

Functionalities of IUCLID Cloud

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1. Technical terms

The following technical terms are used within the context of IUCLID 6 and its interface.

Table 1: Some technical terms

Term	Description
Entity	Entities are data objects in IUCLID that are designed to group together data that serves a unique and specialist purpose. An example of an entity is a <i>Reference substance</i> . In some cases, an entity can be re-used across various different data objects. If such an entity is edited, the change appears immediately in data objects that refer to it. An exception to that is a <i>Dossier</i> , which is a read-only snapshot of data.
Document	A <i>document</i> is a page that contains functionality for creating, viewing or modifying an entity, a record, or a summary. The term <i>document</i> is also used to mean a standard set of data that exists in a <i>Substance</i> as a node in the table of contents. For example, in the OECD harmonised templates there is a document named <i>Acute toxicity: oral</i> .
Field	A <i>field</i> is a location within a data object in which a specific piece of data is stored. The type of data is the same throughout an individual field, for example, the field could contain free text, a value chosen from a drop-down menu, or a number. There can be many fields in one data object. An example of a field is, <i>IUPAC name</i> .
Dataset	A <i>dataset</i> is a collection of documents and/or entities stored within it. It can be of the following types: <i>Substance</i> , <i>Mixture/Product</i> , <i>Template</i> or, <i>Category</i> . For clarity and where appropriate, the type of the dataset should be stated, for example <i>Substance dataset</i> .

2. Common functionalities in the interface

The following functionalities are used throughout the interface.

2.1. Free text template

A free text template is a piece of text designed to help the user to enter all the required information into a text field. It provides a model text, which must then be edited to fit in with the particular circumstances of the user, in that context.

To open a free text template, click on the icon that shows the letter A with an arrow at its lower right, . To copy the text from the template to the field, click on the button labelled *Insert...*. The text should now be edited as required.

2.2. Flag

Certain fields, and sections within documents can be labelled with a flag. A flag can be set to indicate confidentiality and/or an association with a particular regulatory programme.

If a field or a section can have a flag set, whilst editing, a flag icon is shown to the left of its name. The icons are described in the table below.

A section can be a whole record in the table of contents in a substance, for example the record of type *Analytical information*. This whole record can be labelled with a single flag.

By default, no flags are set.

When setting a flag, if a justification of the confidentiality is required, enter it into the field *Justification*, which is a free text field that has a free-text template. Suggestions as to what to enter are provided in a free text template. To open the free text template, click on the icon that shows the letter A with an arrow at the bottom right, . To copy the text from the template to the field, click on the button labelled *Insert*. . The text should now be edited as required.

To set an association with a regulatory programme, tick one or more of the boxes.

The possible states of a flag each have their own icon as shown below.

Table 2: The icons for the states of a flag

Icon	State
	No flag is set.
	A flag is set but confidentiality is not involved.
	A flag is set that involves confidentiality.

The details of any flags set are given in the record of a document.

2.3. Rich text input

Some text fields allow text to be entered in rich text format. This allows for various types of formatting, such as tables. A full description of rich text is out of the scope of this document.

3. Table of contents

The *Table of contents* is shown for entities of type *Substance*, *Mixture/Product* and *Template*. The *Table of contents* has three main functions, as follows:

1. Provides access to specific documents in an entity;
2. Shows the structure of the documents in an entity in a particular regulatory context;
3. Indicates whether a document is mandatory for a particular type of data submission made for regulatory purposes. This is done using a red asterisk on the icon of a document.

The way in which the *Table of contents* is displayed can be set to suit a particular regulatory context, and/or type of data submission made for regulatory purposes, which includes a view for each type of Dossier. The name of the current view is stated in the field *Submission type*, which is above the *Table of contents*.

REACH Complete table of contents, shows all the documents that have any relevance to the REACH regulation, in the structure used for Dossiers submitted under REACH. This view refers to

no specific type of Dossier so the only document that is marked as mandatory is *General information / Identification*.

Whilst entering data intended for submission in a particular type of Dossier, it is recommended to keep the *Table of contents* view set to that Dossier type.

In the *Table of contents* view *Complete table of contents*, sections have been separated out from each other and displayed in sections determined by their origin. Sections not specific to a legislation are displayed in a section referred to as *CORE*, and those from the OECD harmonised templates are in a section named *OECD*. In addition, IUCLID 6 is supplied with the following *EU_BPR*, *EU_CLP* and *EU_REACH*.

This means that under a legislation specific *Table of contents* view such as *REACH Registration above 1000 tonnes*, documents could have originated from either *CORE*, *OECD*, or *EU_REACH*. In addition, some documents can be shown together in the same section under the *Table of contents* view for *REACH*, where under the *Table of contents* view *Complete table of contents*, those same documents are shown in separate sections.

For example, for a submission type of *REACH Registration 10 – 100 tonnes*, if a *Site* is added to section 3.3 *Sites*, it appears under *complete table of contents* in *CORE / section 3.3 Sites*. Similarly, for a submission type of *REACH Registration 10 – 100 tonnes*, if an endpoint study summary is added to section 6.1.1 *Short-term toxicity to fish*, it appears under *OECD* in the harmonised template *C Effects on biotic systems, section 41 Short-term toxicity to fish*.

3.1. Endpoint study record

An *endpoint study record* provides a template with predefined fields in which data is entered to describe a study carried out within the subject area defined by the title of the section, for example *Long-term toxicity to fish*. All entries under the OECD harmonised templates are *endpoint study records*.

3.2. Endpoint summary

An *endpoint summary* provides a means of grouping *endpoint study records* and of providing further information about the grouping. An *endpoint summary* contains links to *endpoint study records* in the field *Link to relevant study records(s)*.

If an endpoint study record is created under *OECD*, and an endpoint summary is created under *CORE* for the same section, when that section is viewed for a particular legislation, both are shown.

3.3. Record

If a *record* contains data that cannot be described as an *endpoint study*, it is referred to just as a *record*.

3.4. Summary

A *summary* as opposed to an *endpoint summary* refers to only *records*, not *endpoint study records*.

3.5. Fixed record

A *fixed record* is created in a section where there can be only one *record*.

3.6. Filter the Table of contents

Filter is a field into which a search term can be entered that is applied immediately to the Table of contents. Any node in the Table of contents that contains the search term anywhere in its name is shown. This includes all records and summaries. The Table of contents hierarchy is expanded as far as is required to show the matching node or nodes. Spaces are interpreted literally. It is not sensitive to case.

The search term can be cleared by clicking on the icon with a cross that is located at the right of the field.

The example below shows filtering for section titles:

search term **biot** shows *OECD / C Effect on biotic systems / 56 Biotransformation and kinetics*

search term **bioti** shows *OECD / C Effect on biotic systems*

3.7. Ordering documents within a section of the Table of contents

The order in which documents are shown within a section of the *Table of contents* can be set manually by selecting and then dragging them.

3.8. Attachments

This is where the relationship between the currently open document and its attachments is managed. Attachments are individual computer files created from outside IUCLID. Attachments can be added, opened, deleted; and remarks can be recorded.

4. Substance

A *Substance* is an entity in IUCLID that is used to store information about something that, in a regulatory context, is considered a single chemical substance.

The fields in a *Substance* are designed to allow the recording of a broad range of different types of information relevant to the regulation of chemical substances. The fields are organised in a *Table of contents*.

In the table of contents, the identity of the *Substance* is defined in section *1 General information*. In section *1.1 Identification*, there are two mandatory fields: *Substance name* and *Legal entity*.

More detail can be provided about the *Substance* identity in section *1.2 Composition*, where one or more compositions can be defined. A composition may contain the identities of *constituents*, *additives* and *impurities*, and their relative proportions. To define the identity of a *Substance* properly for a specific legislation, and to know how to enter sufficient data into the *Substance* entity, see the guidance for that legislation, such as the manuals provided on the ECHA website at the following link.

<http://echa.europa.eu/manuals>

4.1. Related information for a Substance

In Section 0 *Related information* for a *Substance* there are subsections that show how the particular *Substance* relates to other specific entities of type *Template*, *Category*, *Mixture/Product* and *Assessment entity*.

Templates indicates which *Templates* are attached to the *Substance*, as described in section 4 *Template*. *Categories* indicates in which *Categories* the *Substance* has been placed, as described in section 5 *Category*. *Mixtures* indicates in which *Mixture/Products* the *Substance* plays a role, as described in section 3 *Mixture/Product*. *Assessment entities* contains information on how the *Substance* is involved in the assessment process, as described in the next section.

4.2. The Assessment entity

An *Assessment entity* can be thought of as a wrapper for a set of substance property data (across endpoints) that is used for assessment purposes. It enables the definition of consistent sets of properties that are relevant to the assessment of specific compositions/forms of the substance (placed on the market or generated upon use).

The *Assessment entity* aims to provide a tool to assist users in documenting complex assessment cases in IUCLID. When the assessment is straightforward, there is no need to define *Assessment entities*.

Each *Assessment entity* consists of a name, a composition and a list of related endpoint summaries. All endpoint study records that are relevant for the summary of a specific endpoint, are to be actively linked by the assessor to the summary itself.

4.2.1. Introduction to Assessment entity in IUCLID

When clicking on the 0.4 *Assessment entity*, the *Assessment entity* overall pane opens. In the field Approach to fate/hazard assessment, a description of the set(s) of properties of the substance used for the assessment considering the chemical behaviour of the substance in the different foreseen uses, can be provided. Such description provides the overall reasoning where *Assessment entities* are created.

A specific field to provide a description on the approach to fate/hazard assessment for the public is also available.

In the same overall pane, the *Assessment entities* table shows the full list of *Assessment entities* available for the substance. This table is automatically populated as soon as an *Assessment entity* is defined in section 0.4 of the *Substance*. The functionality go to link target navigates to the selected *Assessment entity* and displays the related information.

4.2.2. How to create an Assessment entity

An *Assessment entity* can be created from within the Table of contents of a *Substance*. The options are:

- Registered substance as such
- Specific composition/form of the registered substance
- (group of) constituent in the registered substance

- Transformation of the registered substance

The following fields are displayed for the various types of *Assessment entity*.

4.2.2.1. *Name of the Assessment entity*

The user should indicate the name of the *Assessment entity*. As this name will not be displayed in the tree view, it is suggested to re-name the *Assessment entity* in the tree view accordingly.

4.2.2.2. *Relation to the registered substance*

This depends on the type of *Assessment entity*. It is read-only.

4.2.2.3. *Assessment entity composition*

In this table, the user defines the composition of the *Assessment entity*, to support the understanding of the *Assessment entity* definition. Depending on the type of *Assessment entity*, the user creates link to one of the following:

- an available composition in section 1.2 [*Specific composition/form of the registered substance*];
- a list of *Reference substances* that are part of the compositions in section 1.2 [(*group of constituent in the registered substance*)];
- one of the *Reference substances* available in IUCLID [*transformation of the registered substance*]

4.2.2.4. *Compositions/forms covered by the Assessment entity*

A link to compositions reported in section 1.2 can be made to indicate that the *Assessment entity* is expected to be used for the assessment of those compositions. Such a link is useful for the understanding of the assessment approach.(see the Manual on How to prepare Registration and PPORD Dossiers).

4.2.2.5. *Additional information*

Report specific information not already stated in the overall explanations on why *Assessment entity* has been created (in the field *Approach to fate/hazard assessment*). For example one could use this field to explain the reasoning for grouping constituents as part of a (group of) constituents.

4.2.2.6. *Endpoint summary linked*

To enable transparency and sorting of the information in the IUCLID dataset, all study records and endpoint summaries relevant to an *Assessment entity* should be linked to it. This will for example enable them to be sorted in the view of the IUCLID data set, and to report them in a sorted way in the CSR when using the *Report generator*. From this table, the user can link all endpoint summaries that are relevant for the *Assessment entity*. An explanation of the relevancy of one or several endpoint summary(-ies) for the *Assessment entity* can be provided, when needed, in the field *Notes* when linking it to the *Assessment entity*. In case one or several summaries have a different explanation, a new repeatable block can be added. In each endpoint summary linked,

users are invited to provide the link to all study records relevant for the summary itself. In this way, the *Assessment entity* is indirectly linked to the endpoint studies.

4.2.2.7. Reaction schema

Upload the image of the reaction schema when needed [for *Transformation of the registered substance*].

5. Mixture/Product

A *Mixture/Product* is an entity in IUCLID that is used to store information either about something that, in a regulatory context, is considered a mixture or, under the biocides legislation BPR, a product.

6. Template

A *Template* is an entity that allows data from multiple sections to be inserted into a *Substance* or *Mixture/Product* entity all at once without having to manually recreate all the sections individually and re-enter data.

7. Dossier

A *Dossier* is a write-protected copy of the data stored in a *Substance*, a *Category* or a *Mixture/Product*. Typically, a *Dossier* is used to submit data to a regulatory authority to satisfy a legal obligation arising from a legislation, for example REACH.

7.1. The structure of a Dossier

A *Dossier* is an entity that contains a read-only copy of data from a *Substance* or *Mixture/Product*, plus header information, and in some cases category information. On opening a *Dossier* from the list of search results in the *Navigation* panel, a tab appears labelled *Components*. Under this tab, there is a tree view of the entities in the *Dossier*. The copy of an entity in a *Dossier* has an image of a lock superposed on to its icon to indicate that it is read-only. The original entity is still accessible, but there is no link between it and the copy in the *Dossier*. By default, the tree view is fully collapsed showing only the *Substance* or *Mixture/Product* from which the *Dossier* was created, and any *Legal entity* that may have been included in the *Dossier*. Check that the *Dossier header* contains all the information that was entered into the *Dossier* creation wizard.

The tree view can be expanded to see which entities are in the *Dossier*.

8. Legal entity

In IUCLID, a *Legal entity* is used to store information about a party or person that is involved in the life-cycle of a chemical substance, mixture or product. A *Legal entity* can be used to identify the party that is responsible for a certain activity, such as the manufacturing or import of a substance. The *Legal entity* does not have to be created by the person or party it represents. For example, a

manufacturer can create a *Legal entity* to store information on a third party representative of the substance, or an only representative can create *Legal entities* to identify their suppliers.

A *Legal entity* can be associated with various entities, such as *Substance*. When a User creates an entity, by default, the working legal entity for the User is assigned to the entity. This can subsequently be changed to any of the *Legal entities* to which the User has access, not just the working one.

8.1. General information

The name of the *Legal entity* must be entered, but the other fields are optional. If an attempt is made to create a *Legal entity* with a name that already exists in the database, a warning is given. If the warning is dismissed, a *Legal entity* is created with the name, but with a unique UUID.

The type of the Legal entity and other names are for information purposes. Flags can be set for the *other names*.

8.2. Identifiers

The identifiers can be recorded of type *Legal entity*, *Regulatory programme*, and *Other IT system*. Each type contains a menu from which relevant sub-types of identifier can be selected. For example, *Legal entity* has an option for DUNS. A flag can be set for each identifier.

8.3. Contact information

An address can be defined for a contact of the *Legal entity* and a link can be made to the entity *Contact*.

8.4. Sites

This shows a list of the *Legal entity sites* that have been associated with the *Legal entity*. The association is made from within the *Legal entity site*. Clicking on a record in the list opens the data window for that *Legal entity site*.

9. Legal entity site

A *Legal entity site* is an entity that is used to associate a *Legal entity* and its associated entities with a physical location. This can have important legal implications, especially where the country is concerned. A *Legal entity site* must have a name and must be associated with a *Legal entity*.

10. Reference substance

A *Reference substance* is an entity that is used to define a particular molecular structure, or narrow range of molecular structures in such a way that the definition may be re-used. A *Reference substance* contains chemical identifiers and structural information. For example, there is typically a one to one relationship between *Reference substance* and EC number. A single *Reference*

substance can be referred to from multiple entities wherever a chemical identity needs to be defined, for example in a constituent of a *Substance*.

The use of *Reference substances* is efficient because some chemical substances appear frequently across multiple *Substances* and *Mixture/products*. In addition, *Reference substances* can be shared and exchanged among instances and users of IUCLID. A collection of *Reference substance* entities are available to download free of charge from the IUCLID 6 web site under the section *Support / Get Reference Substances*. If the required *Reference substance* is not available on the web site, or if you otherwise prefer, it is possible to create a *Reference substance* within IUCLID.

10.1. Inventory

A *Reference substance* must at least have a name defined. The name is often the same as an entry in an inventory such as the EC Inventory, but it does not have to be.

If no link is made to an inventory, a reason and a justification can be supplied under *No inventory information available*.

10.2. Reference substance information

Reference substance information is a collection of fields that contain identifiers for the Reference substance and related substances. Identifiers are entered here in addition to any link to an inventory. In the field identifiers of related substances, a block may be created per related substance. Within the block there is a field *Relation*, where the relationship can be described.

A single flag can be applied to all of Reference substance information, for example for confidentiality.

10.3. Molecular and structural information

In Molecular and structural information, enter the molecular formula, the molecular weight, and upload an image that shows the structure in either JPEG, GIF, or PNG format. The field molecular formula accepts text but no characters in subscript, so for example ethane would be C2H4.

A single flag can be applied to all of Molecular and structural information, for example for confidentiality.

11. Contacts

A *Contact* is an entity that records the contact details for a particular person. It can also be used to record something about a *person's* role in a process, for example, as the competent person who is responsible for a safety data sheet (SDS). Links can be made from various other entities to a *Contact*, for example from a *Legal entity*.

Using *Contacts* removes the need to re-enter details where a particular person is involved across multiple processes and *Substances*. The built-in types of contact are *competent person responsible for the SDS*, *emergency contact*, *substance manager*, and *toxicologist*.

12. Chemical inventories

Chemical inventories is used to provide access within IUCLID to inventories of information on chemical identity that originate from outside IUCLID. A *Reference substance* may be linked to an entry in a *Chemical inventory*, to provide information on chemical identity in a standard format.

The EC Inventory contains chemical identifiers such as EC numbers, CAS numbers and molecular formulae.

13. Test materials

Test materials is an entity used to describe the material on which a physical test has been performed. A link can be made to a *Test material* entity from within an endpoint study record.

A *Test material* entity consists of a composition, similar to that used for a *Substance*, a description of the physical form, and some extra information that may be considered confidential, such as a batch number.

The composition can have components of type *constituent*, *impurity* or *additive*. The components are shown in a table that can be edited in the usual way. Each component should be linked to a *Reference substance* and given a concentration range. The field *Composition / purity: other information* is provided to record more qualitative information about the purity. The field *Test material form* is provided to record information about the physical state and characteristics of the material used in the test. Finally, there are two free-text fields where more details can be added. Suggestions as to what to enter are provided in free text templates. To open a free text template, click on the icon that shows the letter A with an arrow at the bottom right. To copy the text from the template to the field, click on the button labelled *Insert*. On saving the *Test materials* entity, watch the message area above the navigation panel for a few seconds whilst the data is checked. If anything is found to be wrong with it, an information message will be shown. For example, if the message is "Concentration: At least one of the values are not set", check the components of the composition.

14. Literature reference

A *Literature reference* is an entity that identifies a particular document that contains information on a *Substance* or a *Mixture/Product*. The only mandatory field is the title, but there are also various other fields that allow a reader to find the document outside IUCLID. A link may be made to a *Literature reference* from an endpoint study record in a harmonised template. The link is made from the field *data source*.

15. Validation assistant

The aim of the Validation assistant is to assist users in the preparation of IUCLID dossiers so that they can be successfully submitted to and processed by the relevant authority. To this end, the Validation assistant carries out validations on the data provided in a IUCLID dataset or dossier according to a set of pre-defined rules to verify that the information was provided as expected. The outcome of the validation is a report, which lists all the rules for which the validation failed.

The Validation assistant currently supports the validation of all dossier types that industry can submit to the European Chemicals Agency (ECHA) under the REACH and CLP regulations. It can be customised to validate other types of dossiers, as needed.