

# IUCLID 5

General introduction

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# IUCLID 5 in a Nutshell

- IUCLID 5 is an IT application built to **store, organise** and **report** on the hazardous properties of chemicals
- IUCLID 5 is intended to serve this purpose for both REACH and other chemical legislative programmes (e.g. OECD HPV and EU Biocides)
- Industry uses IUCLID 5 to prepare data for submission to ECHA to fulfill their obligations under REACH
- IUCLID 5 is the “scientific” database in the Agency both for Agency staff and MSCAs

## Stand-alone or Distributed?

- Distributed (multi-user environment)

For IT-Expert to install.

Installation manuals are available for:

- Windows environment
- Linux environment



- Stand-alone (single computer)

An automatic installer is available.

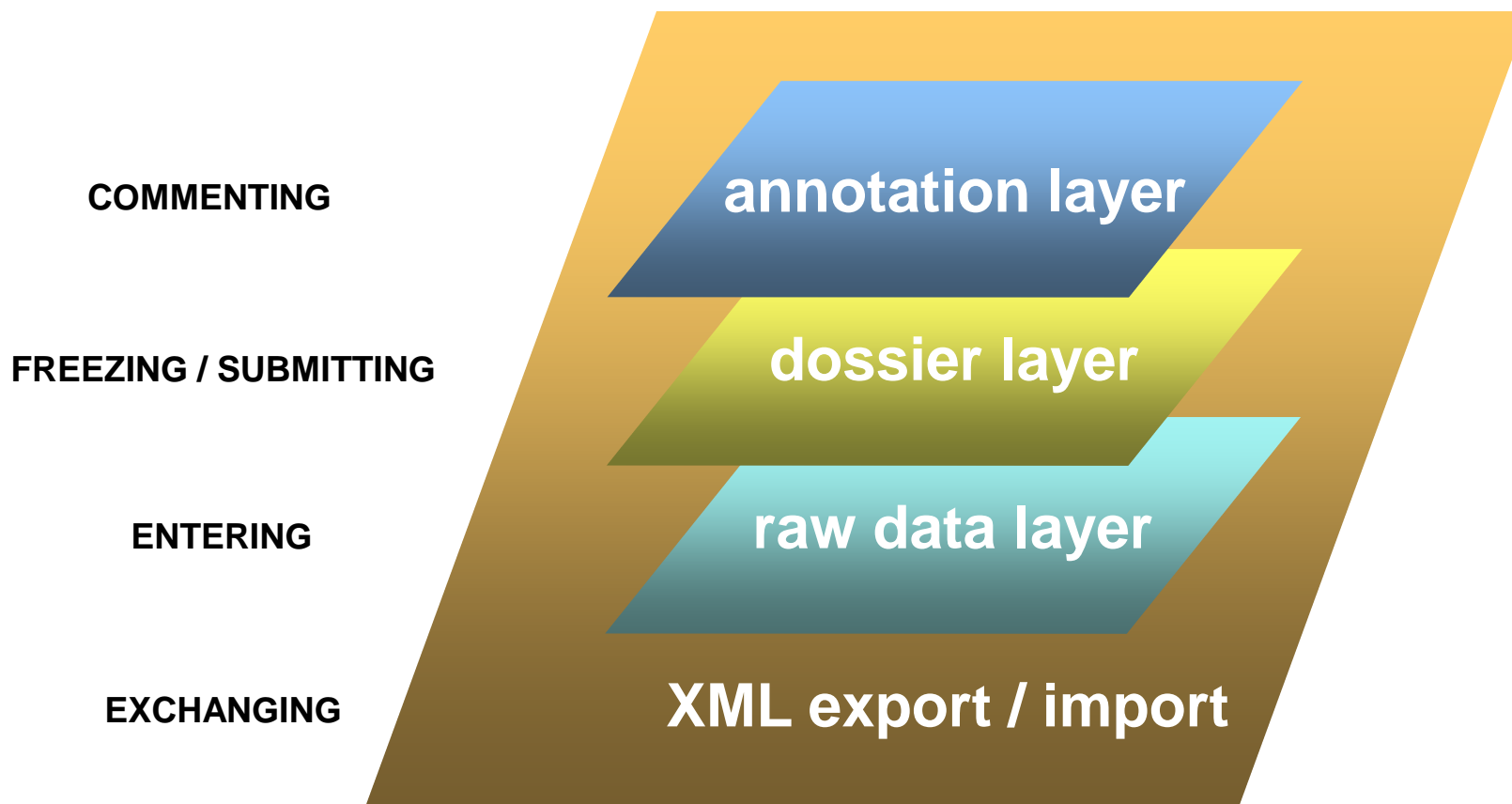
Java and PostgreSQL must first be installed, separately.



- Distributed installations of IUCLID 5 at ECHA
  - Production (PRD)
  - Work in Progress (WRK)
  - Annex XV, SiA, and Annex VI
  - Training
  - Test 1 (latest official release)
  - Test 2 (latest beta version)
- IUCLID on the ECHA Intranet  
<http://echanet/library/ittools/Pages/iuclid5.aspx>

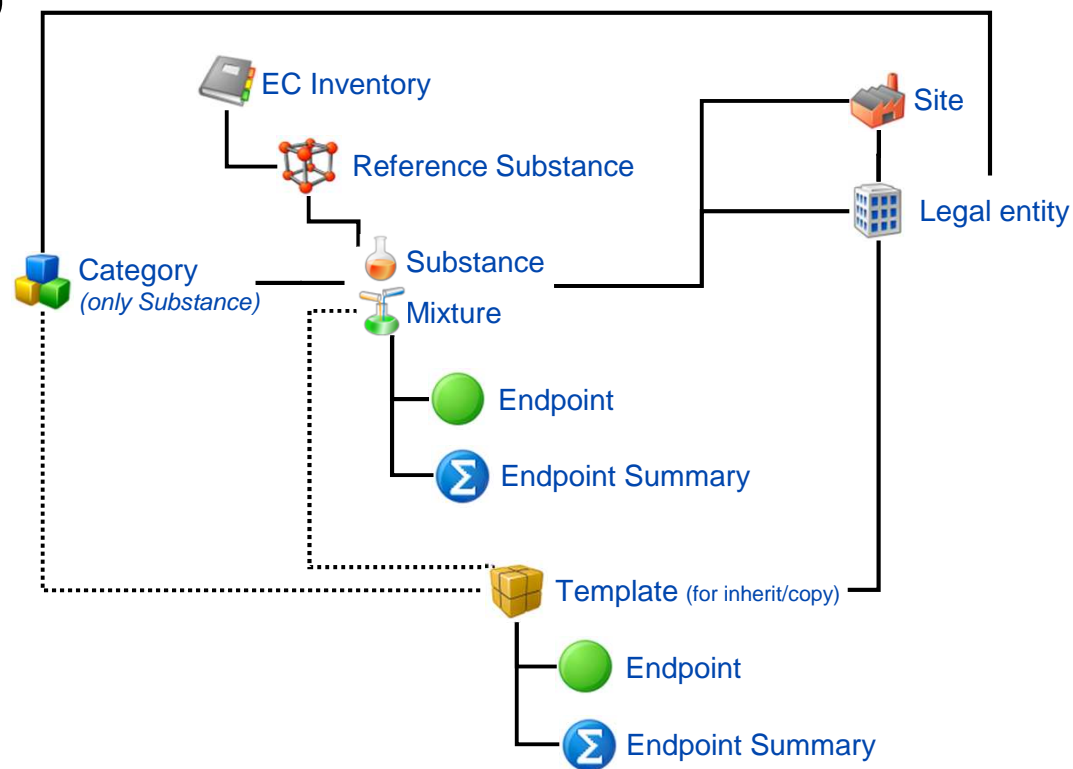
# Abstraction Layers

Multiple data layers in IUCLID 5



# IUCLID 5 – Data Objects

- Substances
- Mixtures
- Endpoints based on OECD harmonized templates
- Endpoint Summaries
- Reference Substances
- Reference Substances
- EC Inventory
- Legal entities
- Legal Entity Sites
- Templates *(for inherit, for copy)*
- Categories *(only for Substances)*
- Attachments
- Annotations



- REACH / CLP
  - Inquiry
  - Registration
  - Registration as only an intermediate
  - Registration in a joint submission
  - PPORD notification
  - C&L notification
  - Substance evaluation
  - Downstream user report
  - Application for Authorisation
  - Notification of a substance in article
  - Annex XV
- OECD HPV chemicals
- EU Biocides
  - Active substances
  - Biocidal products

# Tools and Administration

(Search by UUID)

### Tasks

- Legal entity**  
Create and update company /organisation related information  
[New](#) [Update](#)
- Legal entity site**  
Create and update legal entity sites  
[New](#) [Update](#)
- Substance**  
Create and update substance related information  
[New](#) [Update](#)
- Mixture**  
Create and update mixture related information  
[New](#) [Update](#)
- Template**  
Create and update template related information  
[New](#) [Update](#)
- Category**  
Create and update category related information  
[New](#) [Update](#)
- Dossier**  
View dossier data  
[View](#) [Compare](#)

### Inventories

- Inventory**  
View EC inventory related information  
[View](#)
- Literature reference**  
View and exchange literature reference inventory related information  
[View](#) [Exchange](#)
- Reference substance**  
Create and update reference substance related information  
[New](#) [Update](#)

### Tools and administration

- Manage users, roles, preferences, etc.**  
[User preferences](#), [Set password](#), User management, Role management
- Import**  
Import data from other IUCLID 5 systems  
[Import](#)
- Bulk export**  
Export multiple documents  
[Run](#)

### Plugins

- Query tool**  
Advanced search for endpoint studies, endpoint summaries, substances or mixtures  
[Find](#), Administration
- Chesar**  
Chemical Safety Assessment & Reporting Tool  
[Run](#)
- TCC tool**  
Technical completeness check  
[Run](#)

European Chemicals Agency / Helsinki / Finland | Trainee



# Inventories: Substance ID + Literature References

The screenshot displays the IUCLID 5 web interface. At the top, there is a search bar labeled "(Search by UUID)". Below it, the "Tasks" section includes: "Legal entity" (Create and update company /organisation related information, with [New](#) and [Update](#) links), "Legal entity site" (Create and update legal entity sites, with [New](#) and [Update](#) links), "Substance" (Create and update substance related information, with [New](#) and [Update](#) links), "Mixture" (Create and update mixture related information, with [New](#) and [Update](#) links), "Template" (Create and update template related information, with [New](#) and [Update](#) links), and "Category" (Create and update category related information, with [New](#) and [Update](#) links). A "Dossier" option (View dossier data, with [View](#) and [Compare](#) links) is also present.

The "Inventories" section, highlighted with an orange border, includes: "Inventory" (View EC inventory related information, with [View](#) link) and "Literature reference" (View and exchange literature reference inventory related information, with [View](#) and [Exchange](#) links). Below it is "Reference substance" (Create and update reference substance related information, with [New](#) and [Update](#) links).

The "Tools and administration" section includes: "Manage users, roles, preferences, etc." (with [User preferences](#), [Set password](#), User management, and Role management links), "Bulk export" (Export multiple documents, with [Run](#) link), and "Import" (Import data from other IUCLID 5 systems, with [Import](#) link).

The "Plugins" section includes: "Query tool" (Advanced search for endpoint studies, endpoint summaries, substances or mixtures, with [Find](#) and Administration links) and "Chesar" (Chemical Safety Assessment & Reporting Tool, with [Run](#) link). At the bottom left is the "TCC tool" (Technical completeness check, with [Run](#) link).

The footer shows "European Chemicals Agency / Helsinki / Finla" and the user "Trainee".

# Tasks Panel: Daily Work

The screenshot displays the IUCLID 5 interface with a search bar at the top right containing the text "(Search by UUID)". The main content is organized into several sections, each with a title and a list of tasks:

- Tasks**
  - Legal entity**: Create and update company /organisation related information. [New](#) [Update](#)
  - Substance**: Create and update substance related information. [New](#) [Update](#)
  - Template**: Create and update template related information. [New](#) [Update](#)
  - Dossier**: View dossier data. [View](#) [Compare](#)
  - Legal entity site**: Create and update legal entity sites. [New](#) [Update](#)
  - Mixture**: Create and update mixture related information. [New](#) [Update](#)
  - Category**: Create and update category related information. [New](#) [Update](#)
- Inventories**
  - Inventory**: View EC inventory related information. [View](#)
  - Reference substance**: Create and update reference substance related information. [New](#) [Update](#)
  - Literature reference**: View and exchange literature reference inventory related information. [View](#) [Exchange](#)
- Tools and administration**
  - Manage users, roles, preferences, etc.**: [User preferences](#), [Set password](#), User management, Role management
  - Bulk export**: Export multiple documents. [Run](#)
  - Import**: Import data from other IUCLID 5 systems. [Import](#)
- Plugins**
  - Query tool**: Advanced search for endpoint studies, endpoint summaries, substances or mixtures. [Find](#), Administration
  - TCC tool**: Technical completeness check. [Run](#)
  - Chesar**: Chemical Safety Assessment & Reporting Tool. [Run](#)

The bottom status bar shows "European Chemicals Agency / Helsinki / Finla" and "Trainee".

# Tasks Panel: Plugins

The screenshot displays the IUCLID 5 Tasks Panel interface. At the top, there is a search bar labeled "(Search by UUID)". The panel is organized into several sections, each with a title and a list of tasks:

- Tasks**
  - Legal entity**: Create and update company /organisation related information. [New](#) [Update](#)
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  - Manage users, roles, preferences, etc.**: [User preferences](#), [Set password](#), User management, Role management
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- Plugins** (highlighted with an orange border)
  - Query tool**: Advanced search for endpoint studies, endpoint summaries, substances or mixtures. [Find](#), Administration
  - TCC tool**: Technical completeness check. [Run](#)
  - Chesar**: Chemical Safety Assessment & Reporting Tool. [Run](#)

The bottom of the interface shows the user's role as "Trainee" and the location as "European Chemicals Agency / Helsinki / Finla".

calcium gluconate / calcium gluconate / 299-28-5 / EUROPEAN COMMISSION - European Chemicals Bureau / Ispra (VA) / Italy - IUCLID 5

File Edit Go Window Help

Navigation

Query results Section tree

Query

t

- 2,2-bis(chloromethyl)trimethylene bis(bis...
- calcium gluconate**
- potassium gluconate
- test
- test october
- tris(2-chloro-1-methylethyl) phosphate (IU...
- tris(2-chloro-1-methylethyl) phosphate (IU...
- tris(2-hydroxyethyl)ammonium dodecylsul...
- tris[2-chloro-1-(chloromethyl)ethyl] phos...

**query result & tree view area**

Substance: calcium gluconate / calcium gluconate / 299-28-5 / EUROPEAN COMMISSION - European Chemicals Bureau / Ispra (VA) / Italy - IUCLID 5

**Substance identification**

Chemical name calcium gluconate

Legal entity flags

Legal entity EUROPEAN COMMISSION - European Chemicals Bureau / Ispra (VA) / Italy

**Role in the supply chain**

Role flags

Role:  Manufacturer  Importer  Only representative  Downstream user

**Reference substance**

calcium gluconate / 299-28-5

EC number EC name

206-075-8 calcium gluconate

CAS number CAS name

299-28-5

IUPAC name

**Type of substance**

Composition

Origin

**Trade names**

Name

**data area**

**Information**

Information Modification history Access Consultation Attachments Annotations Validation

Type Substance

UUID IUC5-845ec86e-cdda-4b7d-b935-061201514624

Dossier UUID 0

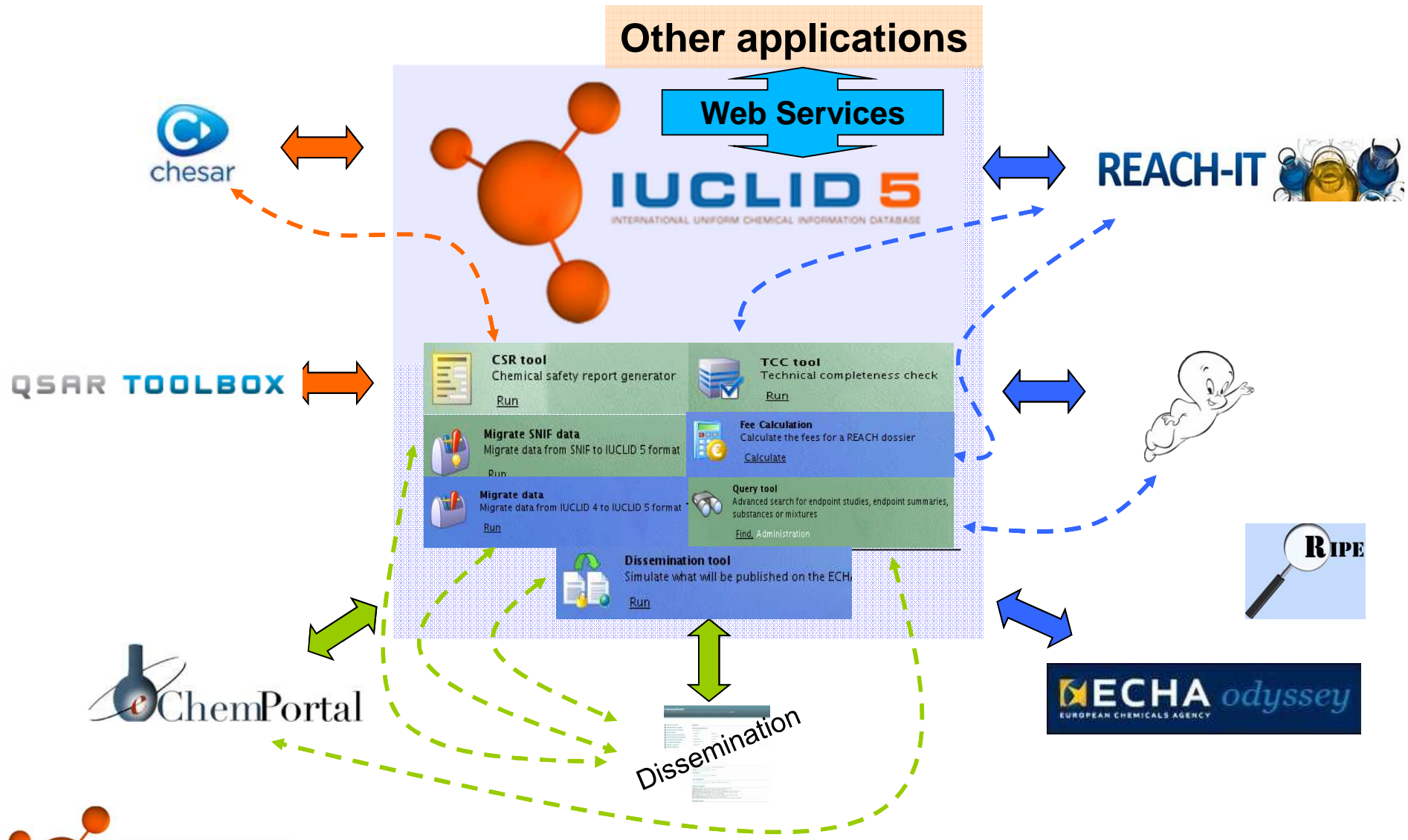
Sealed

Subset of original

**information area**

EUROPEAN COMMISSION - European Chemicals ...

bernar





A *Substance* is a regulatory concept designed to contain as much as possible of the information about a chemical product that is relevant to chemical regulation.

For example:

- the precise chemical composition
- toxicological data
- guidance on its safe use

A “*Substance data set*” is the software entity (object) in IUCLID that is used to store the data of a Substance.

# Chemical Composition of a Substance



## Constituent

A substance typically contains either one or a small number of different principal ingredients that each have a single or narrowly defined molecular structure.

## Impurity

The nature of chemical manufacture means that there are unwanted ingredients.

## Additive

Sometimes, an ingredient is added deliberately in small quantities to perform a specific function, such as a stabiliser.

# Defining Chemical Composition

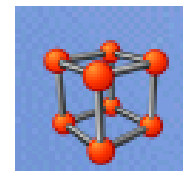


A particular molecule might be present in many Substances. For the sake of efficiency, the chemical identity is defined only once. This is done in a *Reference substance*.

A Reference substance typically has a single or narrowly defined molecular structure.

For example, an impurity in one substance might be a constituent of another.

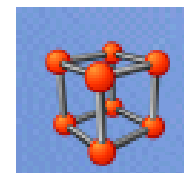




In IUCLID 5, a the chemical composition of a Substance is defined by linking it to Reference substance(s) that each define one of the following:

- **Overall Substance identity and**
  - **Constituent(s)**
  - **Impurity(ies)**
  - **Additive(s)**

# Information in a Reference Substance

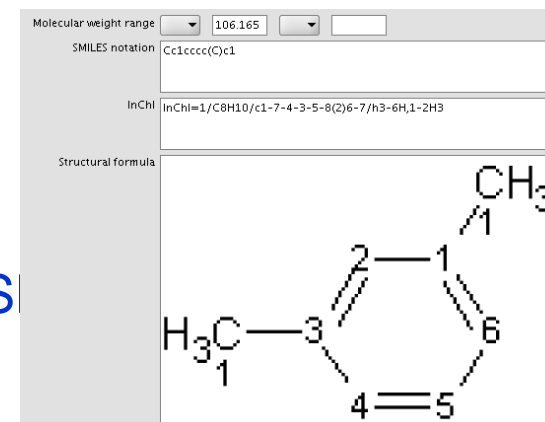


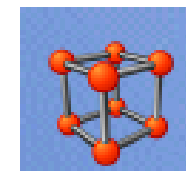
- Name(s), EINECS, ELINCS, CAS, Composition...  
[Identity of the substance Art 10 (a) (ii) – Annex VI, section 2]
- Direct link to EC inventory (if possible)

EC inventory

EC number	233-162-8	CAS number	10049-04-4
EC name	chlorine dioxide		
Molecular formula	ClO <sub>2</sub>		
Description			

- Reference substance gives information on the substance identity e.g. IUPAC name and molecular and structural information, including SMILES notation, InChI, etc.

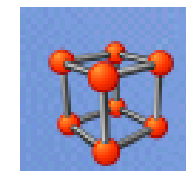




Identification – only one entry

The screenshot displays the IUCLID 5 interface. On the left, a navigation tree shows the '1.1 Identification' section highlighted with a red circle and an arrow pointing to the main data area. The main area is titled 'Substance: 1,2-Benzenedicarboxylic acid, di-C7-11-branched an' and contains the following sections:

- Substance identification**
  - Chemical name: 1,2-Benzenedicarboxylic acid, di-C7-11-branched an
  - Public name: [empty]
  - Legal entity flags: [flag icon]
  - Legal entity: Example Company 1 / Example city / Finland
  - Third party flags: [flag icon]
  - Third party: [empty]
- Role in the supply chain**
  - Role flags: [flag icon]
  - Role:  Manufacturer  Importer  Only rep
- Reference substance**
  - triphenylene / triphenylene / 217-59-4
  - EC number: 205-922-9 | EC name: triphenylene
  - CAS number: [empty] | CAS name: [empty]



## Composition

The screenshot displays the IUCLID 5 interface. On the left, the 'Navigation' pane shows a tree structure with '1.2 Composition' highlighted in red. On the right, the 'Constituents' form is shown, containing the following information:

**Constituents**

<= 100 % (w/w) 1,2-Benzenedicarboxylic acid, di-C7-11-branched and line

Reference substance 1,2-Benzenedicarboxylic acid, di-C7-11-branched

EC number	EC name
271-084-6	1,2-Benzenedicarboxylic acid
CAS number	CAS name
68515-42-4	1,2-Benzenedicarboxylic acid
IUPAC name	

Typical concentration

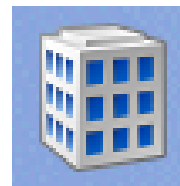
Concentration range   <=  100

Remarks

**Impurities**

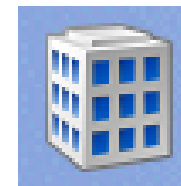
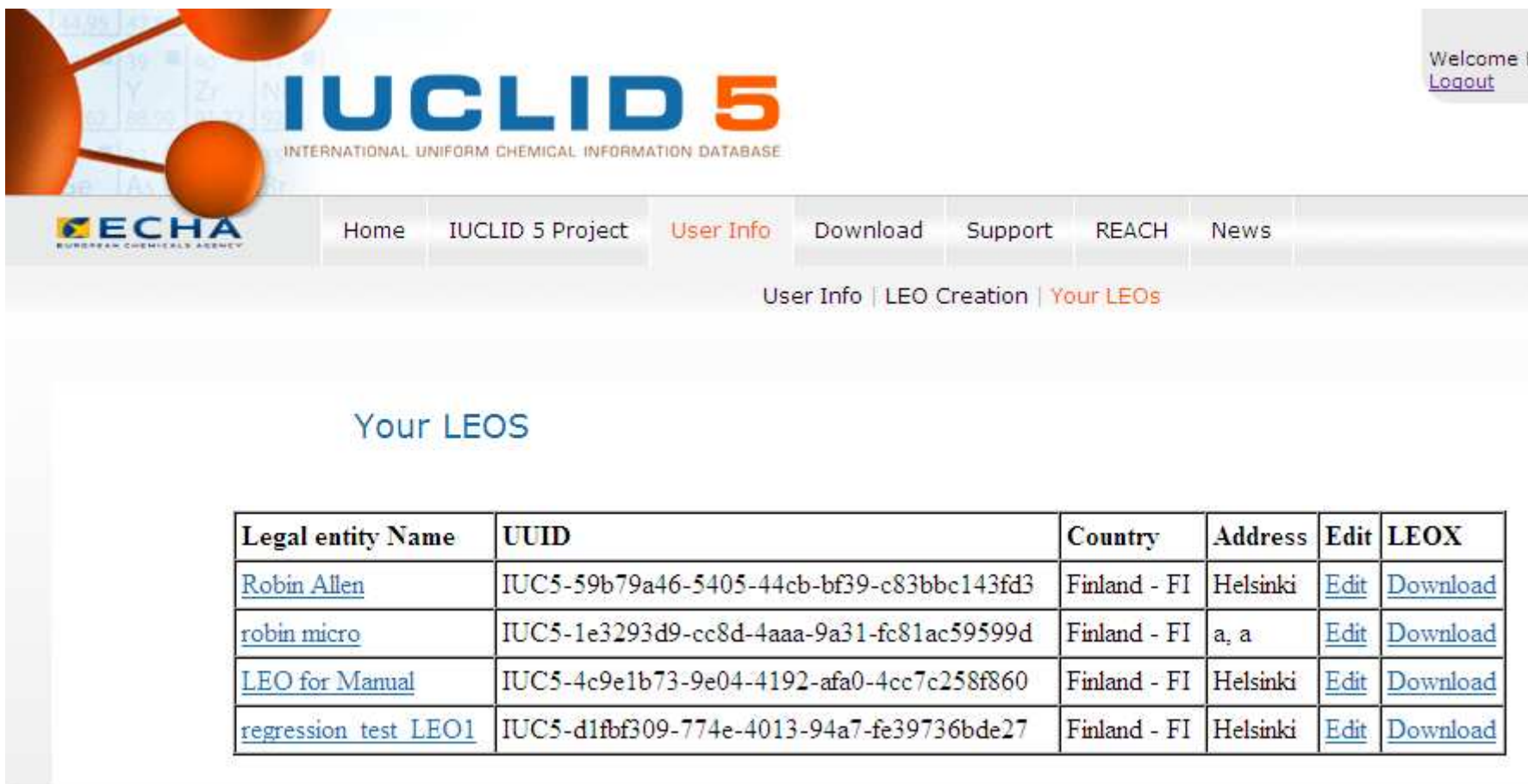
**Additives**

## Legal Entity




- Owner of:
  - Substance
  - Site
  - Dossier
- Not owner of:
  - Reference substance. A reference substances does not have an owner. Anyone is free to use and re-use them.
- For submission under REACH, in REACH-IT the same legal entity must be used as was used to create the dossier and the substance.
- LEOX file, with extension i5z, is used to transfer the legal entity between systems – more later...

# LEOX Management on IUCLID Web Site

Welcome R  
[Logout](#)

**IUCLID 5**  
INTERNATIONAL UNIFORM CHEMICAL INFORMATION DATABASE

 Home IUCLID 5 Project **User Info** Download Support REACH News

User Info | LEO Creation | **Your LEOS**

### Your LEOS

Legal entity Name	UUID	Country	Address	Edit	LEOX
<a href="#">Robin Allen</a>	IUC5-59b79a46-5405-44cb-bf39-c83bbc143fd3	Finland - FI	Helsinki	<a href="#">Edit</a>	<a href="#">Download</a>
<a href="#">robin micro</a>	IUC5-1e3293d9-cc8d-4aaa-9a31-fc81ac59599d	Finland - FI	a, a	<a href="#">Edit</a>	<a href="#">Download</a>
<a href="#">LEO for Manual</a>	IUC5-4c9e1b73-9e04-4192-afa0-4cc7c258f860	Finland - FI	Helsinki	<a href="#">Edit</a>	<a href="#">Download</a>
<a href="#">regression test LEO1</a>	IUC5-d1fbf309-774e-4013-94a7-fe39736bde27	Finland - FI	Helsinki	<a href="#">Edit</a>	<a href="#">Download</a>

**Thank you for  
Your attention**

**IUCLID 5**

INTERNATIONAL UNIFORM CHEMICAL INFORMATION DATABASE



The Development of IUCLID 5 has been supported by the  
Organisation for Economic Cooperation and Development.

IUCLID Version 5 - Est. 2002