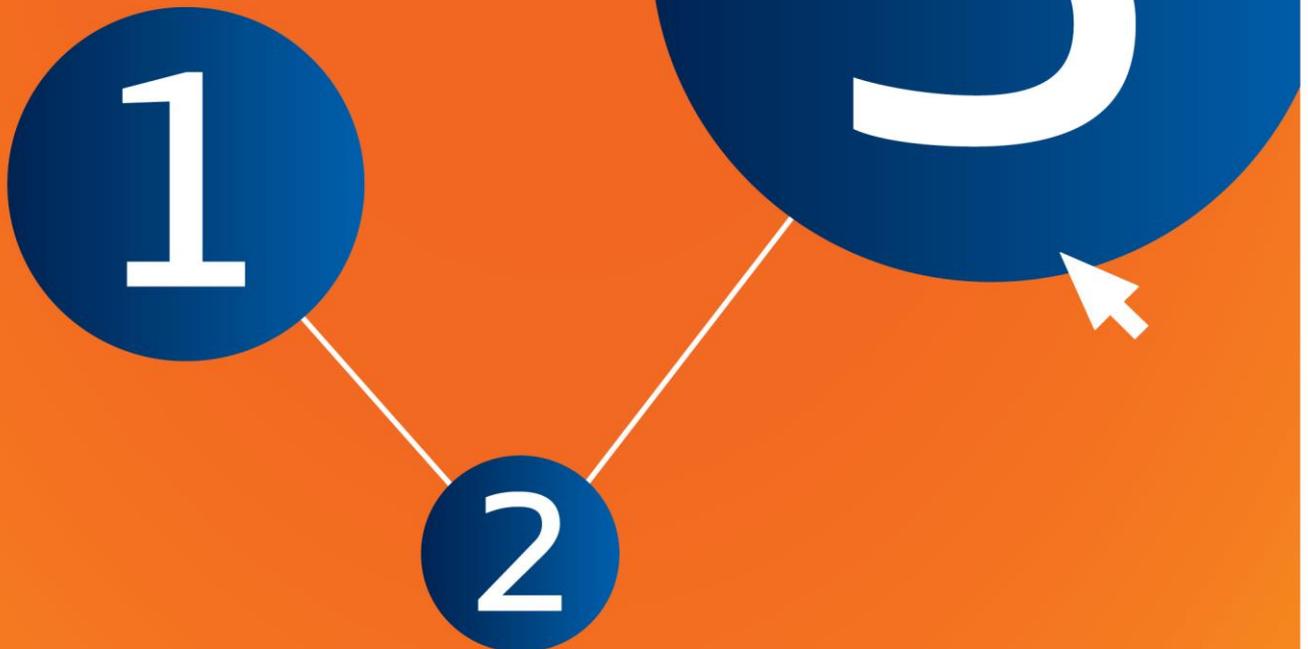


# How to prepare a classification and labelling notification



## Changes to this document

Version	Changes
1.0	First version

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## 1. Introduction

### 1.1. Objective

The purpose of this manual is to assist in the preparation of a IUCLID Classification and Labelling (C&L) notification dossier under the CLP Regulation (EC) No 1272/2008. More particularly it outlines the IUCLID sections and fields to be filled-in in order to prepare a complete C&L notification dossier according to Article 40(1) of the CLP Regulation.

The aim of this users' manual is to help the notifiers to identify which of the numerous IUCLID fields are of prime importance for a successful submission of a C&L notification.

This IUCLID C&L notification dossier can then be submitted to the European Chemicals Agency (ECHA) using the REACH-IT application.

For more details on your duties regarding C&L notification under the CLP Regulation, you can consult the CLP FAQ available at: [http://echa.europa.eu/clp/clp\\_help/clp\\_faq\\_en.asp](http://echa.europa.eu/clp/clp_help/clp_faq_en.asp).

This manual assumes that IUCLID has been installed and you have a valid ECHA account. More information about the different functionalities in IUCLID and how to use those functionalities can be found in the help system built-in IUCLID (see chapter 1.5 *Functionalities of IUCLID*). The manual also assumes that you have all relevant information available.

### 1.2. Overview of the preparation and the submission of a dossier

A IUCLID dossier is non-editable snapshot file of a substance dataset, containing the information to be submitted to ECHA. The steps below indicate the approach for the preparation of a C&L notification dossier in IUCLID:

- Step 1.** Sign-up in REACH-IT and create the *Legal entity* of the notifier (<https://reach-it.echa.europa.eu/>)
- Step 2.** Create the *reference substance* in IUCLID (see chapter 5)
- Step 3.** Create the *substance dataset* in IUCLID for the notified substance (see chapter 6)
- Step 4.** Enter the information requested by the CLP Regulation in the *substance dataset* in IUCLID (see relevant subsections of chapter 6)
- Step 5.** Create a C&L notification dossier in IUCLID (see chapter 7)
- Step 6.** Export the C&L notification dossier from IUCLID (see chapter 8)
- Step 7.** Submit the C&L notification dossier to ECHA via *REACH-IT* (see chapter 9)

The details of the information required to complete each of these sections is explained later in this manual.

### 1.3. Information required for C&L notification

The information to be included in the Substance dataset is described in the CLP Regulation (Article 40(1)).

The requested information comprises the following (the corresponding IUCLID section is indicated in brackets):

- identity of the notifier, i.e. name, contact details (REACH-IT account);

- contact person of the notifier (section 1.1);
- identity of the notified substance as specified in section 2.1 to 2.3.4 of Annex VI to REACH (sections 1.1, 1.2, and 1.4);
- in case you flag the IUPAC name confidential in the C&L inventory: an alternative name to the IUPAC name of the notified substance for publication, and the relevant justification (section 1.1);
- classification of the substance according to the criteria set in the CLP Regulation (section 2.1);
- reason for no classification in case a substance is classified in some but not all hazard classes or differentiations (section 2.1);
- specific concentration limits or M-factors where applicable (section 2.1), together with a justification using the relevant parts of sections 1, 2 and 3 of Annex I to REACH (section 13);
- label elements, i.e. hazard pictograms, signal words and hazard statements (section 2.1).

### 1.3.1. Confidentiality requests

You can flag the IUPAC name of your substance confidential in the C&L inventory ONLY if your substance is:

- a non-phase in substance;
- a substance only used as one or more of the following: as intermediate, in scientific research and development, in product and process orientated research and development.

ECHA can process the IUPAC names flagged confidential in the C&L inventory ONLY upon the following conditions:

- a confidentiality flag is assigned to the IUPAC name;
- an alternative name is given for the publication on ECHA website;
- a justification is attached.

If one of the requested information is missing, the confidentiality claim cannot be processed.

Confidentiality on a IUPAC name in the C&L inventory is different from an alternative name in a Safety Data Sheet or on the label for substance in a mixture (Article 24 of the CLP Regulation).

If you want to use an alternative name in your Safety Data Sheet or on the label, you need to make a request for an alternative name according to Article 24 of the CLP Regulation.

### 1.4. Checks performed by ECHA on the submitted dossiers

All dossiers submitted to ECHA undergo initial technical and administrative checks in order to ensure that they can be handled properly and that the subsequent required regulatory processes can be successfully carried out. Such checks are called business rules (BR).

A dossier can be accepted for processing only if all of the relevant business rules, such as format verification and availability of administrative information are satisfied.

For more information on the business rules check refer to the Annex: *Overview of the business rules checks performed by ECHA on the submitted dossiers.*

### 1.4.1. The Validation assistant

The *Validation assistant* (VA) plugin has been developed to enable you to perform some checks on the dossier before you submit it to ECHA via REACH-IT.

Therefore, before the submission, we strongly advise you to use the *Validation assistant* plugin in two steps:

- i. To check your dataset (before the dossier is created) to be able to correct any failures reported at this level.
- ii. To check the final dossier and address any issues identified in this step.

Using the plugin in both steps is vital for you to minimise any unnecessary failures and potential rejection of your submission.

For instructions on how to run the *Validation assistant*, refer to the help system of IUCLID.

## 1.5. The functionalities of IUCLID

The functionalities of IUCLID are described in detail in the help that is built in to the IUCLID application. To view the help, press the F1 key anywhere inside the application. The help system will try to display the most relevant part of the help content. From there it is possible to navigate to the specific help required. For example, if the export wizard of the application is open, pressing F1 should open the help content at a description of the *Export* functionality. As an alternative to pressing F1, there are links to help in the application interface, wherever there is a help icon in the form of a question mark.

## 2. Legal entity

Submissions to ECHA are done by *Legal entities* which have to be defined including contact details prior to submission. The contact details of the company are stored as a *Legal Entity Object (LEO)*. You can create a LEO both in IUCLID and in the *ECHA accounts* available at <http://echa.europa.eu/support/helpdesks/echa-helpdesk/echa-accounts>.

Note that ECHA will use only the contact details of the legal entity that you have registered in the ECHA accounts or in REACH-IT.

You have already created one legal entity when you installed IUCLID. You can add more legal

entities by right clicking on *Legal entity*  on the IUCLID home page. However, ECHA will not enforce the consistency between the IUCLID legal entity and the ECHA accounts legal entity.

Please note that by the default settings the legal entity is not included in the dossier. If you wish to include the legal entity in your dossier, you can change the default settings during the dossier creation in the dossier creation wizard (see chapter *How to create a Dossier*).

If you include a legal entity in the dossier which will be submitted to ECHA it may be beneficial to check if the legal entities in IUCLID and REACH-IT are the same. For further information on how to create a Legal Entity Object (LEO) and how to synchronise it between IUCLID and REACH-IT, refer to the next chapter.

## 2.1. How to update and synchronise the LEO information

To register your legal entity you should sign-up into the *ECHA accounts* where you can enter and administer your legal entity information.

When you create a LEO a numeric identifier called Universal Unique Identifier (UUID) is generated. Example of a legal entity UUID: *IUC5-a620a92d-32c6-426a-b6ee-fc338cde0932*.

The UUID is different for each LEO, even within the same company in case the company has several LEOs.

You can synchronise the legal entity between IUCLID and REACH-IT by exporting your LEO from ECHA accounts or REACH-IT. Then you can import the file to your local IUCLID installation. It may be beneficial that the UUID is identical between all the applications where the company identity appears (IUCLID, REACH-IT, any web forms submitted to ECHA). Alternatively, if you have not yet created your ECHA account, you may export the LEO from your IUCLID installation and import the file to ECHA accounts when you create an account. Note that a LEO can be imported to ECHA accounts only while you create an account, and not to an existing ECHA account.

To compare the UUIDs between the applications, you can find them inside each application by following the below paths:

- IUCLID: Home page > *Legal entity* > double click your legal entity. The UUID of the company is displayed in the *Information Panel* at the bottom of the IUCLID window.
- ECHA Accounts: Legal Entity tab > General details > Legal Entity UUID
- REACH-IT: Menu > *Company information* > *General information* > *UUID*

For more information on the ECHA account management refer to the ECHA accounts manual available at <http://echa.europa.eu/support/helpdesks/echa-helpdesk/echa-accounts>.

## 3. Contact

In the *Contacts inventory* you can insert the contact details of the relevant competent persons, such as person responsible for the safety data sheet (SDS), toxicologist, etc, which can be attached to the IUCLID dossier. This person may be contacted to provide assistance or ask about the information submitted.

Information on the contact person responsible for your submission must be specified and managed in REACH-IT.

### 3.1. Creating a contact

**Step 1.** To create a *new contact* right-click on the *Contacts*  on the home page and select *New*.

**Step 2.** Complete as many fields as possible under the *General information*.

**Step 3.** To save the contact information click on  from the main menu.

## 4. Chemical inventories

The *Chemical inventories* contains chemical identifiers, which serve as the basis for defining the *reference substances*. The term *inventory* is used to compile all the different chemical inventories that can be available in IUCLID. Currently, the **EC Inventory** is the only inventory used in IUCLID.

The EC Inventory is a combination of three individual inventories:

- **EINECS** (European Inventory of Existing Commercial Chemical Substances) includes substances that were deemed to be on the European Community market between 1st January 1971 and 18th September 1981.
- **ELINCS** (European List of Notified Chemical Substances) includes substances notified under Directive 67/548/EEC, the Dangerous Substances Directive Notification of New Substances (NONS) and placed on the market after 18th September 1981.
- **NLP-list** (No-Longer Polymers list) includes substances that have been on the European Community market between 18th September 1981 and 31st October 1993, and were considered to be polymers under the reporting rules for EINECS but were no longer considered to be polymers according to the 7th amendment of Dir 67/548/EEC.

The entries in the EC Inventory consist of a chemical name and a number (EC name and EC number), a CAS number<sup>1</sup> (if available), molecular formula (if available) and description (for certain types of substances).

## 5. Reference substance

A *Reference substance* enables you to store identification information on a given substance or a given constituent of a substance, such as chemical names (EC name, CAS name, IUPAC name, synonyms, etc.), identity codes (EC number, CAS number), molecular and structural information.

The *Reference substance inventory* gives the possibility to use the same information for the same chemical identity avoiding to re-type it and to ensure that the data is centrally managed and updated. The *Reference substance inventory* is directly maintained by you, in your local installation. Each *reference substance* can be linked to an unlimited number of *substance* or *mixture/product* datasets. For updating the information in a *reference substance*, you can open the *Reference substance inventory*, search for the relevant *reference substance* and update it. The modifications will impact every single dataset linked to that *reference substance*.

To extend the number of entries in your inventory, you can search, download and import available reference substances from the IUCLID website to your local installation. These pre-defined reference substances have been prepared to improve data quality and minimise data entry.

### 5.1. Creating a reference substance

If you do not find a reference substance in the *Reference substance* inventory, you can create a new reference substance.

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<sup>1</sup> In the case of substances listed in the EC inventory with an EC number starting with 4, there may be no CAS number published even though a CAS number may exist for that substance. This is because under the notification scheme for new substances which existed under the previous legislation the CAS number could be claimed confidential and therefore was not published.

There are two types of information that can be reported in a *reference substance*:

1. Information **specific** to the *reference substance*: such information exactly corresponds to the substance/constituent(s) covered by that reference substance;
2. Information **related** to the *reference substance*: this information does not accurately correspond to the substance/constituent(s) covered by that reference substance for any of the following reasons:
  - The information is generic as it also covers other substances/constituents;
  - The information only covers some of the constituents of a reference substance for a substance or a group of constituents;
  - The information refers to a similar constituent/substance;
  - The information is not the latest available information to identify the substance/constituent(s)

Related information should be reported under the *Identifiers of related substances* as it may create an ambiguity on the identity of substance or constituent(s) which a reference substance corresponds to.

To create a reference substance:



- Step 1.** Right-click on the *Reference substance* on the home page and select *New*.
- Step 2.** Enter the name of the reference substance.
- Step 3.** If the **reference substance is listed in the EC inventory** you can assign that entry by clicking the *Add* button.
- Step 4.** If your **reference substance is not listed in the EC inventory**, select a justification from the picklist proposed under the *No inventory information available*.
- Step 5.** Complete as far as possible the remaining fields of the reference substance.

The following information, if available and/or applicable, should be submitted for all the known constituents and additives:

- *EC Inventory* information,
- *CAS number* and *CAS name*,
- *IUPAC name*,
- *Description* (Specify any additional information relevant for the description of the reference substance in this field. This is important especially when the reference substance does not correspond to a well-defined chemical substance. Attached files can be added if necessary.),
- *Synonyms*,
- *Identifiers of related substances*,
- *Molecular formula* (if a molecular formula cannot be derived from the reference substance, a justification should be indicated in the *Remarks* field at the bottom of the section);
- *Molecular weight range*,
- *SMILES notation*,
- *InChI*,
- Upload an image file with the *Structural formula*.

**Step 6.** To save the reference substance click on  from the main menu.

## 6. How to create a Substance dataset

This chapter outlines which information you have to provide through different sections of IUCLID, which depends on the type of submission that you wish to do via a IUCLID dossier.

When entering your data you can use the help system of IUCLID which is built inside the application. To view the help, press the F1 key anywhere inside the application and the most relevant information will be displayed in the help window.

To create a IUCLID **dossier**, you first need to create a substance **dataset**. A substance dataset is a repository of administrative and scientific data for a substance. The information in the dataset can be modified: you can add, remove or change information in the dataset. **The dataset is used as basis for the dossier.** The dossier is a snapshot of the dataset at a certain moment; the information in the dossier cannot be modified.

### To create a dataset:

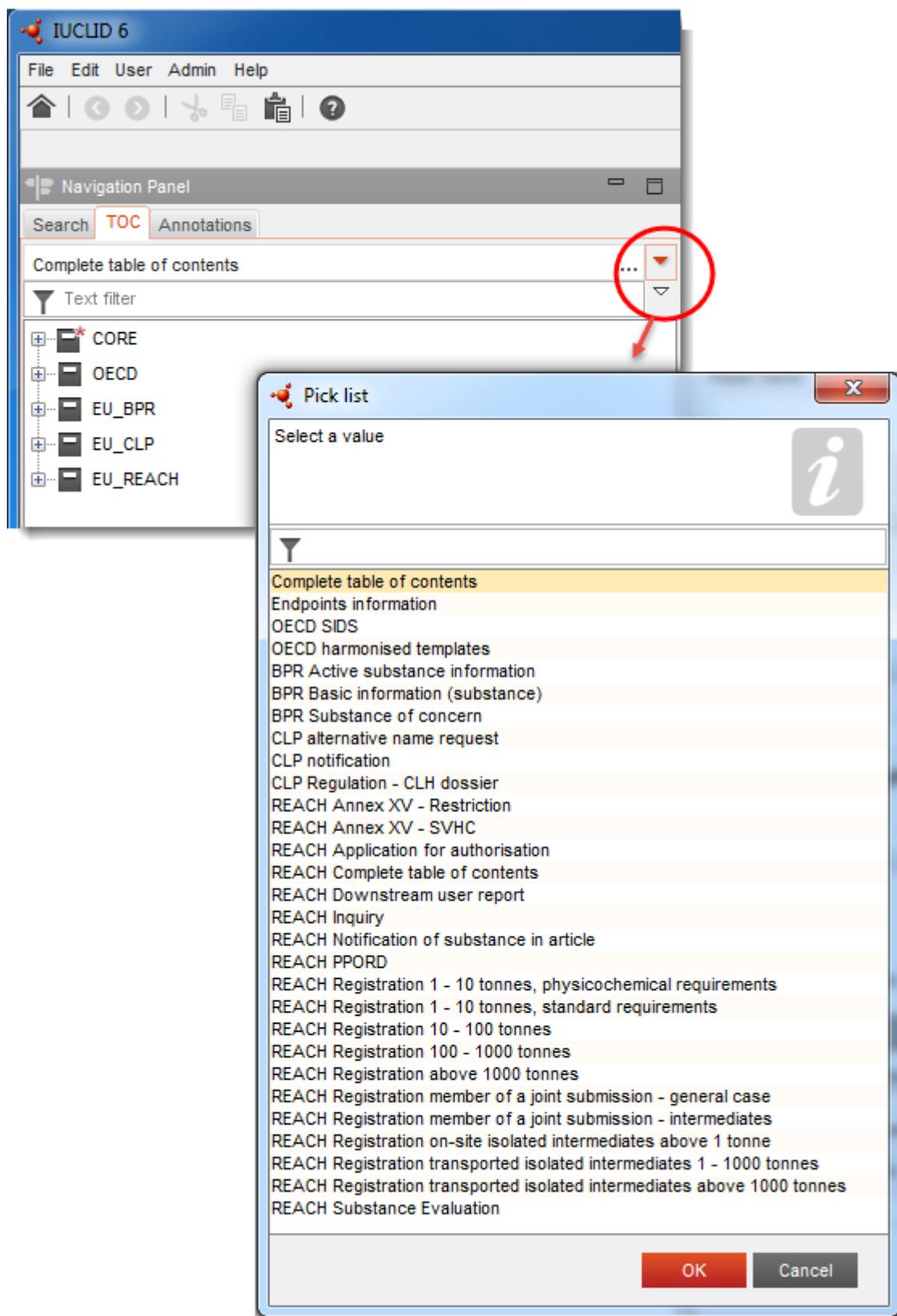
- Step 1.** Right-click on the *Substance*  on the IUCLID home page and then select *New*.
- Step 2.** Fill in the field *Substance name*. Especially if your IUCLID installation contains several datasets, ensure to enter a name that you can easily use to distinguish the substance.
- Step 3.** Assign an existing *legal entity* to the dataset by clicking on the  button. A new window opens where you can search for legal entities within your IUCLID installation. Enter the search criteria, select the appropriate legal entity from the list, and assign it to the substance dataset.
- Step 4.** Save the information by clicking the  icon in the main menu.

For more information on how to fill in the fields in this view, see section 1.1 *Identification*.

### To complete a dataset:

- Step 1.** Once your substance dataset is created it is displayed in the navigation panel on the left part of the screen.
- Step 2.** To open your dataset double-click or right-click and select *Open*.
- Step 3.** When the dataset is open the *Table of contents* (TOC) tab is displayed in the navigation part of the screen.
- Step 4.** To view the table of contents that is relevant for the type of dossier that you are preparing, click on the filled downward arrow () in the TOC tab.
- Step 5.** A list of different submission types appears. Select the specific type of submission from the list.

**Figure 1:** An example of selecting the template from the picklist



**Step 6.** The sections relevant for the submission type are now displayed. Sections including mandatory information to complete are marked with the asterisk (). Note that if you are creating a dataset but do not yet know the exact REACH dossier type that will be prepared, you can select the option *REACH Complete table of contents*. This will display the table of contents containing all sections that are relevant under the REACH Regulation.

Once you have created a dataset for your substance, you can enter data on the substance in this dataset. The following chapters describe what data should be entered into each section of IUCLID for the specific type of submission that this manual refers to. The sections are shown with their name and the numbering used with the relevant IUCLID table of contents view.

When filling in the different parts of a dataset it is important, that:

- when you create many rows in a table, you must fill in the relevant information in each row,
- when *other* is selected in a picklist the adjacent text field marked with 'Other' must be completed,
- when a field is associated with a unit, this must be filled in.

## 6.1. Section 1 General information

In section 1, *General information*, enter information on substance identity and on the dossier submitter. According to the data requirement for a C&L notification, IUCLID sections 1.1 to 1.3 shall be completed by the notifier.

### 6.1.1. Section 1.1 Identification

Section 1.1 contains the identification of the substance, role in the supply chain and the type of (reference) substance.

To complete this section, follow the steps:

**Step 1.** In the *Substance name* field type a name for the substance which you are preparing the dossier for.

**Step 2.** If you have any confidentiality concerns about the substance name, you need to fill in the *Public name* field. In this field you have to indicate a generic name suitable for publication, which appropriately describes the substance.

More information on how to derive a *public name* for a substance for use under the REACH Regulation, you can find at <http://echa.europa.eu/manuals>.

**Step 3.** Assign a *Legal entity* to your substance dataset by clicking on the  button (see chapter *Legal entity*).

### Role in the supply chain:

**Step 4.** Select at least one checkbox in this section according to your role in the supply chain with regards to this substance.

## Identification of substance:

**Step 5.** Click the  button to assign a *reference substance* to your substance dataset.

**Step 6.** A query dialog appears. Search for your reference substance. Click *Assign*.

If you cannot find your reference substance because it has not been created yet, click *New* and create it (see chapter *Reference substance*).

The information to be reported in your reference substance depends on the substance type:

- **Mono-constituent substances:**

A **mono-constituent substance** is a **well-defined substance** for which one constituent is present at a concentration of at least 80 % (w/w). This constituent is the main constituent of the substance. The substance is named according to the chemical name of that main constituent.

If your substance is a **mono-constituent** substance, assign the *reference substance*<sup>2</sup> corresponding to the main constituent in section 1.1.

- **Multi-constituent substances:**

A **multi-constituent substance** is a **well-defined** substance for which more than one constituent is present at a concentration between 10 % and 80 % (w/w). These constituents are the main constituents of the substance. A multi-constituent substance is normally named as a *reaction mass* of the main constituents.<sup>3</sup>

If your substance is a **multi-constituent** substance, assign the *reference substance*<sup>4</sup> corresponding to the reaction mass of the main constituents of your substance in section 1.1.

- **UVCB substances:**

**UVCB substances** (i.e. substances of Unknown or Variable composition, Complex reaction products or Biological materials) are substances that cannot be sufficiently identified by their chemical composition.

If your substance is a **UVCB** substance, assign a *reference substance*<sup>5</sup> corresponding to the UVCB substance in section 1.1.

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<sup>2</sup> Note that for the reference substance: *Molecular formula*, *Molecular weight range* and *Structural formula* must be provided. In addition, the *SMILES notation* should also be provided if available.

<sup>3</sup> Certain multi-constituent substances corresponding to reaction masses of isomers may sometimes be more conveniently named using a chemical name where the isomeric form is not specified rather than as a "reaction mass".

<sup>4</sup> Note that the *Molecular formula*, *Molecular weight range* and *Structural formula* of the reference substance must be provided or a justification for not providing this information must be given in the *Remarks* field. In addition, the *SMILES notation* should also be provided if available.

<sup>5</sup> Note that the *Molecular formula*, *Molecular weight range* and *Structural formula* of the reference substance must be provided or a justification for not providing this information must be given in the *Remarks* field. In addition, the *SMILES notation* should also be provided if available.

**Type of substance:**

**Step 7.** Select the appropriate *Type of substance* from the picklist.

We also recommend you to read the *Guidance for identification and naming of substances under REACH and CLP* available at <http://echa.europa.eu/guidance-documents/guidance-on-reach>.

**Step 8.** Select the *Origin*, e.g. organic or inorganic, from the picklist.

**Step 9.** If relevant, you can include additional identifiers for your substance under *Other identifiers*. Such identifiers may include Trade names of the substance, identifiers by which the substance was previously known but have later been replaced/refined, or identifiers which are used to identify the substance under other regulatory schemes. Chemical (scientific) synonyms should not be listed here, but should be indicated in the reference substance information.

**Step 10.** You can add information of the contact person(s) for this substance from the previously defined contacts (see chapter *Contact*).

**Step 11.** To save the information click  from the main menu.

**6.1.2. Section 1.2 Composition**

Section 1.2 is used for describing the identity of your substance at a compositional level. In this section, you will report the identity and concentration of the constituents of the composition, including any impurities and additives. The state and form of your composition(s) is reported in this section.

You are advised to ensure that the information included in IUCLID section 1.1 and section 1.2 is sufficient to clearly report your substance identity and is consistent between both sections. In particular, this information reported may not be so generic that it would describe more than one substance.

Each substance dataset must contain at least one composition record which refers to the composition manufactured, imported or used by the registrant/notifier/applicant. Depending on the type of substance and dossier to be prepared, it may be necessary to report more than one composition. This is in particular the case where compositional differences affect the hazard profile and classification of the substance.

Each composition is reported as a record in IUCLID. To create a new record:

**Step 1.** Right-click on the *1.2. Composition* in the TOC from the navigation panel on the left part of the screen.

**Step 2.** From the picklist select *New record*.

**Step 3.** A new record to report a new composition is created.

Next, fill in the information on your substance composition.

**General information:**

**Step 1.** Provide a descriptive *Name* for the composition. This is especially relevant if you report multiple compositions.

- Step 2.** The default selection in the *Type of composition* field is *legal entity composition of the substance*. This refers to a composition manufactured, imported or used by the registrant/notifier/applicant. Each dataset should contain at least one composition of this type. Only modify this value where you intend to report a composition with a different purpose. For more information on what composition types that can be reported for that submission please refer to the specific instructions for the submission type that you are preparing.
- Step 3.** Indicate the physical *State/form* of the composition by selecting the appropriate value in the picklist. Where the substance covers different physical states or forms, a separate composition should be created for each of them.
- Step 4.** You can give more detailed information on the composition under the *Description of composition*. This is particularly important when several compositions are reported in order to clarify the differences between the compositions. Providing further considerations on how the composition has been defined is also advisable when the composition covers wide concentration ranges or polymorphs or isomers. For substances that cannot be described with well-defined and quantified constituents (e.g. UVCB substances), further information to identify the composition is provided in this field, including the identity of the starting materials and a description of the production process used to manufacture the substance.
- Step 5.** You can provide supporting attachments under the *Attached description*.
- Step 6.** In the *Justification for deviations* field, provide where relevant, the justification for deviating from the rules for reporting the composition of substances as specified in the legal text and indicated in the *Guidance for identification and naming of substances under REACH and CLP* available at <http://www.echa.europa.eu/web/guest/guidance-documents/guidance-on-reach>.

### Degree of purity:

- Step 7.** Provide the degree of purity of the composition, together with the unit of measurement. For instance, a substance with a purity of between 95-98% (w/w) will be given as shown below. Note: The degree of purity should correspond to the overall concentration of the (main) constituents in the composition.

**Figure 2: Degree of purity**

The screenshot shows a web form element titled "Degree of purity". It features a range input field with "95" on the left and "98" on the right, separated by a double-headed arrow. To the right of the range is a dropdown menu showing "% (w/w)". There are also small navigation icons (back, forward) and a "..." menu icon.

### Constituents:

- Step 8.** Include the *constituents* for the composition by clicking the  button. Each composition must have, as a minimum, one constituent. The number of constituents to be reported will depend on the type of substance. To add more constituents, click the , and then the new repeatable blocks will appear.
- Step 9.** Assign a *reference substance* to the newly created constituent by clicking the  button. Search for the appropriate reference substance and add it by selecting it and clicking *Assign*; alternatively, create a new reference substance to specify the

*constituent* (see *Reference substance*). Ensure that the reference substance contains a chemical name in the IUPAC name field, and the appropriate EC and CAS identifiers, as available.

**Step 10.** Indicate the *Typical concentration* and the *Concentration range* (minimum and maximum values, and unit of measurement) for every constituent.

**Figure 3: Constituent**

The screenshot shows a software window titled 'Constituents' with a sub-header 'Styrene / Styrene / 100-42-5 / 202-851-5, ca. 98 % (w/w), >= 96 - <= 99.5 % (w/w)'. Below the header, there is a 'Reference substance' section with a search bar containing 'Styrene / Styrene / 100-42-5 / 202-851-5'. A table below lists inventory details:

Inventory	Inventory number	Inventory name
EC Inventory	202-851-5	styrene
CAS number	CAS name	
100-42-5	Benzene, ethenyl-	
IUPAC name		
Styrene		

Below the table, there are input fields for 'Typical concentration' (set to 'ca.' and '98' with a unit dropdown of '% (w/w)') and 'Concentration range' (set to '>=' and '96' for the lower bound, '<=' and '99.5' for the upper bound, with a unit dropdown of '% (w/w)').

### Impurities and additives:

**Step 11.** To complete the information regarding *Impurities* and *Additives* follow the same procedure.

**Step 12.** Where the impurity or additive is considered relevant for classification and labelling of the substance, the relevant box must be ticked.

**Step 13.** The function of each *additive* has to be provided by making a selection in the picklist *Function*. Only selections beginning with the word *stabiliser* are applicable under REACH and CLP.

To report **unknown impurities**, create a generic reference substance (see *Reference substance*) and insert in the *IUPAC name* field the phrase *unknown impurities*. In the *Remarks* field of the impurity block, specify the nature, number and relative amounts of the impurities as far as possible. Also provide the *Typical concentration* (with unit of measurement) and *Concentration range* (with unit of measurement) for the *unknown impurities*.

**Figure 4: Unknown impurities**

**Impurities** ^

Unknown impurities / Unknown impurities, ca. 0.05 % (w/w), >= 0.04 - <= 0.08 % (w/w)

Reference substance  
Unknown impurities / Unknown impurities

Inventory	Inventory number	Inventory name
...	...	...

CAS number	CAS name
...	...

IUPAC name  
Unknown impurities

Typical concentration  
ca. 0.05 % (w/w)

Concentration range  
>= 0.04 <= 0.08 % (w/w)

Remarks  
3 unknown organic impurities for which the individual concentration does not exceed 0.03% according to the HPLC analysis (see section 1.4). Based on the fragmentation pattern in the HPLC-MS analysis (see also section 1.4), the structure of these impurities might include one chlorine and two bromine atoms

**Figure 5: Additive**

The screenshot shows the 'Additives' window with the following details:

- Reference substance:** 4-tert-butylbenzene-1,2-diol / 4-tert-butylbenzene-1,2-diol / 98-29-3 / 202-653-9
- Inventory table:**

Inventory	Inventory number	Inventory name
EC Inventory	202-653-9	4-tert-butylpyrocatechol
CAS number	CAS name	
98-29-3	1,2-Benzenediol,4-(1,1-dimethylethyl)-	
IUPAC name		4-tert-butylbenzene-1,2-diol
- Typical concentration:** ca. 0.01 % (w/w)
- Concentration range:** >= 0.005 - <= 0.02 % (w/w)
- Function:** stabiliser: inhibitor
- Details of function in composition:** This stabiliser is added to styrene in order to prevent its polymerisation

When reporting information on the composition, where there is any deviation from the rules for identifying a mono-constituent, multi-constituent or UVCB substance, you will need to provide explanations for the deviations in the field *Justification for deviations*. Such deviations include, for example, reporting a mono-constituent composition that includes a main constituent with a concentration of less than 80 %.

The composition to be reported depends on the substance type:

#### **Mono-constituent substances:**

**For mono-constituent** substances, you have to complete the following information:

- Report only the main constituent under the *Constituents* in section 1.2. Assign the same reference substance for this constituent as in section 1.1.
- Report individually any impurities under the *Impurities* in section 1.2.
- Report any additive necessary to stabilise your composition under the *Additives in* section 1.2. Specify the stabilising function of the additive from the picklist *Function*.
- Report the concentration range (both minimum and maximum values) and the typical concentration for the main constituent, any impurity and any additive.

Note: The typical concentration and concentration range values reported for the main constituent of a mono-constituent substance should normally not be less than 80% (w/w).<sup>6</sup>

- Report a degree of purity for your composition corresponding to the concentration range of the main constituent.

### Multi-constituent substances:

For **multi-constituent** substances, you have to complete the following information:

- Report the main constituents under the *Constituents* in section 1.2.  
Note: The main constituents should be the same for all compositions reported.
- Report any other constituent below 10% under *Impurities* in section 1.2.
- Report any additive necessary to stabilise your composition under *Additives* in section 1.2. Specify the stabilising function of the additive from the picklist *Function*.
- Report the concentration range (both minimum and maximum values) and the typical concentration for the main constituents, any impurity and any additive.  
Note: The typical concentration and concentration range values of each main constituent should normally be  $\geq 10$  and  $< 80\%$ .<sup>7</sup>
- Report a degree of purity for the composition corresponding to the overall concentration range of the main constituents.

### UVCB substances:

For **UVCB** substances, you have to complete the following information:

- Report the description of the manufacturing process, as well as other information relevant for the substance identification, in the field *Description of the composition*.  
Note: To facilitate the reporting of the manufacturing process, suggestions as to what to enter are provided in a free text template for the field *Description of composition*. To open the free text template, click on the icon that shows the letter A with an arrow at the bottom right, . A pop-up window appears. Click *Option 2: composition of a UVCB substance*. To copy the text from the template to the field, click on the button labelled *Insert*. The text should then be edited so that it contains only the relevant data.
- Report the appropriate individual constituents or groups of constituents under *Constituents*.  
Note: To provide information on the constituents or groups of constituents in your substance, you must not reuse, in section 1.2, the reference substance already assigned for your substance in section 1.1.
- Do not report any constituent under the *Impurities* header of the composition (impurities are not considered relevant for UVCBs).

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<sup>6</sup> Any deviation from the "80% rule" should not be applied, unless a valid justification is provided. This justification should be provided in the *Justification for deviations* field for each composition where such a deviation is applied.

<sup>7</sup> Any deviation from the "80% rule" should not be applied, unless a valid justification is provided. This justification should be provided in the *Justification for deviations* field for each composition where such a deviation is applied.

- Report any additive necessary to stabilise your composition under the *Additives* header. Specify the stabilising function of the additive.
- Report the concentration values of the individual constituents, groups of constituents and any additive as a concentration range (both minimum and maximum values) and typical concentration.
- Report the appropriate degree of purity for your UVCB substance (the degree of purity should normally be 100% for UVCBs which do not include any additive, as the concept of *impurity* is not considered relevant for these substances).

### Reporting the characterisation of nanomaterials:

This sub-section is filled in when *solid: nanomaterial* has been selected in the *State/form* picklist for that composition. It includes fields to report key characteristics of compositions that are nanoforms.

**Step 14.** Select the *Shape* of the nanoform from the available options in the picklist.

**Step 15.** Provide size ranges for the three *Dimensions* *x*, *y*, *z* and the unit of measurement (e.g. nm). Provide the *Percentile* (e.g. D50) of the size distributions to which the size ranges refer to. Additional information on shape of the nanoform can be provided in the *Remarks* field.

**Step 16.** Provide the ranges of specific surface areas of the nanoform, together with the unit.

**Step 17.** Under *Surface treatment applied*, indicate whether surface treatment was applied, and the type of treatment as relevant.

**Step 18.** Where surface treatment was applied, provide information on the treatment. Click on the  button to create a surface treatment block and indicate a name for the surface treatment.

**Step 19.** Next, in the table *Surface treatment* report the identity of the surface treatment agents layer-by-layer. Click on the *Add* button to create a new row for each layer. This action will open a dialogue window, where you indicate the layer number, and link a reference substance that describes the surface treatment agent applied by clicking the  button.

**Step 20.** Indicate the nature of the *External layer* by selecting one of the options available in the picklist. Provide the % (w/w) *Total fraction of core particle* that is representative of this nanoform. This value refers to the weight fraction of the core particle relative to the total weight of the surface-treated particle. Any supporting information, such as illustrations of the particle structure can be attached.

Note that several surface treatment blocks can be created within the same composition. This refers to the situation where several nanoforms with similar surface treatment exist, but where the dossier submitter has determined that this does not impact the chemical identity or the hazard profile of this composition.

When the nanoforms of the substance vary significantly in shape, specific surface area or surface treatment applied, then separate composition records are created to reflect these differences.

**Step 21.** To save the information click  from the main menu.

### 6.1.3. Section 1.3 Identifiers

In this section you can insert identifiers for regulatory programmes. In particular, this section should be used to report the following identifiers when available: REACH registration number, REACH pre-registration number, REACH inquiry number, notification number (NCD), CLP notification number.

To enter your data, you must first create a new record by right-clicking on the section name and selecting a *new fixed record*.

- Step 1.** Press *Add* button to add a new identifier to the *Regulatory programme identifiers* table.
- Step 2.** Depending on the type of submission, select the appropriate identifier from the *Regulatory programme* picklist.
- Step 3.** Enter the relevant number in the *ID* field.
- Step 4.** Click on *OK* and the added regulatory programme identifiers will appear in the table.
- Step 5.** If you need to provide more than one programme identifier, create a new row by repeating the previous steps.
- Step 6.** To save the information click  from the main menu.

### 6.1.4. Section 1.4 - Analytical information

Use section 1.4 of IUCLID to specify, if available, some of the information requested under Article 40 (1- b) of the CLP Regulation, on the identity of the substance to be notified.

- Step 1.** In the section tree of your Substance dataset, right-click the section 1.4 *Analytical information* and add *New record*.
- Step 2.** Under the *Optical activity* field, provide information on the existence or not of optical activity
- Step 3.** In the *Remarks* field, provide information on typical ratio of (stereo) isomers, whenever applicable (Figure 6).

If your substance is optically active you should also specify the value for the specific rotation (in degrees) indicating also the temperature of measurement (in °C) and the wavelength of the incident light source (in nanometres). The direction of rotation should also be specified as either + or -. If a sample solution is used the concentration and solvent name should also be provided.

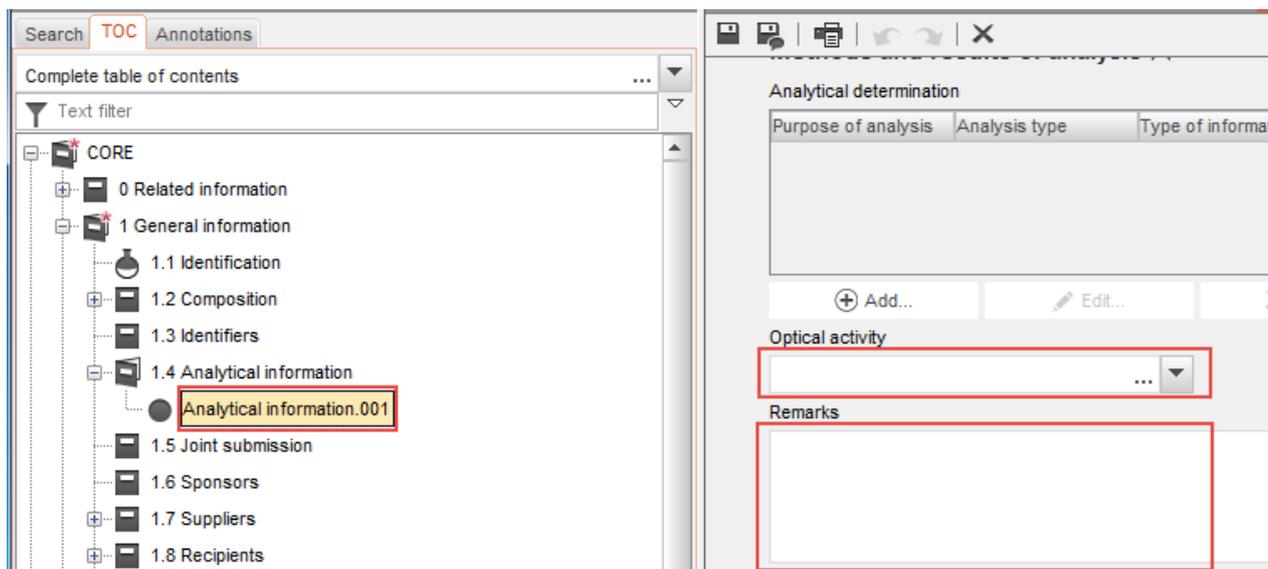
Typically specific rotation is specified as follows:

$$[\alpha]_t^{\lambda^{\circ}}$$

Where:  $[\alpha]$  = specific rotation

t = temperature in °C

$\lambda$  = wavelength of incident light; for sodium D lamp (598 nm) this is indicated simply by D

**Figure 6: Optical activity information**

Analytical methods and spectral data are not requested in a C&L notification under the CLP Regulation.

## 6.2. Section 2 C&L and PBT assessment

The information on the substance C&L according to the GHS should be included in IUCLID section 2.1

### 6.2.1. Section 2.1 GHS

Use this section to specify the Classification and Labelling (C&L) information of your substance resulting from the application of the criteria of the CLP Regulation (1272/2008).

It is highly recommended to consult Annex I of the CLP Regulation for the classification criteria and the following guidance document for more detailed instructions on the application of the C&L criteria available at <http://echa.europa.eu/web/guest/guidance-documents/guidance-on-clp>.

In this section you can create several records to indicate more than one C&L for different compositions and forms of a substance. Note that when a new record is created you must fill in the data in all requested fields.

To create a new record:

- Step 1.** Right-click on the section *2.1 GHS* in the *TOC* from the navigation panel on the left part of the screen.
- Step 2.** From the picklist select *New record*.
- Step 3.** A new record to report the classification and labelling information is created.

Harmonised classification has to be respected and you should not modify any of those harmonised hazard classes/differentiations, unless you have data based on which a stricter classification (hazard classes and/or differentiations) applies. Therefore, if your substance has a harmonised classification for some hazard classes/differentiations, you should classify for other hazards according to available and reliable data and upgrade the harmonised classification towards a stricter classification, if necessary.

To complete this section, follow the steps:

### General information:

- Step 1.** Enter a descriptive *Name* for the GHS record. This is particularly relevant in the case that multiple GHS records are created, to easily distinguish the different records.
- Step 2.** If you submit a dossier for a substance which is **not classified** you should select the checkbox *Not classified*. In this case, you should not enter any hazard category or hazard statement in the GHS record.
- Step 3.** Select a composition(s) in the *Related composition* field for which the GHS record is relevant by clicking the *Add* button.

If you have several compositions (several records in section 1.2) and several GHS records (i.e. several classification and labelling pairs), then it is mandatory that you link each GHS record to the related composition(s) by using the *Related composition* field.

Several compositions can be linked to the same C&L record if they have the same classification.

### Classification:

In this block you must select a *Hazard category* and *Hazard statement* for each hazard class of differentiation, otherwise, you must fill in the *Reason for no classification*.

The *Reason for no classification* should be selected according to the following principles:

- *data lacking* should be selected if you do not have relevant data or other adequate and reliable information that can be compared with the classification criteria;
- *inconclusive* should be selected if you have data or other information which is not reliable (e.g. data of poor quality) or if you have several equivocal study results or information. In these cases, the available data/information cannot be regarded as a firm basis for classification;
- *conclusive but not sufficient for classification* should be selected in cases where a substance is tested with the appropriate high quality reflected in the study or where other high quality information is available, and based on that, it is concluded that the classification criteria are not fulfilled.

For each of the classifications, or the reasons for no classifications, reported in this section, a justification should be provided in the field *Justification for (no) classification*. This field is

available in the endpoint summary for some specific endpoints for which classification can be derived:

- 4.13 Flammable
- 4.14 Explosiveness
- 4.15 Oxidising properties
- 6 Ecotoxicological information
- 7.2 Acute Toxicity
- 7.3 Irritation / corrosion
- 7.4 Sensitisation
- 7.5 Repeated dose toxicity
- 7.6 Genetic toxicity
- 7.7 Carcinogenicity
- 7.8 Toxicity to reproduction
- 7.9.1 Neurotoxicity
- 7.9.2 Immunotoxicity.

**Note that the CLP regulation foresees certain waivers:**

If a substance is classified for certain physical hazards, it does not need to be classified for certain others. For example: explosives, organic peroxides, self-reactive substances and mixtures as well as pyrophoric or oxidising solids should not be considered for classification as flammable solids since flammability is an intrinsic hazard in these classes.

If a substance has a particular physical state, e.g. it is a gas, it does not need to be classified for hazards that are only associated with other physical states, e.g. as an oxidising solid or corrosive to metals.

In case of the above classification waivers apply, you should select *conclusive, but not sufficient for classification* as a reason for no classification.

**and interconnections:**

If a substance is classified for skin corrosion Cat.1, the risk of severe damage to eyes is considered implicit (but not the vice versa). In this case, the substance should be classified for serious eye damage 1.

**Classification - Physical hazards:**

**Step 4.** Specify the *Hazard category* (e.g. Expl. Div. 1.1) and *Hazard statement* (e.g. H201: Explosive; mass explosion hazard) for the *Physical hazards* by selecting the appropriate values from the picklists.

The CLP Regulation implements the Globally Harmonized System of Classification and Labelling of Chemicals (GHS). However, not all the hazard categories and corresponding hazard statements from the GHS have been implemented into the CLP regulation. Therefore, please note when populating IUCLID section 2.1 - GHS that not all the available entries are relevant for CLP (e.g. Flammable liquids/Flammable liquid 4/H227: Combustible liquid).

**Classification - Health hazards:**

**Step 5.** Specify *Hazard category* (e.g. Acute Tox. 1) and *Hazard statement* (e.g. H300: Fatal if swallowed) for the *Health hazards* by selecting the appropriate values from the picklists.

In case you have conclusive data which enables you to specify the nature of *Reproductive toxicity* effects (i.e. damage to fertility and/or the unborn child), you should indicate that in the field *Specific effect* by including the appropriate additional *Hazard statement* code(s).

The following additional codes are specified in Annex VI, 1.1.2.1.2: to the CLP Regulation:

- H360F - May damage fertility.
- H360D - May damage the unborn child.
- H360FD - May damage fertility. May damage the unborn child.
- H360Fd - May damage fertility. Suspected of damaging the unborn child.
- H360Df - May damage the unborn child. Suspected of damaging fertility.
- H361f - Suspected of damaging fertility.
- H361d - Suspected of damaging the unborn child.
- H361fd - Suspected of damaging fertility. Suspected of damaging the unborn child.

For more instructions on the selection of these codes, please consult the guidance on the application of the CLP criteria available at <http://echa.europa.eu/web/guest/guidance-documents/guidance-on-clp>.

The Route of exposure for Reproductive toxicity should only be specified if it is conclusively proven that no other routes of exposure cause the hazard. Supporting evidence should be attached in section 13 (unless it is already specified in Annex VI to the CLP Regulation).

**Figure 7: Specify the nature and the route of exposure for reproductive toxicity**

Reproductive toxicity ^			
	Hazard category	Hazard statement	Reason for no class
Reproductive toxicity	Repr. 1A ...	H360: May damage ferti ...	
Specific effect	H360F May damage fertility		
Route of exposure	Oral ...	Remarks	
Effects on or via lactation	...	...	

In case you have conclusive data which enables you to explicitly specify the hazard of *Carcinogenicity* via inhalation (or it is specified in Annex VI to the CLP Regulation) you should include the corresponding additional hazard statement code (H350) in the free text field next to *Route of exposure*.

The route of exposure for carcinogenicity should only be specified if it is conclusively proven that no other route of exposure causes the hazard. Supporting evidence should be attached in section 13 (unless it is already specified in Annex VI to the CLP Regulation).

**Figure 8: Specify the hazard of carcinogenicity via inhalation**

Carcinogenicity ^			
	Hazard category	Hazard statement	Reason for
Carcinogenicity	Carc. 1A ... ▼	H350: May cause cancer <state r ... ▼	
Route of exposure	Inhalation ... ▼	H350	

**Step 6.** For the following hazard class or differentiation: *Specific target organ toxicity - single exposure (STOT SE)* and *Specific target organ toxicity - repeated exposure (STOT RE)* you should fill in *Hazard category*, *Hazard statement* and *Affected organs*, otherwise, the field *Reason for no classification* should be filled in.

It is recommended to include no more than three primary target organs for practical reasons and because the classification is for specific target organ toxicity. If more target organs are affected it is recommended that the overall systemic damage should be reflected by the phrase *damage to organs*.

If the affected organ is unknown, indicate *unknown* in the field *Affected organs*. For these and other classes/differentiations, you are also advised to indicate the *Route of exposure*, where applicable.

You can specify more than one STOT SE /STOT RE by adding additional blocks by clicking on the  symbol.

The route of exposure should only be specified if it is conclusively proven that no other route of exposure causes the hazard. Supporting evidence should be attached in section 13 (unless it is already specified in Annex VI to the CLP Regulation).

**Figure 9: Specify the affected organ**

The screenshot shows two panels for specifying target organ toxicity. The top panel, titled 'Specific target organ toxicity - single', contains the following fields: 'Hazard category' set to 'STOT Single Exp. 1', 'Hazard statement' set to 'H371: May cause damage to o...', 'Affected organs' set to 'Kidneys', and 'Route of exposure' set to 'Oral'. The bottom panel, titled 'Specific target organ toxicity - repeated', contains: 'Hazard category' set to 'STOT Rep. Exp. 1', 'Hazard statement' set to 'H372: Causes damage to orga...', 'Affected organs' set to 'liver', and 'Route of exposure' set to 'Oral'. Both panels have a 'Remarks' field.

The CLP Regulation implements the Globally Harmonized System of Classification and Labelling of Chemicals (GHS). However, not all the hazard categories and corresponding hazard statements from the GHS have been implemented into the CLP regulation. Therefore, please note when populating IUCLID section 2.1 - GHS that the following entries under the health hazards are not relevant for CLP.

Hazard class	Hazard category	Hazard statement
Acute toxicity - oral	Acute Toxicity 5	H303
Acute toxicity - dermal	Acute Toxicity 5	H313
Acute toxicity - inhalation	Acute Toxicity 5	H333
Skin corrosion / irritation	Skin Mild Irritation 3	H316
Serious eye damage / eye irritation	Eye Irritation 2A Eye Irritation 2B	H320
Aspiration hazard	Asp. Toxicity 2	H305

**Classification - Specific concentration limits:**

**Step 7.** If your substance has harmonised *Specific concentration limits*, you need to specify them by filling in at least one of the two range fields in the *Concentration range (%)* and in addition, you also need to indicate the relevant *Hazard categories*.

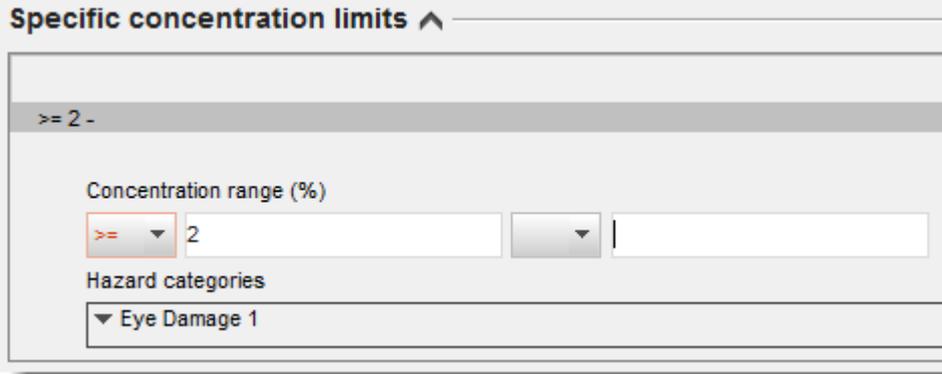
You can specify more than one concentration limit by adding additional blocks by clicking on the  symbol.

If you propose to set specific concentration limit(s) under the strict condition of Article 10 of the CLP Regulation, you have to provide a scientific justification in section 13.

For each specific concentration limit (SCL), you should specify:

- a concentration range (at least one of the two range fields);
- at least one hazard statement related to the SCL.

**Figure 10: Specific concentration limits**



The CLP Regulation implements the Globally Harmonized System of Classification and Labelling of Chemicals (GHS). However, not all the hazard categories and corresponding hazard statements from the GHS have been implemented into the CLP regulation. Therefore, please note when populating IUCLID section 2.1 - GHS that the following hazard categories under the specific concentration limits are not relevant for CLP.

Hazard category
Flammable Liquid 4
Acute Toxicity 5
Skin Mild Irritation 3
Eye Irritation 2A
Eye Irritation 2B
Asp. Toxicity 2

Classification - Environmental hazards:

**Step 8.** Specify *Hazard category* (e.g. Aquatic Acute 1) and *Hazard statement* (e.g. H400: Very toxic to aquatic life) for the *Environmental hazards* by selecting the appropriate values from the picklists.

The CLP Regulation implements the Globally Harmonized System of Classification and Labelling of Chemicals (GHS). However, not all the hazard categories and corresponding hazard statements from the GHS have been implemented into the CLP regulation. Therefore, please

note when populating IUCLID section 2.1 - GHS that the following entries under the environmental hazards are not relevant for CLP.

Hazard class	Hazard category	Hazard statement
Hazardous to the aquatic environment	Aquatic Acute 2	H401
	Aquatic Acute 3	H402

If a substance meets the criteria for classification to the aquatic environment as both, Aquatic Acute 1 AND Aquatic Chronic 1 (or other category):

- select from the picklist in the field *Hazardous to the aquatic environment (acute / short-term)*, the category *Aquatic Acute 1* and the hazard statement *H400*;
- select from the picklist in the field *Hazardous to the aquatic environment (long-term)*, the category *Aquatic Chronic 1* (or relevant category) and the hazard statement *H410* (or relevant hazard statement).

When a substance is classified as *Aquatic Acute 1* and/or *Aquatic Chronic 1*, multiplying factor(s) (M-factor) has/have to be assigned. Where appropriate, *M-factors* shall be set for acute and long-term hazards separately. This means that there can be two different *M-factors* for one substance.

If you propose to set such M-factors you have to provide a scientific justification in section 13.

**Figure 11: Specify the Environmental hazards**

The screenshot shows the 'Aquatic environment' section in the IUCLID software. It contains a table with two columns: 'Hazard category' and 'Hazard statement'. The first row shows 'Aquatic Acute 1' and 'H400: Very toxic to aquatic life.'. The second row shows 'Aquatic Chronic 1' and 'H410: Very toxic to aquatic life with long-term effects'. Below the table, there are two input fields for 'M factor acute' (value 10) and 'M factor chronic' (value 100).

**Labelling:**

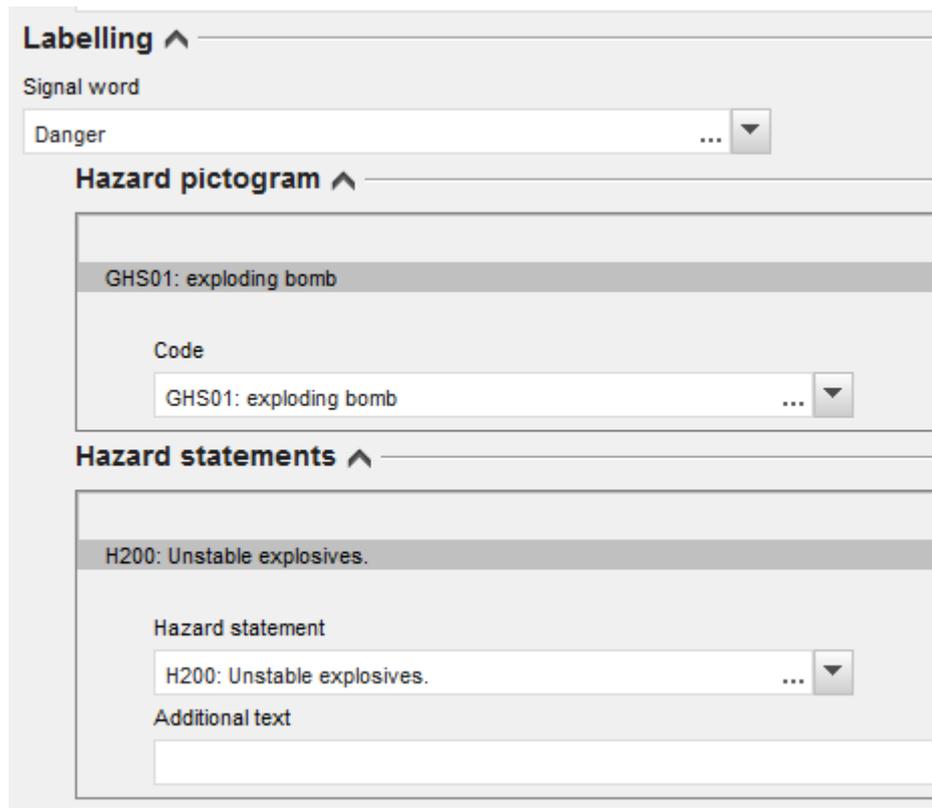
**Step 9.** Specify the *Signal word* by selecting the appropriate value from the picklist. If no signal word applies to your substance, then you need to select *No signal word* from the picklist.

**Step 10.** If applicable, please select a *Hazard pictogram* from the picklist. You can select more than one pictogram by clicking on ⊕.

**Step 11.** You should select at least one *Hazard statement* from the picklist and provide *Additional text* where applicable or, if no hazard statement applies to your substance, then you need to select *No hazard statement*.

You can always specify more than one hazard statement for the labelling by clicking on .

**Figure 12: Labelling for section 2.1**



The screenshot shows a web-based interface for labelling. It is divided into three main sections:

- Signal word:** A dropdown menu with 'Danger' selected.
- Hazard pictogram:** A dropdown menu with 'GHS01: exploding bomb' selected. Below it, a 'Code' field also contains 'GHS01: exploding bomb'.
- Hazard statements:** A dropdown menu with 'H200: Unstable explosives.' selected. Below it, a 'Hazard statement' field also contains 'H200: Unstable explosives.', and an empty 'Additional text' field is visible.

The principles of precedence for the hazard pictograms are stated in Art. 26 of CLP Regulation, for example, if the hazard pictogram 'GHS06' applies, the hazard pictogram 'GHS07' shall not appear on the label. Please consult CLP Regulation and/or the guidance on the application of the CLP criteria to ensure consistency of the between the classification and labelling sections.

According to Art. 27 of CLP Regulation, some hazard statements are not required in the label because of redundancy. A few examples are listed below. For additional information please consult the guidance on the application of the CLP criteria.

Hazard classification	Associated hazard statement(s)	Associated hazard statement that could appear on the label
Skin Corr. 1B and Eye Dam. 1	H314; H318	H314
Aquatic Acute 1 and Chronic 1	H400; H410	H410

Aquatic Acute 1 and Chronic 2	H400; H411	H410
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The CLP Regulation implements the Globally Harmonized System of Classification and Labelling of Chemicals (GHS). However, not all the hazard categories and corresponding hazard statements from the GHS have been implemented into the CLP regulation. Therefore, please note when populating IUCLID section 2.1 GHS that the following hazard statements for labelling are not relevant for CLP.

<b>Hazard statement (in Labelling section):</b>
H227: Combustible liquid
H303: May be harmful if swallowed
H305: May be harmful if swallowed and enters airways
H313: May be harmful in contact with skin
H316: Causes mild skin irritation
H320: Causes eye irritation
H401: Toxic to aquatic life
H402: Harmful to aquatic life
H303+H313: May be harmful if swallowed or in contact with skin
H303+H333: May be harmful if swallowed or if inhaled
H313+H333: May be harmful in contact with skin or if inhaled
H303+H313+H333: May be harmful if swallowed, in contact with skin or inhaled
H315+H320: Causes skin and eye irritation

**Step 12.** If applicable, please select a *Precautionary statements* from the picklist.

**Step 13.** If applicable, please specify the *Additional labelling requirements*. These include supplemental CLP hazard statements and additional labelling elements resulting from the application of CLP Article 25. Please consult the CLP Regulation and Guidance for further information on the additional labelling requirements.

**Notes:**

**Step 14.** If applicable, you can select note(s) from the picklist.

### 6.3. Section 13 Assessment reports

Section 13 can be used to attach the scientific justification requested under Article 40(1e) of the CLP regulation:

- if you want to set specific concentration limit(s) (SCL) or an M-factor under the strict conditions of Article 10 of the CLP Regulation, you have to attach a scientific justification for it,

- for the scientific justification, you should use the relevant parts of the Chemical Safety Report format according to Annex I to REACH. There is no need for a justification if the SCL value is given in Table 3.1 of Annex VI to the CLP Regulation (“the harmonised list”),
- further, this section should be used to demonstrate that a hazard is only caused by specific route(s) of exposure (unless specified in the harmonised list (Annex VI to CLP) or to submit the reasons for Classification and Labelling deviating from existing entries in the C&L inventory (Article 16(1) of the CLP regulation).

Use this section to attach, if needed, the justification requested under Article 16(1).

It should be noted indeed that in the case you do not agree with the classification and labelling (excluding the harmonised ones in Table 3.1 of Annex VI) already present in the C&L inventory, you have to provide a reason for this specific hazard class or differentiation. The reason can include for example an:

- indication that an impurity/additive has an impact on the C&L; or/and
- indication of the substance form/state; or/and
- indication that you have relevant data/information supporting your classification of the substance.

You then need to attach the document containing the justification in IUCLID as part of the substance dataset as follows:

- Step 1.** Right-click section 13 *Assessment Reports* from the navigation panel on the left part of the screen.
- Step 2.** From the picklist select *New record*.
- Step 3.** A new endpoint study record section appears. Re-name the new endpoint study record to "Justification for a SCL or M factor in accordance with Article 10 of the CLP Regulation" or "Justification for route of exposure or Reason for not agreeing with a notified C&L (article 16)" and save it.

To complete this section follow the steps:

- Step 1.** In the *Type of report* picklist, choose *REACH Chemical safety report (CSR)* or *other*. If *other* is selected then you have to fill in the adjacent field.
- Step 2.** In the *Document/report* field click the  button. In the pop-up window, click *Browse*, find the relevant document, and attach it. Use the *Remarks* field to specify further the nature of the document. Then click *OK*.

Repeat the steps if you need to attach more documents in this section.

## 7. How to create a Dossier

Once you have included all relevant information in your substance dataset, the next step is to create a dossier.

Before creating a dossier you are advised to check the completeness of your substance dataset by running the *Validation assistant*. For more information on how to run the Validation assistant refer to the help system of IUCLID.

This may also be a good time to verify if the quality of the dataset can be improved before creating a dossier, please check the webpage *How to improve your dossier* on the ECHA

website: <http://echa.europa.eu/support/how-to-improve-your-dossier>

- Step 1.** To create a dossier open the list of available substance datasets by clicking on the *Substance*  on the IUCLID home page.
- Step 2.** All available substances (within the limits of the search results managed in the user's preferences) are displayed in the navigation panel on the left part of the screen. If a substance does not appear in the list you can search for it using the search panel. If the list is very long, you can also filter by typing (part of) the name of the substance in the filter field.
- Step 3.** Select the substance for which you want to create a dossier.
- Step 4.** Right-click on the substance in the query results list. From the pop-up menu select *Create dossier*.
- Step 5.** After selecting the *Create dossier* option the dossier creation wizard is displayed. Follow the steps in the dossier creation wizard.

Only two steps are displayed in the dossier creation wizard as the default option: *Select submission type* (1) and *Complete the dossier header* (5). If you wish to change the default settings to have more options you can select the checkbox *Use advanced settings*.

- Step 1. **Select the submission type.**** Choosing the correct dossier template by selecting the submission type is essential for a successful submission. Before exporting your dossier you have to make sure that the selected template corresponds with the intended submission.  
When the checkbox *Use advanced settings* is selected follow the steps 2-4, if the default settings are kept (recommended approach), go to step 5 directly.
- Step 2.** Define the confidentiality level by selecting the data protection flags. If you have included any confidentiality or regulatory programme flags in your substance dataset, please make sure that the relevant information is included in your dossier by selecting the appropriate flags in this step. If you are unsure it is recommended to select the defaults option 'all fields - including confidential test material'. ECHA will assess the confidentiality of the information and the justifications provided. You can find more information on the publication of part of the dossier on the ECHA website at <http://echa.europa.eu/manuals>.
- Step 3.** Select whether the annotations should be included in the dossier.
- Step 4.** Verify and select which documents and entities will be included in your dossier. To this end, select in the Entities list the substance entity which will be preceded by . The documents and entities connected to the substance will be listed in the References to window; documents to be included are already checked. Certain documents, such as section 1.1, will always be included in a dossier, and cannot be excluded in this step. Likewise, depending on the submission type, some documents will not appear in the list and cannot be included as they are not relevant for the selected submission type. If you are unsure of the information to be included, you can select Next and rely on the default settings for that submission type.
- Step 5. **Complete the dossier header**** by entering additional administrative information.

Information contained in the dossier header is crucial for business rules checking when you submit your dossier. Missing or incorrect information can result in that your submission cannot be accepted for further processing and will be automatically removed from the system. In this

case you need to create a new dossier with corrected information and submit it again. For more information refer to the Annex: *Overview of the business rules checks performed by ECHA on the submitted dossiers*.

The following subchapters describe how to fill in the administrative information in the dossier header.

## 7.1. Administrative information

Enter an appropriate *Dossier name* which enables you to easily identify the dossier when searching and exporting it from IUCLID.

When relevant, enter a *Dossier submission remark*. This remark can include further information on the reason for the submission (e.g. detail which information has been updated).

## 8. How to export a Dossier

To start the export process, first search for the *Dossier*  in the navigation panel of the IUCLID application. When the Dossier is shown in the list of search results, right-click on its entry, and then select *Export* from the menu.

For details on the export wizard, see the help that is built in to the IUCLID application.

## 9. Submit Dossier

To submit your dossier to ECHA you must sign-up in REACH-IT with the legal entity details of the submitting entity, and follow the instructions provided there for your specific type of submission.

You can access REACH-IT from ECHA website: <http://www.echa.europa.eu/> or go directly to the REACH-IT website: <https://reach-it.echa.europa.eu/>.

## 10. Update Dossier

If you need to update your dossier, you do not need to re-type again all your substance data. Instead you can update the information in the substance dataset. To edit the substance dataset, select it from the navigation panel and fill in or update the relevant data. When the dataset is ready you can create a dossier (see chapter *How to create a Dossier*).

## Annex 1. Overview of the business rules checks performed by ECHA on the submitted dossiers

Business rules are a set of dossier format and administrative pre-requisites that must be fulfilled before ECHA can establish that the dossier can be handled properly and that the required regulatory processes can be successfully carried out. Business rules do not assess the completeness or compliance of the data provided. If the dossier submission fails at the business rule level, the dossier will be automatically removed from the system, and a new submission is required before any regulatory processes can be initiated. You can see the outcome of the business rules check in the submission report in REACH-IT.

This document will guide you through the basic requirements of creating the substance dataset and the IUCLID dossier header. In addition, it is recommended to use the IUCLID Validation Assistant plugin on the substance dataset and also on the final dossier before exporting it from IUCLID and submitting it to REACH-IT. Right-click on your substance dataset or on the dossier in the IUCLID navigation panel and select *Validate*. This plugin will check most of the business rules. However, some of the business rules depend on the information that is stored within the REACH-IT database, and therefore the plugin cannot simulate all the business rules checked by the Agency.

Business Rules applicable only for the CLP notifications		
Location (IUCLID/REACH-IT)	Rule description	Relevance
<b>IUCLID substance dataset</b>	A dossier must be created from a substance dataset. It cannot be created out of a mixture or product dataset.	All dossier types
<b>IUCLID section 1.1 – Identification</b>	A reference substance must exist in section 1.1.	All dossier types
<b>IUCLID section 1.1 - Identification</b>	At least one of the following fields must be provided for the reference substance in section 1.1: EC/List number CAS number Molecular formula AND molecular weight AND structural formula SMILES notation Remarks	CLP Notifications
<b>IUCLID section 1.1 – Identification; section 1.2 – Composition</b>	Each reference substance in section 1.1 and 1.2 must contain a substance identifier. An acceptable substance identifier is: EC/List number CAS number IUPAC name  Any EC/List number defined in section 1.1 and 1.2 of IUCLID must exist in the REACH-IT EC inventory.  If you use a reference substance to report unknown constituents/impurities, they must be “identified” by inserting “Unknown constituent/impurity” in the IUPAC name field.	All dossier types

	If categories are used, this rule is applied to all the category member substances.	
<b>IUCLID section 1.1 – Identification</b>	In an update submission, the substance must be identified by an EC/List number.	CLP Notifications
<b>IUCLID section 1.2 - Composition</b>	At least one composition must be defined in section 1.2. The following requirements are also to be fulfilled: All created compositions must contain at least one constituent. All constituents must be linked to a reference substance.	All dossier types
<b>IUCLID section 1.2 – Composition</b>	All compositions created in section 1.2 must have the composition type indicated. At least one of the compositions in section 1.2 must reflect the composition of the substance manufactured/imported by the registrant. This composition must be marked as the “Legal entity composition of the substance”.  If the composition type “other” is selected from the list, the relevant information must be provided in the adjacent free text field.	All dossier types
<b>IUCLID section 1.1 – Identification; section 1.2 – Composition</b>	If the substance is defined as mono-constituent, the first ‘legal entity composition of the substance’ in section 1.2 has to have a matching substance identity when compared with the reference substance in section 1.1.	All dossier types
<b>IUCLID section 1.1 - Identification; section 1.2 - Composition</b>	If the substance is defined as a multi-constituent substance, the reference substance in section 1.1 cannot be identical to any of the constituents defined in the first composition of type ‘legal entity composition of the substance’ in section 1.2.	All dossier types
<b>IUCLID section 1.2 - Composition</b>	All constituents of a multi-constituent or of a UVCB substance must identify distinct reference substances.	All dossier types
<b>IUCLID section 1.1 - Identification; section 1.3 – Identifiers</b>	The EC number assigned to the Inquiry number you have indicated in section 1.3 must match with the EC number linked to the reference substance in Section 1.1	CLP Notifications
<b>IUCLID section 1.2 – Composition</b>	At least one value and a unit must be provided for the ‘Degree of purity’ for each ‘Legal entity composition of the substance’ in section 1.2.	CLP Notifications
<b>IUCLID section 1.2 – Composition</b>	The full ‘Concentration range’ (lower and upper value together with a unit) must be provided for each constituent, impurity and additive of a legal entity composition in IUCLID section 1.2. When reporting a constituent, impurity or additive at exactly 0% or 100%, provide this value, together with the unit, in the field ‘Typical concentration’ and leave the ‘Concentration range’ fields empty.	CLP Notifications
<b>IUCLID section 1.2 - Composition; section 2.1 - GHS</b>	When creating a substance dataset containing multiple compositions of type ‘Legal entity composition of the substance’ in section 1.2, all of them must be linked to a classification and labelling record in section 2.1.	CLP Notifications

<p><b>IUCLID section 1.2 - Composition; section 2.1 - GHS</b></p>	<p>When you are reporting several compositions in section 1.2 and several records in classification and labelling (C&amp;L) in section 2.1 then each composition must be assigned to the corresponding C&amp;L record, through the section 2.1 field 'Related composition'.</p>	<p>CLP Notifications</p>
<p><b>IUCLID section 1.2 - Composition</b></p>	<p>When submitting CLP notifications, only compositions of type 'Legal entity composition of the substance' are allowed.</p>	<p>CLP Notifications</p>
<p><b>IUCLID section 1.3 - Identifiers</b></p>	<p>When submitting an update to a previously notified substance (NONS), it is not enough to provide the Registration number, but the matching NCD number must also be indicated.</p>	<p>CLP Notifications</p>
<p><b>IUCLID section 2.1 - GHS</b></p>	<p>At least one set of classification and labelling information must be provided in GHS format under section 2.1.</p>	<p>CLP Notifications</p>
<p><b>IUCLID section 2.1 - GHS</b></p>	<p>If at least one classification is provided in a C&amp;L record in section 2.1 then:  a 'Signal word' must be provided in the 'Labelling' block of the same record.  a 'Hazard statement' or a 'CLP supplemental hazard statement' must be provided in the 'Additional labelling requirements' block of the same record.</p> <p>If no classification is provided, the tick box 'Not classified' should be selected and no hazard statements and no signal words should be provided.</p>	<p>CLP Notifications</p>
<p><b>IUCLID section 2.1 - GHS</b></p>	<p>For each 'Specific concentration limit' block that is created in a C&amp;L record in IUCLID section 2.1, at least one of the two fields under 'Concentration range (%)' must be provided. In addition, at least one selection must be made under 'Hazard categories'.</p> <p>If no classification is given in a C&amp;L record, the tick box 'Not classified' should be marked and no specific concentration limits should be indicated in that record.</p>	<p>CLP Notifications</p>
<p><b>IUCLID section 2.1 - GHS</b></p>	<p>If the substance is classified, a 'Hazard category' and a 'Hazard statement' must be provided, or a 'Reason for no classification' for each hazard class in IUCLID section 2.1 should be indicated.</p> <p>If the substance is not classified, the tick box 'Not classified' should be marked and no classification should be provided in that record.</p>	<p>CLP Notifications</p>
<p><b>IUCLID section 2.1 - GHS</b></p>	<p>If the substance is classified, at least one block for 'Specific target organ toxicity - single' and 'Specific target organ toxicity - repeated' must be provided in IUCLID section 2.1. For each block, a 'Hazard category', a 'Hazard statement', and 'Affected organs' must be provided, or indicate a 'Reason for no classification'.</p> <p>If the substance is not classified, the tick box 'Not classified' should be marked and no classification.</p>	<p>CLP Notifications</p>
<p><b>IUCLID dossier header</b></p>	<p>Once a reference number for a registration/notification is granted, it is not allowed to submit another initial submission for the same</p>	<p>CLP Notifications</p>

	substance from the same legal entity. If you need to modify/add data, an update submission is required.	
<b>IUCLID dossier header</b>	<p>Updates can be submitted in the following cases:</p> <p>Following the successful registration / notification of this particular substance, after having received a reference number (spontaneous update).</p> <p>Following a technical completeness check (TCC) failure (requested update).</p> <p>Following a request for further information by the Agency (spontaneous or requested update as specified in the request).</p> <p>In any other case, an initial submission is required.</p>	All dossier types - Updates
<b>IUCLID dossier header</b>	<p>If you wish to submit a spontaneous update then the following conditions must be fulfilled:</p> <p>In the dossier header tick the boxes 'The submission is an update' and 'Spontaneous update'.</p> <p>Insert the submission number to the last successful submission as the 'Last submission number'.</p> <p>Select an appropriate justification for updating by first creating a block under 'Spontaneous update' and then making a selection in the pick-list. If you selected 'other:', you are required to give the reason in the adjacent free text field.</p>	CLP Notifications
<b>IUCLID dossier header</b>	<p>If you wish to update your dossier following a request by the Agency then the below conditions must be fulfilled:</p> <p>In the dossier header tick the boxes 'The submission is an update' and 'Further to a request from a regulatory body'.</p> <p>Insert the submission number to the last successful submission as the 'Last submission number'.</p> <p>Provide the annotation number in the field 'Number'. The annotation number can be found in REACH-IT under the Key documents in the letter that motivated the update.</p>	CLP Notifications
<b>IUCLID dossier header</b>	<p>Legal entity change cannot be performed by submitting and update to the dossier. The 'Legal entity change' module in REACH-IT is to be used to carry out the administrative changes related to ownership of the registration/notification.</p>	CLP Notifications
<b>IUCLID dossier template</b>	<p>The dossier template used in IUCLID must correspond with the intended submission type in REACH-IT.</p>	All dossier types
<b>REACH-IT</b>	<p>A new dossier cannot be submitted when the previous submission for the same substance is still being processed.</p>	All dossier types - Updates
<b>REACH-IT</b>	<p>It is not allowed to submit a CLP notification while a registration dossier for the same substance is currently undergoing a submission process.</p>	CLP Notifications
<b>REACH-IT</b>	<p>No submissions can be made from the account of a legal entity, which at the time of submission undergoes the legal entity change (merge) process.</p>	All dossier types

	Legal entity change functionality is available in REACH-IT.	
<b>REACH-IT</b>	It is not allowed to upload a new dossier for the same substance, when the previous submission is still being processed.	CLP Notifications
<b>REACH-IT</b>	Parallel submissions are not allowed for the same annotation number. You cannot submit a dossier quoting the same annotation number while another dossier is still being processed.	CLP Notifications
<b>REACH-IT</b>	It is not allowed to submit an initial/update CLP notification, if the substance has already been registered by the submitting legal entity.	CLP Notifications

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