the tool bar menu:

The Migration main page is displayed:

To set the migration tool and to perform the migration itself, proceed as follows (the numbers are referring to the screenshot here above):
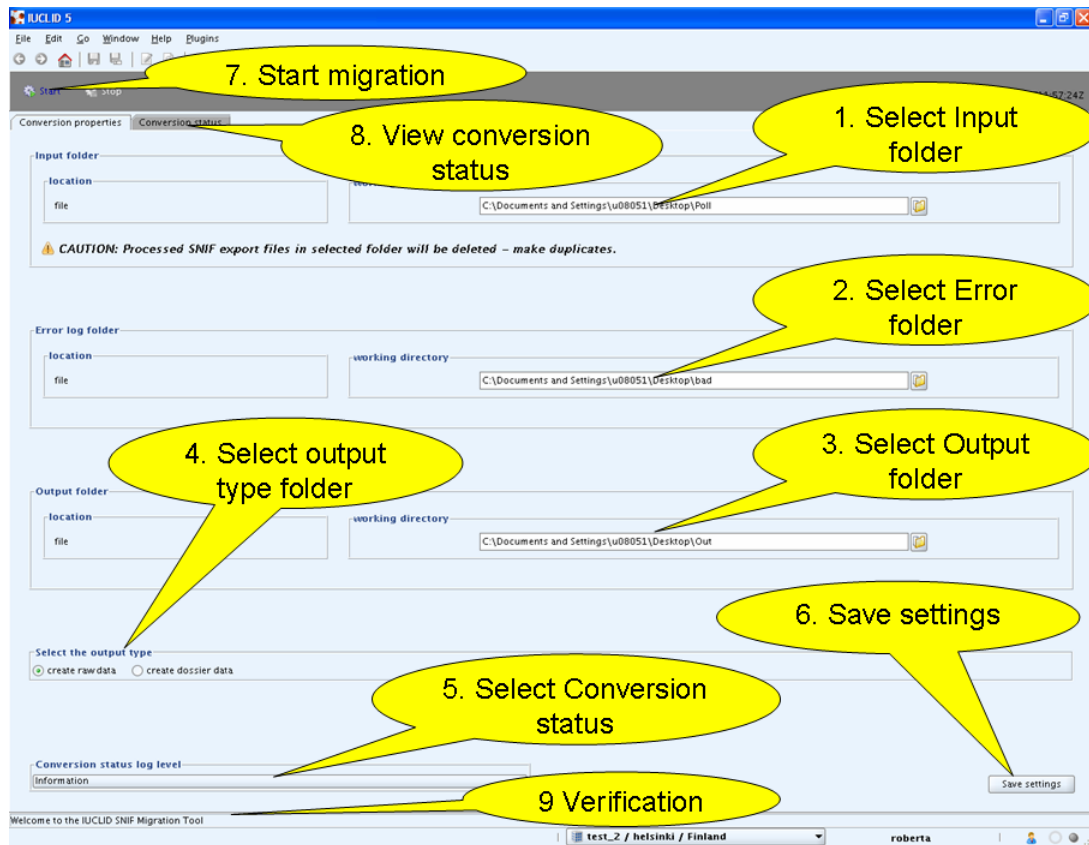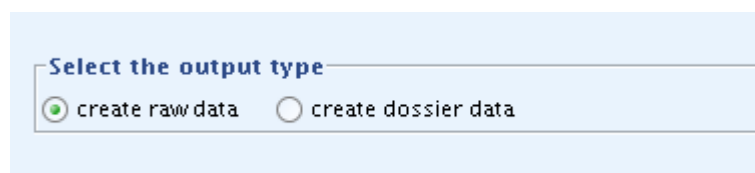
1. **Select Input folder**: Click the **File finder** button to create the link to the working directory and select the previously created folder, in which the SNIF export file(s) is(are) stored.

    Caution

    As indicated in the user interface under Input folder, the SNIF export file will be deleted when the migration process is successfully completed. It is recommended to keep copies of your original export files in another folder.

2. **Select Error log folder**: Click the **File finder** button to create the link to the working directory and select the folder (previously created) where the file containing the error migration report shall be stored.

3. **Select Output folder**: Click the **File finder** button to create the link to the working directory and select the folder (previously created) where the output file shall be stored, i.e. the IUCLID 5 export file containing the migrated data. The name of the created IUCLID 5 export file consists of the name of the original SNIF export file plus the file extension is ".i5z". For example, the source file 11111111.00s would appear as IUCLID 5 export file 11111111.i5z.

4. **Select Output type**: Select between the creation of a Substance dataset or a Dossier, by clicking the related radio-box button:

    -   "create raw data" will generate Substance dataset(s)

    -   "create dossier data" will generate Dossier(s) (be aware that the Dossier template generated will be "Complete")

    Note

    If you need to generate both the Substance and Dossier datasets, the migration tool should be run twice: the first time with "create raw data" checkbox selected and the second time with the "create dossier data" checked.

    Caution

When generating both the raw data and Dossier dataset, be aware of the fact that the name of the resulting file in the OUT folder will be exactly the same. Therefore if you run the migration tool twice, the second file generated will overwrite the previous one created. Please take care of importing/moving the first file to avoid loosing of data.

5. **Conversion status log file**: Select the level of detail that will be reported in the conversion log. In order of decreasing detail the levels are:
   - Debugging
   - Information (default selection)
   - Warning
   - Error

6. Click the **Save settings** button to keep the settings for any further migration sessions.

7. Click the **Start** button in the upper left to start the migration process.

   Tip

   The conversion can always be stopped at any given point in time by clicking the **Stop** button . When the conversion is started again at a later stage, the migration tool will process the remaining files.

8. Click Tab **Conversion status** to view the status of the transformation process.

9. Verify if the migration process is finished: The following message is displayed on the bottom line: "Conversion done. Terminated after running ....".
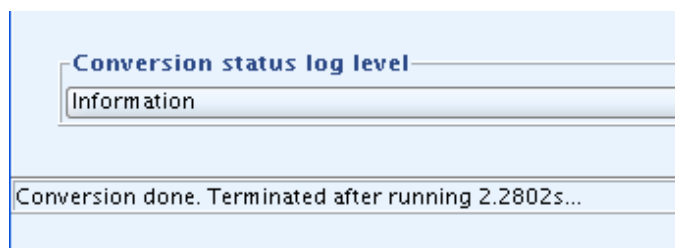
3.2. Import of the Substance/Dossier dataset

Once the migration process has been completed, go Home to the Task panel and start to import the newly created IUCLID 5 export file containing the transformed dataset(s). In the Task panel, click the **Import** button. The Import assistant will guide you through the following steps of the import process:

1. Select the IUCLID 5 import file created out of the corresponding SNIF export file from the OUT folder (or simply drag and drop it) and click one of the radio buttons to set one of the following Overwrite modes:
   - never
   - if newer than existing (default selection)

- always
- ask user
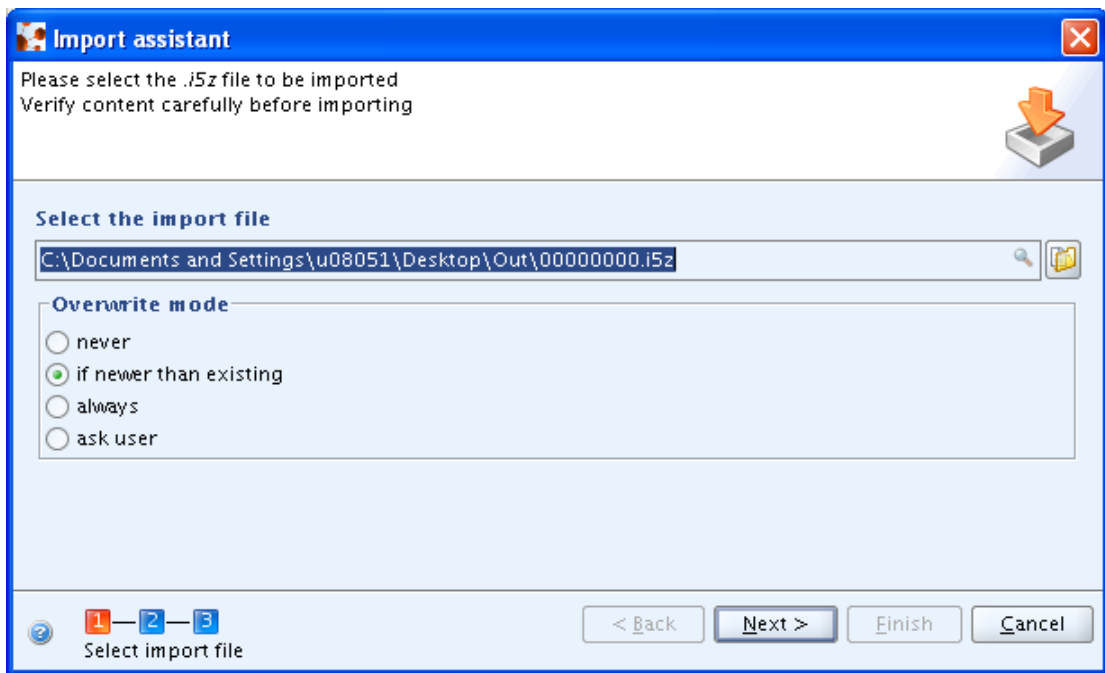
2. Verify the content of the import file.
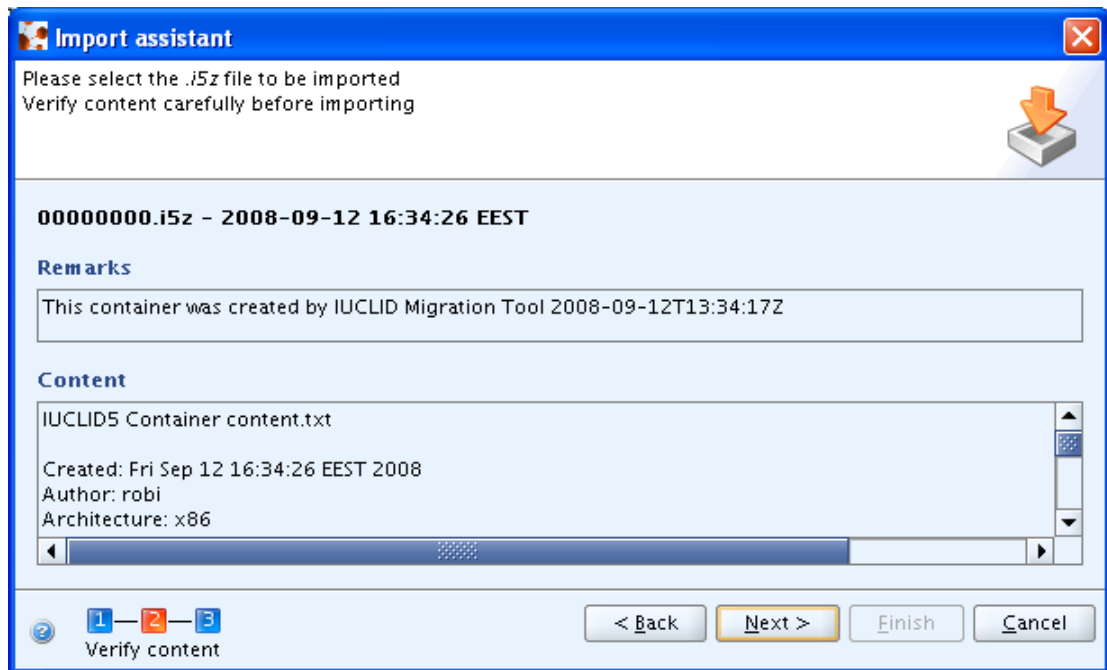
3. Prepare the import: The import file is analysed. Wait until the record counter reach the end of the procedure (it may take some minutes. Then proceed as described in the IUCLID 5 End User Manual guidance (D.14. Import (Import data from other IUCLID 5 systems))

   Tip

   Once the import process has started, you can continue any other IUCLID job. To open the background jobs indicator showing the progress of the import, select the command **Background jobs** from the **Window** menu on the menu bar or click the background job indicator on the very right of the bottom line.

   Caution

   If the migration or import process fails, the source export file may be damaged or contain invalid characters. In the **Error log folder**, check whether a log file has been created for that export file. As a workaround you can try to re-import the export file into your DES/NCD installation. This may clean it and remove the invalid characters. Create a new export file then and try the migration again.

3.3. Bulk import

In the following, guidance is given on how to include several export files in a bulk import. Go Home 🏠 to the Task panel if you are not already there.

1. Under **Import** ⬇️, click **Bulk Import**.

Import
Import data from other IUCLID 5 systems
Import, Bulk import
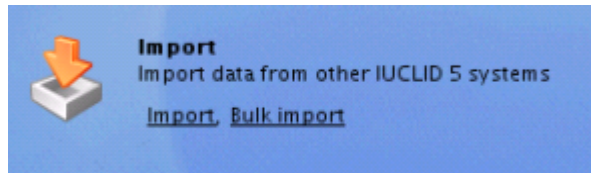
2. Click the **Add** button ➕ and select the files you wish to import. Change the Overwrite mode unless the default setting "if newer than existing" should be kept. Then click the **Next** button.

Bulk import assistant
Please select the .i5z files to be imported
and verify the import results

Import	Pathname	Filename	Size	Modified
✔	C:\SNIF\Migration\O...	85040021.i5z	165.47 KB	2008-06-12 20:15:1...
✔	C:\SNIF\Migration\O...	87080004.i5z	129.65 KB	2008-06-12 20:15:3...
✔	C:\SNIF\Migration\O...	84060013.i5z	152.52 KB	2008-06-12 20:15:0...
✔	C:\SNIF\Migration\O...	11111111.i5z	190.53 KB	2008-06-12 20:18:1...
✔	C:\SNIF\Migration\O...	00010605.i5z	166.88 KB	2008-06-12 20:14:5...
✔	C:\SNIF\Migration\O...	11222222.i5z	177.48 KB	2008-06-12 20:15:0...

Overwrite mode
- ○ never
- ◉ if newer than existing
- ○ always

1 — 2
Select import files/directories

[< Back] [Next >] [Finish] [Cancel]

Be aware that the bulk import will start immediately after clicking the **Next** button and will proceed until completion. The **Finish** button in Step 4 is only to close the Import assistant and is only active when the import is completed. Click the **Close** button in the Import protocol window and then the **Finish** button to close the Import assistant.
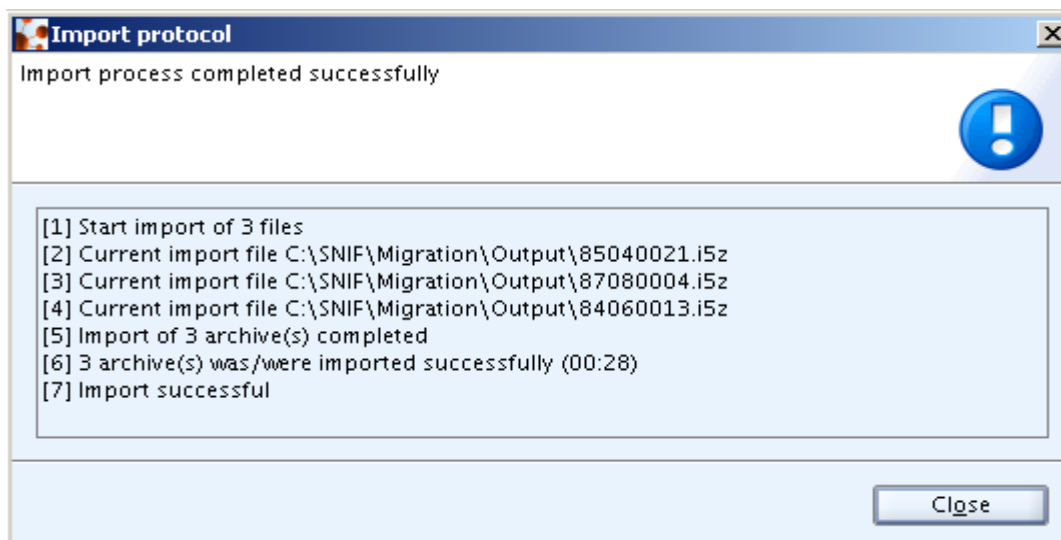
Tip:

Execution of the bulk import may take some time depending on the amount of data being imported and the hardware system used. You can follow the progress of the import by selecting the Background jobs indicator from the Window menu.
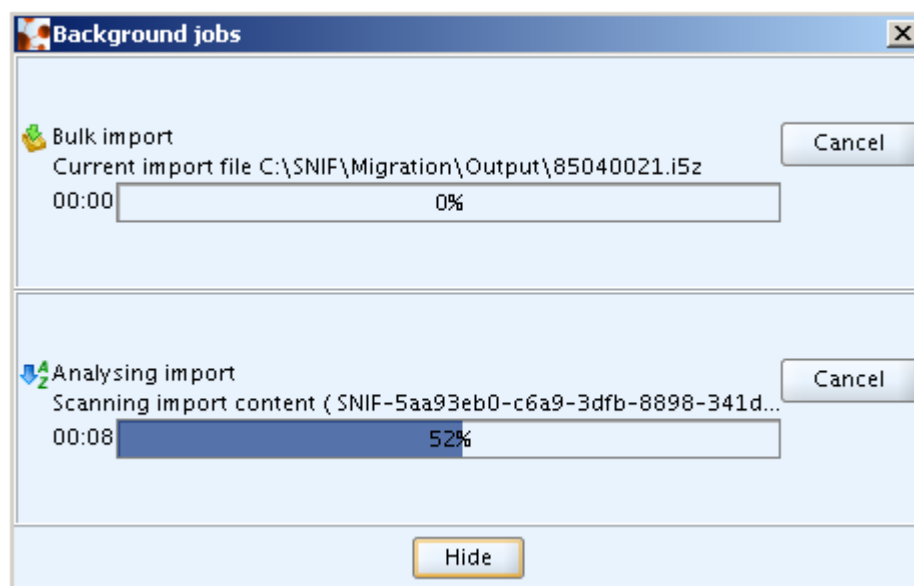
More information on bulk import (i.e. importing more than one data set at the same time) into IUCLID 5 can be found in the IUCLID 5 End User Manual ("D.14.10 Bulk import").

After the successful import of the migrated data, the datasets of the output type raw data appear in your IUCLID 5 **Substance** list:

After the successful import of the migrated SNIF file(s), the dataset(s) of the output type Dossier appear in your IUCLID 5 task **Dossier** list:

4. Post-processing – Migration report

In this chapter, instructions are given on how to check the Migration report and what peculiar migration issues should be taken into account when deciding on whether post-processing of any IUCLID 5 dataset migrated from SNIF is necessary.

The information on the migration process is recorded and stored in a so called Migration report. After the import of the migrated SNIF file(s), the Migration report is attached to the newly created IUCLID 5 Substance dataset as a PDF document. This report is intended to assist the user in the decision on what data need to be checked and/or manually moved to a specific target field. In cases where the information cannot be migrated into any field in IUCLID 5, an entry in the Migration report document will be created where the exact place of the problem is specified and the non-migrated data is deposited.

The Migration report contains detailed information on all migration stages and steps, as well as messages about possible migration errors or failures.

> **Note**
>
> The migration report is not available for data migrated to Dossiers, therefore it is suggested to always create a Substance dataset to be able to check the migration results.

4.1. Checking the Migration report

You can access the Migration report as follows:

1. Open the IUCLID 5 Substance dataset
2. With the first section *1.1 Identification* or any other sections 1 to 3 being displayed, expand the Information window at the bottom, i.e. below the Data entry window, and click the **Attachments** Tab.

3. Double-click the PDF document displayed to open it.

The migration report is composed by the following two chapters:

a) **Mapping results**: For each single DES/NCD section, a report of the mapping and migration result is given.

b) **Validation rules**: For those SNIF sections which include data that had to be transformed / checked based on specific IUCLID 5 validation rules, a validation message is output in the log file.

Here below, some examples of mapping results are given:

a) Mapping results

- *Migration successful*

When the "Migration successful" sentence is displayed, it means that the listed SNIF data field is migrated without any error or failure.

- *FAILURE: no data*

If the sentence "FAILURE: no data" is displayed, the listed SNIF section(s) do not contain any data to migrate.

```
18. 1.3.20 Impurities  [1.3.20]
    Impurities: Typical percentage ( by weight) [030]:
    SNIF record 1    IUCLID5 xpath
    eu.eca.iuclid.common.business.substance.Substance:/substanceCompositions[1]/substanceImpurities[1]/proportionT
    ypical/precision
    FAILURE: No data
    SNIF record 2    IUCLID5 xpath
    eu.eca.iuclid.common.business.substance.Substance:/substanceCompositions[1]/substanceImpurities[1]/proportionT
    ypical/precision
    FAILURE: No data
    SNIF record 4    IUCLID5 xpath
    eu.eca.iuclid.common.business.substance.Substance:/substanceCompositions[1]/substanceImpurities[1]/proportionT
    ypical/precision
    FAILURE: No data
```

- *FAILURE: Failed to map the data*

If the sentence "FAILURE: Failed to map the data" is displayed, the indicated SNIF section contains data that cannot be migrate into the destination field. This may happen when the SNIF file reports a different value than the ones specified in the NCD/DES picklist. If this is the case, the original SNIF value entry is reported in brackets.

```
13. 0.4.20 Labelling (by Competent Authority) [0.4.20]
    Risk phrases [020]:
    SNIF record 1    IUCLID5 xpath
    eu.eca.iuclid.common.business.substance.Substance:/csfLabelForSubstance[1]/labelRPhrases
    FAILURE: Failed to map the data (C - s n f t)
```

b) Validation results (Second part of the migration report)

- *Text 'xxxxxxxx' exceeds the maximum field capacity of '256' characters and has been cut off*:

This message (or similar messages) indicates that the text present in the SNIF file is longer that the one present in the IUCLID 5 destination field. If this happens, you will find the suspension points indication "…" in the IUCLID 5 dataset.

For example, in IUCLID 5 the following text has been cut off:
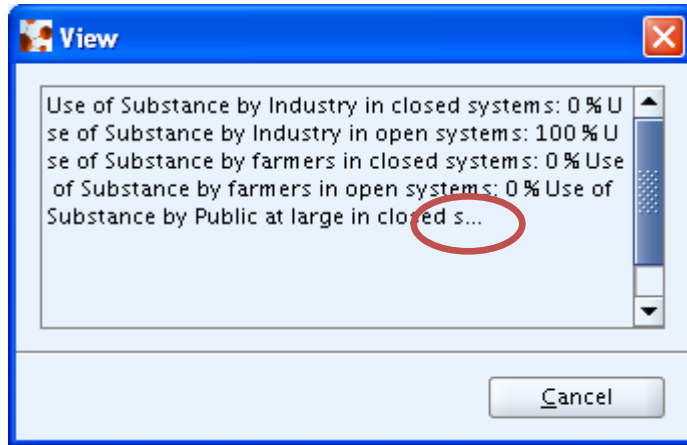
In the migration report the full text is entirely reported in the validation result part:
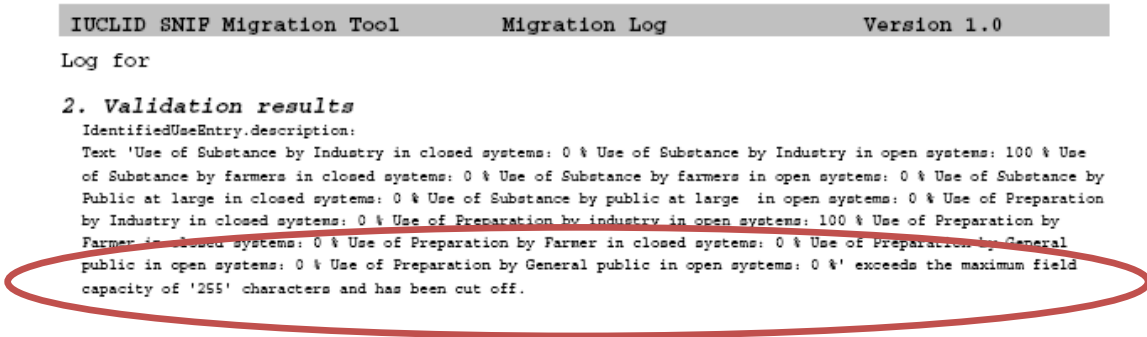
4.2. Technical migration issues

Independent of any possible need of updating the scientific content, guidance given in the following subchapters:

- general migration issues and
- specific migration issues

addresses the technical migration issues which can occur.

Tip

A unique record name is created automatically when an endpoint is migrated into sections 4 to 13 of IUCLID 5. This name consists of the title of the IUCLID 5 section, followed by an indication that the data source was a SNIF export file ("SNIF"), the original record order number and the original source section number, as shown in the screenshot below. This makes it easier if you search for a specific record.
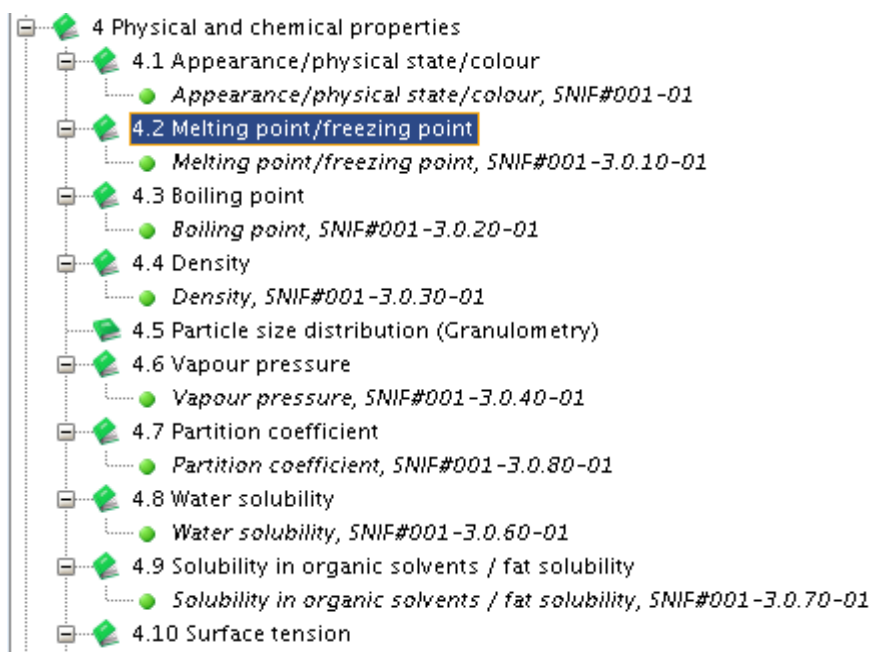
5. General migration issues

Because of the different structure between IUCLID 5 and NCD/DES the following applies in all (or most of all) SNIF export file sections:

- Numeric range fields
- Flags
- List of values – picklists
- Concatenation of single DES/NCD fields
- Mapping of NCD text field (unlimited) with IUCLID 5 field limited to 255 or 2000 characters
- Mapping the Notifier / Manufacturer / Importer information
- Mapping the Classification and labelling
- Mapping the Endpoint sections

5.1. Numeric range fields

SNIF file and IUCLID 5 in some cases have different numeric range fields.

- In DES/NCD only the lower value subfield is preceded by a qualifier subfield, while both the lower and upper value fields in IUCLID 5 come with qualifier subfields.

- The single qualifier subfield in DES/NCD allows to select all operator types, i.e. =, <, <=, >, =>, ca. or blank (i.e. no entry), whereas the following validation rules apply in IUCLID 5:

  o Lower qualifier field only allows to select >, =>, ca. or blank (i.e. no entry);

  o Upper qualifier field only allows to select <, <=, ca. or blank (i.e. no entry).

- Completing the upper qualifier and numeric field is only allowed, if either a lower value is already entered to specify a numeric range or if the upper value is preceded by either operator "<" or "<=".
- No "equal to" sign (=) is provided. Instead, this is indicated by no operator being selected, i.e. the qualifier field is simply left empty. This is consistent with single numeric fields, where no "equal to" sign is provided either.

Therefore different rules have been implemented to correctly migrate the data between the two different applications.

a) Mapping SNIF qualifier and single numeric field to IUCLID 5 numeric range field block

The mapping definitions made for any single qualifier plus numeric field are based on the following rationale:

- Migrate qualifier to lower qualifier field if SNIF phrase is ca., > or >=
- Migrate qualifier to upper qualifier field if SNIF phrase is < or <=
- Migrate numeric field to lower numeric field if SNIF phrase is ca., >, >=, = or NULL (i.e. no phrase selected)
- Migrate numeric field to upper numeric field if SNIF phrase is < or <=

Examples:

DES/NCD		IUCLID 5			
Qualifier	Value	LoQualifier	LoValue	UpQualifier	UpValue
ca.	20	ca.	20		
	20		20		
>	20	>	20		
>=	20	>=	20		
<	20			<	20
<=	20			<=	20

b) Mapping of a numeric range block (NCD/DES) to a numeric range field block (IUCLID 5)

The mapping definitions made for numeric range fields are based on the following rationale:

- Migrate lower qualifier to lower qualifier field if SNIF phrase is ca., > or >=
- Migrate lower qualifier to upper qualifier field if SNIF phrase is < or <= and upper value field is empty
- Migrate upper qualifier to upper qualifier field if SNIF phrase is < or <=
- Migrate upper qualifier to lower qualifier field if SNIF phrase is ca. and lower value field is empty
- Migrate lower numeric field to lower numeric field if SNIF phrase is ca., >, >=, = or NULL (i.e. no phrase selected)
- Migrate upper numeric field to upper numeric field if SNIF phrase is < or <=
- Migrate upper numeric field to upper numeric field if SNIF phrase is ca., = or NULL and lower value field is not empty
- Migrate lower numeric field to upper numeric field if SNIF phrase is < or <= and upper value field is empty

- Migrate upper numeric field to lower numeric field if SNIF phrase is ca., >, >=, = or NULL and lower value field is empty

- Migrate lower qualifier + numeric field to Remarks field if SNIF phrase is < or <= (which are not allowed in the lower qualifier field of IUC5) and upper value field is not empty

- Migrate upper qualifier + numeric field to Remarks field if SNIF phrase is > or >= (which are not allowed in the upper qualifier field of IUC5) and lower value field is not empty

DES/NCD				IUCLID 5			
LoQualifier	LoValue	UpQualifier	UpValue	LoQualifier	LoValue	UpQualifier	UpValue
ca.	20			ca.	20		
	20				20		
>	20			>	20		
>=	20			>=	20		
<	20					<	20
<=	20					<=	20
		ca.	20	ca.	20		
			20		20		
		>	20	>	20		
		>=	20	>=	20		
		<	20			<	20
		<=	20			<=	20
ca.	20	<	30	ca.	20	<	30
	20		30		20		30
>	20	<	30	>	20	<	30
>=	20	<30		>=	20	<	30
<	20		30				30*
				plus text entry in appropriate Remarks field: "< 20 (lower limit)"			
<=	20		30				30*
				plus text entry in appropriate Remarks field: "<= 20 (lower limit)"			
	20	>	30		20*		
				plus text entry in appropriate Remarks field: "> 30 (upper limit)"			
	20	>=	30		20		
				plus text entry in appropriate Remarks field: ">= 30 (upper limit)"			
<	20	>=	30				
				plus text entry in appropriate Remarks field: "< 20 (lower limit) >= 30 (upper limit)"			

5.2. Flags

In NCD/DES the confidentiality is indicated as an activated checkbox, whereas In IUCLID 5, several flags are available. It has been decided to always migrate each NCD/DES confidentiality flag as IUCLID 5 [CBI] (Confidential Business Information).
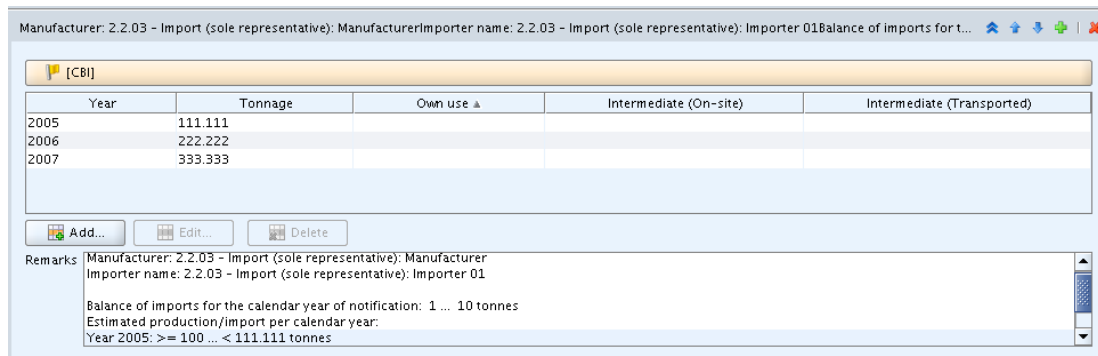
5.3. List of values – picklists

In NCD/DES the "list of values" associated with a text box provides the user with a selection of predefined rational values (picklist). The content of the picklist is tailored to the individual entry field. The mapping to the correspondent IUCLID 5 picklist applies the following rules:

- in case the two picklist entries are matching, the same picklist entry in IUCLID 5 is selected

- in case the picklist entry is not matching any entries in IUCLID 5, the picklist entry "Other:" is selected. The original entry is displayed in the related text field

- in case no picklist is present in IUCLID 5, the original text is reported in IUCLID in the corresponding field

5.4. Concatenation of single DES/NCD fields

A specific rule was used to add a specific default text before the migrated value from DES/NCD to IUCLID 5 and/or if several DES/NCD fields should be migrated to the same target field.

5.5. Mapping of text field from NCD (unlimited) to IUCLID 5 (limited to 255 or 2000 chars)

Specific rules were defined to migrate correctly text that exceeds the maximum field length in IUCLID 5. In the endpoint sections (4-13), if the maximum length is reached, alternative target fields are defined preceded by an appropriate default text. In chapters 1, 2 and 3 instead, the excess text is indicated in the migration report (see here above).

5.6. Mapping the Notifier / Manufacturer / Importer information

In IUCLID 5 the philosophy is that Legal entities should have a unique identifier across different IUCLID installations, even if this is very difficult to enforce during migration.

The SNIF migration plugin, takes only the information related to the owner of the notification to create the Legal entity owner of the IUCLID 5 dataset.

Other companies may have been specified in DES/NCD, in particular when the notifier is an importer or a sole representative, and should indicate the name(s) and address(es) of the manufacturer(s) outside the EEA and/or the importer(s) and the name(s) of the contact person(s) that he represents in section 0.2.20. The SNIF migration tool creates a unique Legal entity for each manufacturer and or importer indicated in DES/NCD and migrate this information directly to IUCLID 5 section 1.7 (suppliers).

In this way, the number of Legal entities created is controlled and the existing Legal entities all represent unique companies.

Legal entity sites are migrated from DES/NCD to IUCLID 5 section 3.3.

5.7. Mapping the Classification and labelling

In DES/NCD there are several instances of the classification and labelling. The one migrated into IUCLID 5 is the most updated one:

- if the Technical Progress Committee proposal is agreed, it would be the one to be migrated
- if instead this is not agreed, the migrated one is the C&L defined by the "Classification and Labelling Group Proposal".
- If both the previous C&L sections are not defined, the migrated one is the "Final proposal for C&L proposed by the "lead CA" (DES/NCD 10.2.2).
- If all three previous sections are not finalised, the migrated one should be DES/NCD 0.4.10 Classification (by Competent Authority) and the DES/NCD 0.4.20 Labelling (by Competent Authority).
- If all previous sections are not defined, the migrated one should be DES/NCD 9.2.01 Classification (by notifier) and 9.2.02 Labelling (by notifier).

5.8. Mapping the Endpoint sections

The migration tool makes the following default selections when a record is created:

- GPL compliance: always turned to YES
- The specifications of the original NCD section numbers are reported in the name of the corresponding endpoint(s) in IUCLID 5.
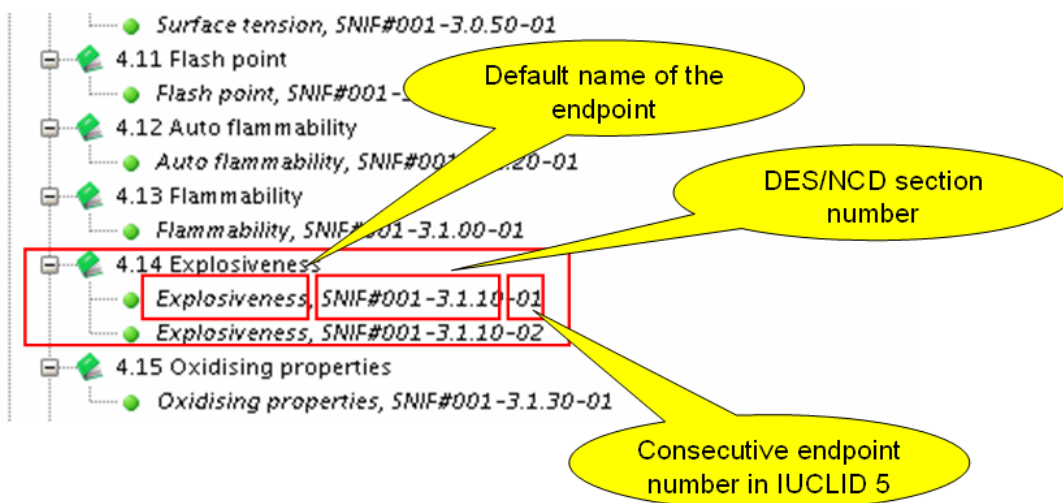
- The date of the study submitted is generally considered as the one of the dossier creation

6. Specific information on how data are migrated from DES/NCD to IUCLID 5

In this chapter, each NCD/DES section is addressed and specific migration issues are described. Be aware that the notification number is reported in IUCLID 5 section 1.3 in the table "regulatory programme".

6.1. DES/NCD Section 0: Details of the notification

0.1.00 Details of the notification: all information related to:

- Member State responsible of notification
- Date of notification
- Lead dossier notification number

is migrated to the Annotation layer of IUCLID 5 belonging to section 1.1. and can be viewed by selecting the 'Annotation' tab in the information pane.

0.2.10 Notifier: A Legal entity is created for the notifier and linked to IUCLID 5 section *1.1 Identification.* This Legal entity is the owner of the Substance dataset. The role in the supply chain is also indicated in the same IUCLID 5 section.

0.2.20 Manufacturer/importer: Legal entities for Manufacturer(s) and/or importer(s) are created in IUCLID 5 and linked to section *1.7 Suppliers.* If more than one manufacturer/importer are specified, new repeatable block entries are created in section 1.7.

0.3.00 Name to be included in ELINCS: The codes indicating the view of the authority with regard to the publication of the trade name / IUPAC name are migrated to IUCLID 5 section *1.2 Composition* in the "brief description" field. The EC number is migrated to section *1.2 Composition* in the field "Name".

6.2. DES/NCD Section 1: Identity of the substance

<u>1.1.00 Name - 1.3.10 component(s)</u>: A Reference substance for each component indicated in these sections is created in IUCLID 5 and linked respectively to section 1.1 and 1.2

Note

Be aware that the information related to DES/NCD field "Typical concentration of substance(% by weight)" is reported only in the Migration report due to an inconsistency between the format of these two fields (DES/NCD allows entering a text string, IUCLID 5 allows only a valid number). Therefore the user should enter manually a valid typical concentration substance number.

<u>1.3.20 Impurities</u>: A Reference substance for each impurity is created in IUCLID 5 and linked to section 1.2 under "impurities"

<u>1.3.40 Additives</u>: A Reference substance for each additive defined is created in IUCLID 5 and linked to section 1.2 under "additives".

Note

The information related to component(s), impurity(-ies) and additive(s) is used to create entries in IUCLID 5 section *1.2 Composition*. As data exchange is an essential task, data integrity should be ensured to avoid multiple entries for the same chemical substance in the table of Reference substances. During the migration process, the migration tool checks whether the Reference substance already exists. In detail the process is as follows:

1. If the same CAS number exists, the existing Reference substance is used.
2. If no CAS number is found in your Reference substance inventory, a new Reference substance is created in IUCLID 5.

In the first case, information on the substance identification in the NCD/SNIF dataset is ignored. Of course information that is targeted to section *1.2 Composition* is still transferred. It is therefore suggested to download and import in your local IUCLID 5 installation all relevant References substances from the IUCLID 5 web site before proceeding with the migration. Moreover the predefined Reference substances contain all relevant information including the SMILES notation, which is required in Annex VI of the REACH legislation.

<u>1.3.50 Spectral data, 1.3.61 Chromatography, 1.4.10 Detection: components, 1.4.20 Detection: impurities, 1.4.30 Detection: additives, 1.5.10 Composition of the tested substance</u>: all these data are migrated to IUCLID section *1.4 Analytical information* where appropriate repeatable blocks are created.

6.3. DES/NCD Section 2: Information on substance

2.0.10 Process(es) used in production, 2.1.50 Process(es) related to the use of the substance: Data are migrated to IUCLID 5 section *3.1 technological process.*

2.0.20 Exposure related to production, 2.1.60 Exposure estimates related to use of the substance, 2.1.70 Fields of application with approximate breakdown (partially): Data are migrated to IUCLID 5 section *3.8 Exposure estimates*.

2.0.30 Production site(s): A site is created and linked to IUCLID 5 section *3.3 sites*.

2.1.00 Proposed uses, 2.1.70 Fields of application with approximate breakdown (partially): Dare are migrated to IUCLID 5 section *3.5 Identified uses an exposure scenarios* (Regarding "desired effect codes", information is migrated to the annotation layer).

2.1.40 Form under which the substance is marketed, 2.1.70 Fields of application with approximate breakdown (partially): Data are migrated to IUCLID 5 section *3.4 Form in the supply chain*.

2.1.80 Identity of recipients: A Legal entity is created for each recipient and linked to IUCLID 5 section *1.8 Recipients*.

2.1.90 Waste quantities and composition of waste resulted from the proposed uses: Data are migrated to IUCLID 5 section *3.7 Waste from production and use*.

2.2.00 Estimated production in and/or imports into the EU, 2.2.03 Estimated imports in case of sole representative (partially): Data are migrated to IUCLID 5 section *3.2 Estimated quantities.* Be aware that in the table only the highest tonnage is indicated: the complete string related to the production is displayed in the following remark field.

2.2.03 Estimated imports in case of sole representative (partially): Data related to the production of the manufacturer are migrated to IUCLID 5 section *1.7 Suppliers* in the Remarks field.

2.3.00 Recommended Methods and Precautions for Handling and Storage, 2.3.30 Recommendations for Transport, 2.3.40 Fire hazards (recommendation for appropriate extinguishing agents and nature of the products of combustion or pyrolysis), 2.3.50 Other dangers, particularly reaction with water, 2.3.60 Dust explosion, 2.4.00 Emergency measures in the case of accidental spillage, 2.5.00 Eye and skin injury emergency treatment, 2.6.00 Packaging of the substance and/or preparation: Data are migrated to IUCLID 5 section *11 Guidance on safe use* in the corresponding field if present or in the "Remarks" one.

6.4. DES/NCD Section 3: Physico-chemical properties

The table below provides a mapping between the DES/NCD section 3 related to Physico-chemical properties and IUCLID 5 endpoints.

As general advice, be aware that the information contained in one single endpoint in NCD/DES might be migrated into several endpoints in IUCLID 5, depending on the information present in the original endpoint.

3.0.00 Nature of the substance	*4.1 Appearance/physical state/colour*
3.0.10 Melting temperature/freezing temperature	*4.2 Melting point/freezing point*
3.0.20 Boiling temperature	*4.3 Boiling point* *4.2 Melting point/freezing point*
3.0.30 Relative density	*4.4 Density*
3.0.40 Vapour pressure	*4.6 Vapour pressure*
3.0.50 Surface tension (of aqueous solution)	*4.10 Surface tension*
3.0.60 Water solubility	*4.8 Water solubility*
3.0.70 Fat solubility	*4.9 Solubility in organic solvents / fat solubility*
3.0.80 Partition coefficient n-octanol/water	*4.7 Partition coefficient*
3.0.90 Flash point	*4.11 Flash point*
3.1.00 Flammability	*4.13 Flammability*
3.1.10 Explosivity	*4.14 Explosiveness*
3.1.20 Self ignition temperature (auto-flammability)	*4.12 Auto flammability*
3.1.30 Oxidising properties	*4.15 Oxidising properties*
3.1.40 Additional physico-chemical properties	*4.1 Appearance/physical state/colour* *4.5 Particle size distribution (Granulometry)* *4.8 Water solubility* *4.11 Flash point* *4.14 Explosiveness*
3.1.50 Particle size	*4.5 Particle size distribution (Granulometry)*
3.1.60 Molecular weight distribution (additional test required for polymers)	*4.23 Additional physico-chemical information*
3.1.70 Thermal Stability (additional test required for polymers)	*4.19 Stability: thermal, sunlight, metals* *4.23 Additional physico-chemical information*
3.1.80 Extractivity (additional test required for polymers)	*4.23 Additional physico-chemical information*

6.5. DES/NCD Section 4: Toxicological studies

The table below provides a mapping between the DES/NCD section 4 related to Toxicological studies and IUCLID 5 endpoints.

As general advice, be aware that the information contained in one single endpoint in NCD/DES might be migrated to several endpoints in IUCLID 5, depending on the information present in the original endpoint.

4.1.11 Acute toxicity: Administered orally	*7.2.1 Acute toxicity: oral*
4.1.12 Acute toxicity: Fixed-dose toxicity procedure	*7.2.1 Acute toxicity: oral*
4.1.20 Acute toxicity: Administered by inhalation	*7.2.2 Acute toxicity: inhalation*
4.1.30 Acute toxicity: Administered cutaneously	*7.2.3 Acute toxicity: dermal*
4.1.50 Acute toxicity: Skin irritation	*7.3.1 Skin irritation / corrosion*
4.1.60 Acute toxicity: Eye irritation	*7.3.2 Eye irritation*
4.1.70 Acute toxicity: Skin sensitisation	*7.4.1 Skin sensitisation*
4.2.10 Subacute toxicity (28/90 day test)	*7.5.1 Repeated dose toxicity: oral* *7.5.3 Repeated dose toxicity: inhalation* *7.5.4 Repeated dose toxicity: other routes* *7.5.2 Repeated dose toxicity: dermal*
4.3.10 Mutagenicity: Bacteriological test	*7.6.1 Genetic toxicity in vitro*
4.3.21 In vitro mammalian cytogenicity (B10)	*7.6.1 Genetic toxicity in vitro*
4.3.22 In vitro mammalian cell gene mutation (B17)	*7.6.1 Genetic toxicity in vitro*
4.3.23 Unscheduled DNA synthesis, mammalian cells in vitro (B18)	*7.6.1 Genetic toxicity in vitro*
4.3.25 In vitro mammalian cell transformation (B21)	*7.6.1 Genetic toxicity in vitro*
4.3.26 Gene mutation - Saccharomyces cerevisiae (B15)	*7.6.1 Genetic toxicity in vitro*
4.3.27 Mitotic recombination - Saccharomyces cerevisiae (B16)	*7.6.1 Genetic toxicity in vitro*
4.3.28 6th amendment data	*7.6.1 Genetic toxicity in vitro*
4.3.30 Mutagenicity: Non-bacteriological in vivo	*7.6.2 Genetic toxicity in vivo*
4.3.31 In vivo mammalian bone marrow cytogenetics (B11)	*7.6.2 Genetic toxicity in vivo*
4.3.32 In vivo mammalian bone marrow micronucleus (B12)	*7.6.2 Genetic toxicity in vivo*
4.3.33 In vivo mammalian germ-cell cytogenetics (B23)	*7.6.2 Genetic toxicity in vivo*
4.3.34 Rodent dominant lethal	*7.6.2 Genetic toxicity in vivo*
4.3.35 Mouse spot testing	*7.6.2 Genetic toxicity in vivo*
4.3.36 Mouse heritable translocation test	*7.6.2 Genetic toxicity in vivo*
4.3.37 Sex linked recessive lethal in Drosophila	*7.6.2 Genetic toxicity in vivo*
4.4.20 Reproductive studies: one generation toxicity test	*7.8.1 Toxicity to reproduction*
4.4.30 Reproductive studies: two or three generations	*7.8.1 Toxicity to reproduction*
4.4.40 Developmental toxicity - Teratogenicity	*7.8.2 Developmental toxicity / teratogenicity*
4.5.10 Assessment of toxicokinetic behaviour	*7.1.1 Basic toxicokinetics*
4.5.20 Toxicokinetic study	*7.1.1 Basic toxicokinetics*
4.6.10 Chronic toxicity test	*7.5.1 Repeated dose toxicity: oral* *7.5.2 Repeated dose toxicity: dermal* *7.5.3 Repeated dose toxicity: inhalation* *7.5.4 Repeated dose toxicity: other routes*
4.6.20 Carcinogenicity test	*7.7 Carcinogenicity*
4.6.30 Combined chronic toxicity/carcinogenicity test	*7.5.1 Repeated dose toxicity: oral* *7.5.2 Repeated dose toxicity: dermal* *7.5.3 Repeated dose toxicity: inhalation* *7.5.4 Repeated dose toxicity: other routes*
4.7.00 Additional toxicological studies	*7.9.3 Specific investigations: other studies*

6.6. DES/NCD Section 5: Ecotoxicological studies

The table below provides a mapping between the DES/NCD section 5 related to Ecotoxicological studies and IUCLID 5 endpoints.

As general advice, be aware that the information contained in one single endpoint in NCD/DES might be migrated to several endpoints in IUCLID 5, depending on the information present in the original endpoint.

5.1.01 Acute toxicity for fish	*6.1.1 Short-term toxicity to fish*
5.1.02 Acute toxicity for Daphnia	*6.1.3 Short-term toxicity to aquatic invertebrates*
5.1.03 Growth inhibition test on algae	*6.1.5 Toxicity to aquatic algae and cyanobacteria*
5.1.06 Inhibition of microbial activity	*6.1.7 Toxicity to microorganisms*
5.1.07 Long term toxicity to Daphnia magna	*6.1.4 Long-term toxicity to aquatic invertebrates*
5.1.08 Higher plant test	*6.3.3 Toxicity to terrestrial plants*
5.1.09 Toxicity for earthworms: artificial soil test	*6.3.1 Toxicity to soil macroorganisms except arthropods*
5.1.10 Fish, prolonged toxicity study (14 day)	*6.1.2 Long-term toxicity to fish*
5.1.11 Fish, prolonged toxicity study (incl. Reproduction)	*6.1.2 Long-term toxicity to fish*
5.1.12 Fish, early life	*6.1.2 Long-term toxicity to fish*
5.1.13 Avian oral toxicity test	*6.3.5 Toxicity to birds*
5.1.14 Avian reproduction test	*6.3.5 Toxicity to birds*
5.2.11 Ready biodegradability	*5.2.1 Biodegradation in water: screening tests*
5.2.12 Biochemical/chemical oxygen demand (BOD/COD)	*5.2.1 Biodegradation in water: screening tests*
5.2.13 Inherent biodegradability	*5.2.1 Biodegradation in water: screening tests*
5.2.14 Biodegradation in wastewater simulation test	*5.2.2 Biodegradation in water and sediment: simulation tests*
5.2.21 Hydrolysis as a function of pH	*5.1.2 Hydrolysis*
5.3.10 Absorption/desorption screening test	*5.4.1 Adsorption / desorption*
5.4.10 Bioconcentration factor (BCF)	*5.3.1 Bioaccumulation: aquatic / sediment*
5.5.00 Additional ecotoxicological tests	*6.6 Additional ecotoxicological information*

6.7. DES/NCD Section 6: Possibility of rendering the substance harmless

6.1.00 Possibility of rendering the substance harmless: For industry/skilled trades, 6.2.00 Possibility of rendering the substance harmless: For the public at large: Data are migrated to IUCLID 5 section *11 Guidance on safe use* in the corresponding field if present or in the "Remarks" one.

6.8. DES/NCD Section 7: Risk assessment

7.0.00 Risk assessment: Data are migrated to IUCLID 5 section *13 Risk assessment report.*

6.9. DES/NCD Section 9: Declarations

9.1.01 Declaration concerning the unfavourable effects of the substance on man and environment, 9.2.03 Safety data sheet proposed by the notifier: Data are migrated to IUCLID 5 section *13 Risk assessment report.*

9.2.01 Classification proposed by the notifier, 9.2.02 Labelling proposed by the notifier: see the classification and labelling philosophy here above.

9.2.04 Update Log: Information is migrated to the annotation layer belonging to IUCLID 5 section *1.1 identification*

6.10. DES/NCD Section 10: Follow up classification and labelling

See the classification and labelling philosophy here above.

European Chemicals Agency

IUCLID 5 Support

SNIF Migration plugin User Manual
November 2008 v 1.0

http://iuclid.eu