



Developing a registration dossier with IUCLID

Christel Musset

European Commission, DG JRC
Institute for Health and Consumer Protection (IHCP)
European Chemicals Bureau (ECB)

Workshop on REACH Implementation Project 3
25 September 2006





Outline

What is IUCLID?

Preparing a registration dossier with IUCLID 5

The registration dossier is ready: what comes next?



Outline

What is IUCLID?

Preparing a registration dossier with IUCLID 5

The registration dossier is ready: what comes next?



REACH & IUCLID: which link? (1)

- Art. 110 of the REACH proposal specifies:
 - “The Agency shall specify formats and make them free of charge, and software packages and make them available on its website for any submissions to the Agency”
 - “For the purposes of registration, the format of the technical dossier referred to in Article 10(a) shall be IUCLID”



REACH & IUCLID: which link? (2)

- IUCLID is the IT system (software & database)



- designed to prepare REACH-compliant registration dossiers to be submitted to the European Chemicals Agency
- it will be made available to Industry free of charge



What is IUCLID?

- **IUCLID** is a database system for managing hazard data on chemical substances and reporting to the Authorities
- It was initially developed in 1993 to meet the EU requirements of the Existing Substances Regulation (793/93/EEC)
- New version **IUCLID 5** in development: **major upgrade** of IUCLID 4, both in technology and functionality
- **Data format** agreed at international level (OECD format) – The same pool of data stored in IUCLID can be re-used for other legislations
- Will come with a **migration tool** to transfer existing data to the new format



Outline

What is IUCLID?

Preparing a registration dossier with IUCLID 5

The registration dossier is ready: what comes next?

What is meant by registration dossier?

- Requirements are defined in **Art. (10)** of the REACH proposal
 - Technical dossier
 - company identity & substance identity
 - manufacture & uses – guidance on safe use - C&L - exposure information if applicable
 - study summaries - robust study summaries - proposals for testing
 - various statements
 - Chemical safety report (>10 tonnes)

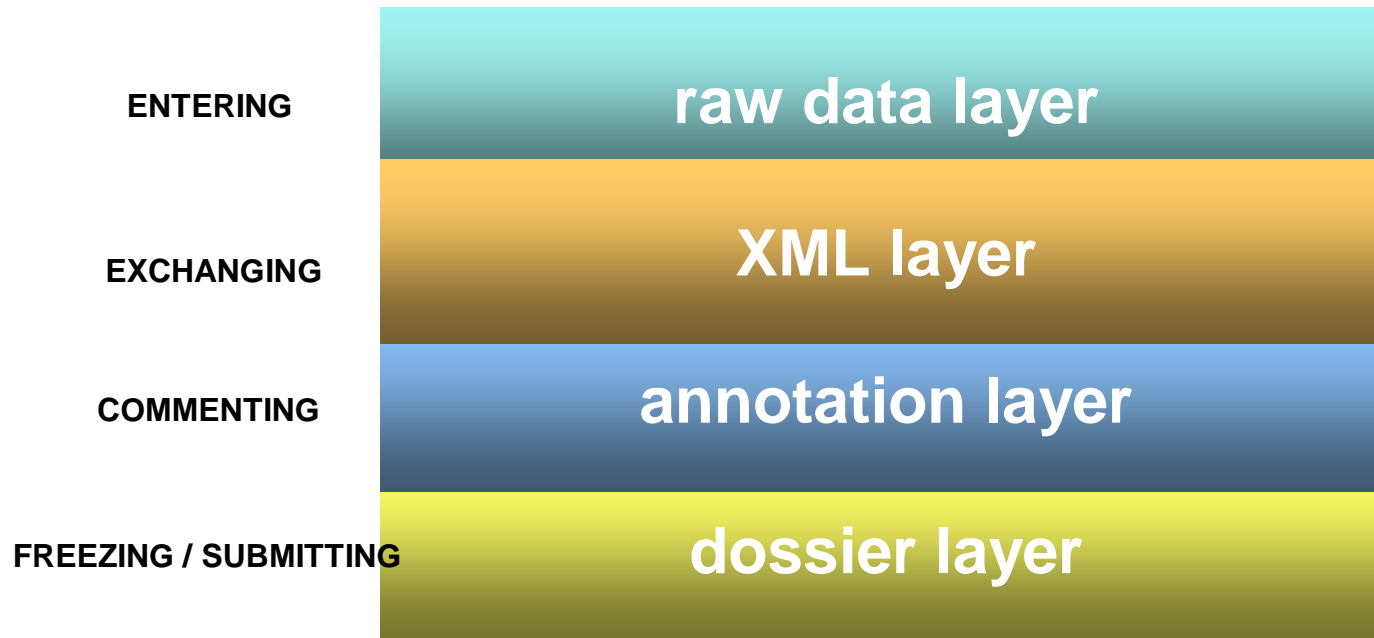
- **Technical dossier**: database format
 - data are filled in a structured format in the IUCLID database
- **Chemical safety report**: document (e.g. MS Word);
 - document created and edited outside IUCLID

One single
package to be
submitted to
Agency

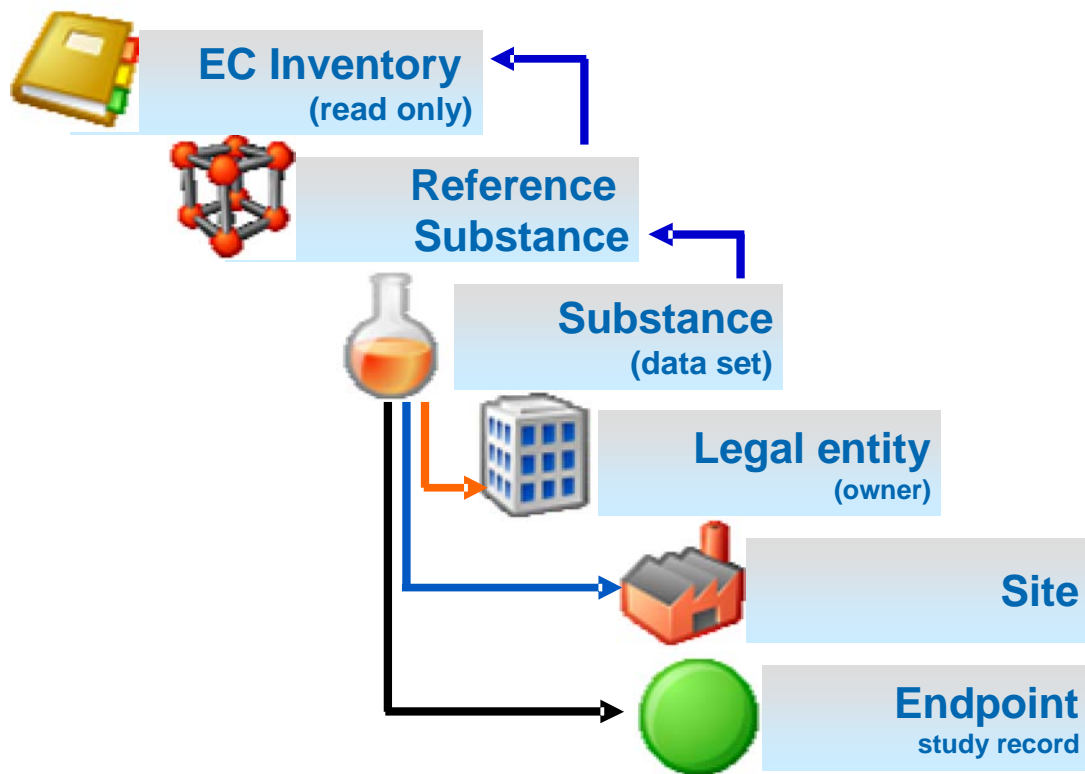


Preparing the registration dossier

- Step wise approach:
 - from **data collection** via manual data entry or electronic **exchange** with other applications e.g. MSDS, EH&S systems, ...**data review and commenting**,
 - to **selection of relevant data** to be submitted in the registration dossier
- IUCLID 5 is structured to cover all these steps



IUCLID 5 structure



IUCLID 5 main menu

The screenshot shows the IUCLID 5 main menu interface. It is organized into several sections: **Tasks**, **Inventories**, and **Tools and administration**. Each section contains icons and text for various functions. Orange callouts are placed around the interface to highlight specific features: 'company information' points to the 'Legal entity' task; 'substance properties' points to the 'Substance' task; 'sites of production or use' points to the 'Legal entity sites' task; 'substance identification' points to the 'Reference substance' task; 'data exchange' points to the 'Import' task; 'Migration of existing data' points to the 'Migration tool'; and 'list of substances in EINECS, ELINCS, ...' points to the 'Inventories' task.

Section	Task Name	Description	Callout
Tasks	Legal entity	Create and update company-/organisation-related information. New, Update	company information
	Legal entity sites	Create and update legal entity sites. New, Update	sites of production or use
	Substance	Create and update substance related information. New, Update	substance properties
	Template	Create and update template related information. New, Update	
Inventories	Inventories	View EC inventory related information. View	list of substances in EINECS, ELINCS, ...
	Reference substance	Create and update reference substance related information. New, Update	substance identification
Tools and administration	Migration tool	Do migration related work. Run migration tool	Migration of existing data
	Import	Import data from other IUCLID5 systems. Import	data exchange
	Manage users, roles, preferences etc.	User preferences, Set password, User management, Role management	



Company information

- “Legal entity” = information on manufacturer / importer [Art 10 (a) (i)]

Legal entity: TestCompany

General information Identifiers Contact information Sites

Legal entity name TestCompany

Legal entity type company

Remarks

The legal entity name should be unique in the IUCLID database: for example, two companies should not carry the same name. In practice, a legal entity may have other names, they are then enlisted in the "other name" attribute.

help text

- Company information is stored in a “directory” – interest:
 - Re-usability: the same information can be re-used in all registration dossiers submitted by the company without typing again the information
 - Central management of the information: no inconsistency!
 - updated once for all substances
 - exchanged with partners within a joint submission



Substance identity (1)

- Names, EINECS, ELINCS, or CAS nb, Composition... [Art 10 (a) (ii)]
- Direct link to the EC inventory if the substance is listed

EC inventory

EC number	<input type="text" value="203-576-3"/>	CAS number	<input type="text" value="108-38-3"/>
EC name	<input type="text" value="m-xylene"/>		
Molecular formula	<input type="text" value="C8H10"/>		
Description	<input type="text"/>		

- Structural information

Molecular weight range

SMILES notation

InChI

Structural formula

13





Substance identity (2)

- Composition

confidentiality
setting

description of
constituents,
and %

(main) impurities,
and %

additives, nature
and %

Degree of purity

[CBI]

>= 97 < 99 % (w/w)

Constituents

106-42-3 / p-xylene									
7732-18-5 / Water									

Impurities

108-88-3 / Toluene									

Additives

--	--	--	--	--	--	--	--	--	--

(Robust) study summaries (1)

- Annexes VII to X: from chapter 3 to chapter 7

- + 1 General Substance Information
- + 2 Manufacture, use and exposure



- + 8 Preliminary: Effectiveness against target organisms
- 9 Guidance on safe use
- 10 Literature search
- 11 Assessment Reports

- Sub-chapters



- 5 Ecotoxicological Information
 - 5.1 Aquatic toxicity
 - 5.1.1 Short-term toxicity to fish
 - 5.1.2 Long-term toxicity to fish
 - 5.1.3 Short-term toxicity to aquatic invertebrates
 - 5.1.4 Long-term toxicity to aquatic invertebrates
 - 5.1.5 Toxicity to aquatic algae and cyanobacteria
 - 5.1.6 Toxicity to aquatic plants other than algae
 - 5.1.7 Toxicity to microorganisms
 - 5.1.8 Toxicity to other aquatic organisms

(Robust) study summaries (2)

- Long-term toxicity to aquatic invertebrates (extract)

waiving (annex XI)

experimental result
estimated
read-across
QSAR

...

(annex XI)

Study: Long-term toxicity to aquatic invertebrates.001

Administrative Data Data source Materials and methods

Results and discussions Overall remarks, attachments Applicant's summary and conclusion

Purpose flag: key study

Data waiving: []

Justification for data waiving: []

Study result type: experimental result

Reliability: 1 (reliable without restriction)

Rationale for reliability: []

Data source

Reference

Reference type	Author	Year	Title	Bibliographic s
grey literature	Author name	1978		
publication	Smith J.	1998	Toxicity of m-xylene in xxxxxxxx	The Lancet

Add... Edit... Delete Move up Move down

Data access: data published

(Robust) study summaries (3)

- Conclusions and summaries can be inserted and formatted with a text editor – ready to be exported to the Chemical safety report

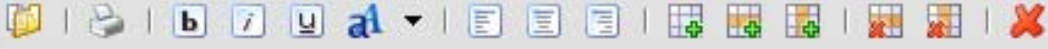
Long-term exposure

Dermal DN(M)EL in mg/kg bw/day

Inhalation DN(M)EL in mg/m³

Oral DN(M)EL in mg/kg bw/day

Discussion



Exposure data are available for Scenarios 1, 2 and 3. For Scenario 4, due to the very large panel of use, the EASE model is preferred model is considered to be the worst case). Occupational exposure data are summarised in the next table.

Scenario	Estimated inhalation exposure ppm (mg/m ³)		Estimated skin exposure (mg/cm ² /day)
	Long term (8-hour TWA)	Short term	
1-Production	20 (69)	30 (103)	0-0.1
2-Intermediate	20 (69)	30 (103)	0-0.1
3-Formulation and industrial use of	300 (1,032)		0.03-0.3



Creation of the registration dossier (1)

- The user selects the type of dossier, depending on the tonnage range, in a pre-defined list (picklist)

Dossier template:

Complete

OECD

REACH Annex 14 type of dossier

REACH Applic. Autho. (Art. 59)

REACH C&L notification (Art. 110) Art. 35 for DU

REACH DU Report (Art. 35)

REACH Intermediate: transported isolated 1-1000t (Art. 16)

REACH Intermediates: on site isolated above 1t (Art.15)

REACH Intermediates: transported isolated above 1000t (Art. 16)

REACH Notification of substance in article (Art. 6(3))

REACH PPORD (Art. 7)

REACH Registration Annex V - complete (ton1+)

REACH Registration Annex V - min. requirement (ton1+)

REACH Registration Annex VI (ton 10+)

REACH Registration Annex VII (ton 100+)

REACH Registration Annex VIII (tons 1000+)

Creation of the registration dossier (2)

- + 1 General Substance Information
- + 2 Manufacture, use and exposure
- 3 Physical and chemical properties
 - + 3.1 Appearance/physical state/colour
 - + 3.2 Melting point/freezing point
 - + 3.3 Boiling point
 - + 3.4 Density (Bulk density, density or relative density)
 - 3.5 Particle size distribution (Granulometry)
 - + 3.6 Vapour pressure
 - + 3.7 Partition coefficient
 - + 3.8 Water solubility
 - + 3.9 Solubility in organic solvents / fat solubility
 - 3.10 Surface tension
 - + 3.11 Flash point
 - 3.12 Auto flammability
 - 3.13 Flammability
 - 3.14 Explosiveness
 - 3.15 Oxidising properties
 - 3.16 Oxidation reduction potential
 - 3.17 Stability in organic solvents and identity of reaction products
 - 3.18 Reactivity towards container material
 - 3.19 Thermal stability
 - 3.20 Non-saturated pH
 - 3.21 Dissociation constant
 - 3.22 Viscosity
 - 3.23 Additional physico-chemical information

Creation of the registration dossier (3)

- A list gives an overview of the elements that will figure in the dossier

Documents selected for dossier creation:

Export	Filter	Document	Endpoint	Last modification	Origin
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Substance 3-nitrotoluene / 3-nitrotoluene...	---	2006-07-17 14:02:45 ...	
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Reference substance 3-nitrotoluene	---	2000-02-11 00:00:00 ...	
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Legal entity European Chemicals Bureau / I...	---	2006-05-27 10:08:59 ...	
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Legal entity EUROPEAN COMMISSION - Eur...	---	2000-02-11 00:00:00 ...	
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Study Appearance/physical state/colour.0...	3.1 Appearance/physical state/colour	2006-07-17 14:02:45 ...	Substance 3-nitrotoluen...
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Study Repeated dose toxicity: inhalation.001	6.5.3 Repeated dose toxicity: inhalation	1994-05-30 00:00:00 ...	Substance 3-nitrotoluene
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Study Toxicity to reproduction.001	6.8.1 Toxicity to reproduction	1994-05-30 00:00:00 ...	Substance 3-nitrotoluene
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Study Repeated dose toxicity: dermal.001	6.5.2 Repeated dose toxicity: dermal	1994-05-30 00:00:00 ...	Substance 3-nitrotoluene
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Study Acute toxicity: oral.001	6.2.1 Acute toxicity: oral	1994-05-20 00:00:00 ...	Substance 3-nitrotoluene
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Study Toxicity to microorganisms.001	5.1.7 Toxicity to microorganisms	1994-05-28 00:00:00 ...	Substance 3-nitrotoluene
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Study Water solubility.001	3.8 Water solubility	1994-03-07 00:00:00 ...	Substance 3-nitrotoluene
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Study Bioaccumulation: aquatic.001	4.3.1 Bioaccumulation: aquatic	1994-05-28 00:00:00 ...	Substance 3-nitrotoluene
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Study Solubility in organic solvents / fat so...	3.9 Solubility in organic solvents / fat ...	1994-03-07 00:00:00 ...	Substance 3-nitrotoluene
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Study Acute toxicity: other routes.001	6.2.4 Acute toxicity: other routes	1994-05-30 00:00:00 ...	Substance 3-nitrotoluene
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Study Acute toxicity: dermal.001	6.2.3 Acute toxicity: dermal	1994-05-20 00:00:00 ...	Substance 3-nitrotoluene
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Study Biodegradation in water and sedime...	4.2.2 Biodegradation in water and sedi...	1994-05-28 00:00:00 ...	Substance 3-nitrotoluene
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Study Eye irritation.001	6.3.2 Eye irritation	1994-05-30 00:00:00 ...	Substance 3-nitrotoluene
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Study Flash point.001	3.11 Flash point	1994-03-07 00:00:00 ...	Substance 3-nitrotoluene
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Study Short-term toxicity to aquatic invert...	5.1.3 Short-term toxicity to aquatic in...	1994-05-31 00:00:00 ...	Substance 3-nitrotoluene
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Study Partition coefficient.001	3.7 Partition coefficient	1994-03-07 00:00:00 ...	Substance 3-nitrotoluene
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Study Long-term toxicity to aquatic invert...	5.1.4 Long-term toxicity to aquatic in...	1994-05-31 00:00:00 ...	Substance 3-nitrotoluene
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Study Toxicity to aquatic plants other than...	5.1.6 Toxicity to aquatic plants other t...	1994-05-28 00:00:00 ...	Substance 3-nitrotoluene
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Study Boiling point.001	3.3 Boiling point	1994-05-28 00:00:00 ...	Substance 3-nitrotoluene
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Study Genetic toxicity in vitro.001	6.6.1 Genetic toxicity in vitro	1994-05-30 00:00:00 ...	Substance 3-nitrotoluene
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Study Density (Bulk density, density or r...	3.4 Density (Bulk density, density or r...	1994-05-28 00:00:00 ...	Substance 3-nitrotoluene

not included (because of filter settings)
 partially included (reduced information)
 completely included
 cannot be included (error)

Select the documents



Creation of the registration dossier (4)

- When the selection of the elements of the dossier is complete, the creation process can be finalised
- Data transferred in the dossier are frozen (read-only information)
- The dossier is ready for submission: a summary of its content is displayed

Dossier name	REACH Registration Annex V - complete (ton1+) / 108-88-3 / / 2006-06-17
Dossier template identifier	REACH Registration Annex V - complete (ton1+)
Dossier template version	2006-05-03
Original substance or preparation	toluene / toluene / 108-88-3 / testEntity1 / Ispra / Italy
Submitting legal entity	testEntity1 / Ispra / Italy
Dossier submission remark	Registration dossier prepared for toluene.



Outline

What is IUCLID?

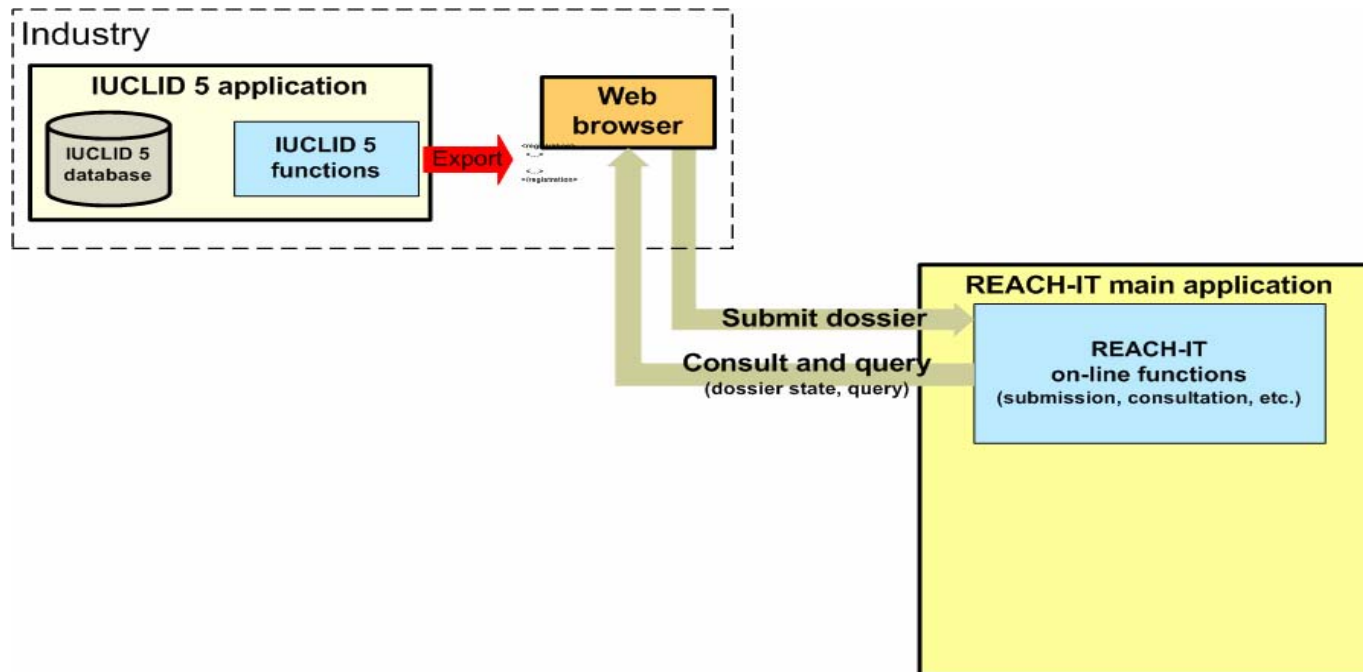
Preparing a registration dossier with IUCLID 5

The registration dossier is ready: what comes next?



From IUCLID 5 to the Agency

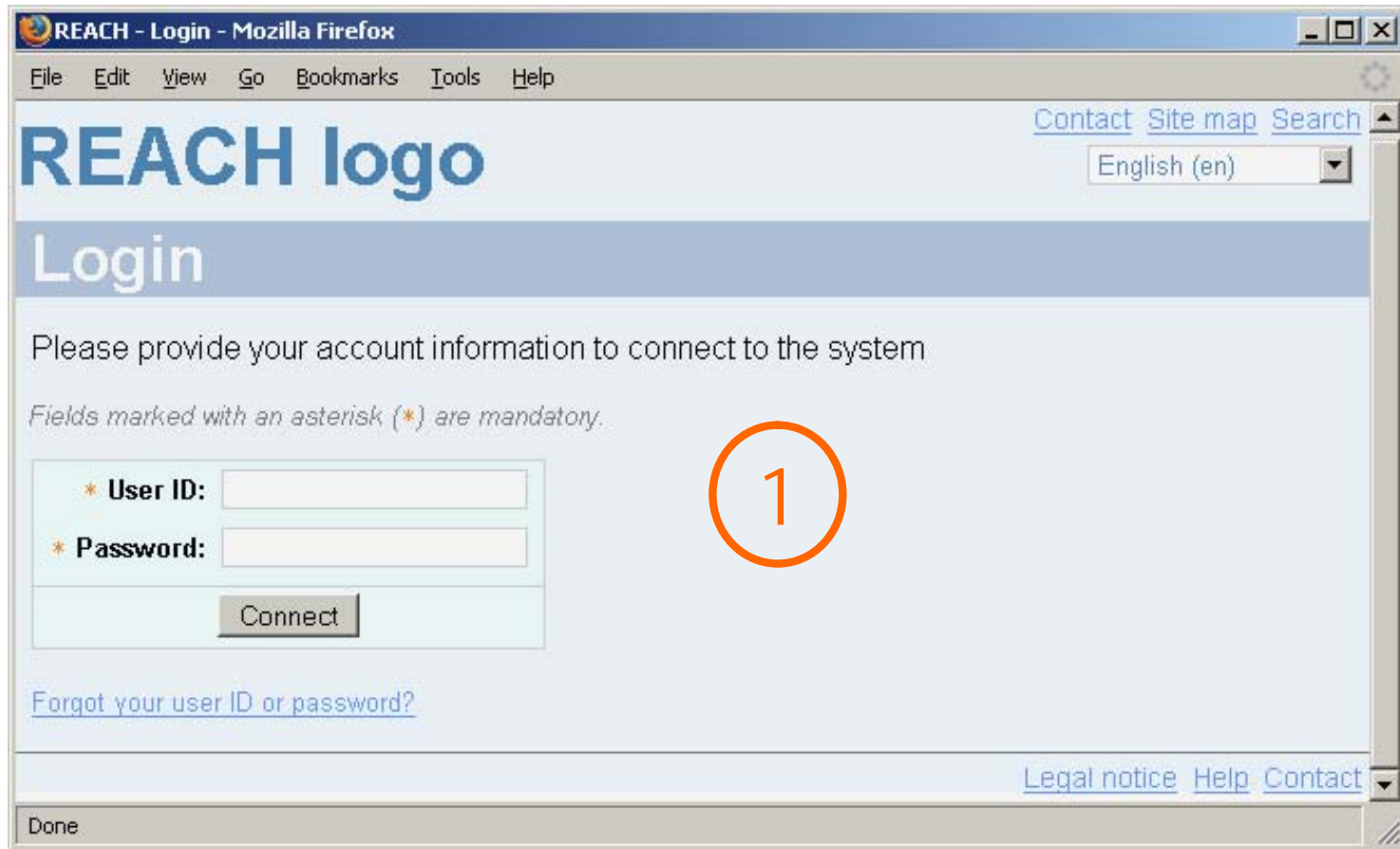
- The registration dossier prepared in IUCLID 5 is exported and submitted to the European Chemicals Agency web site





Dossier submission (1)

1. The user connects to the Agency web site and gives his credentials (ID & password)





Dossier submission (2)

- The user then selects the submission page in the home menu, and submits his registration dossier





Dossier follow-up

- The user may consult the Agency website to get an overview of his submitted dossiers

Substance name

Registration number

Submission date

REACH - Company dossiers - View - Mozilla Firefox

REACH logo

You are connected as *jd (Jane Doe)* on behalf of *The Chemical Company, Inc.* - [Logout](#)

Company > Dossiers > View

Your company has submitted the following dossiers

Trade name	Substance name	EC number	Submission number	Submission date	Reference number	
Naphthol	Naphthalene	202-049-5	20070927-RT67	27/09/2007	REG-20070927-RT67-9	More ...
Neopentane	Neopentane	207-343-7	20070323-TH89	23/03/2007	REG-20070323-TH89-8	More ...
Phosphoryl	Phosphoryl trichloride	233-046-7	20080123-RT67	23/01/2008	REG-20080123-RT67-3	More ...
S-Dichloride	Sulphur dichloride	234-129-0	20070713-RT13	13/07/2007	REG-20070713-RT13-6	More ...
S-Tetrachloride	Sulphur tetrachloride		20080123-CL45	23/01/2008	CLL-20080123-RT67-3	More ...

[Next page \[6 - 10 \]](#)

You can filter the dossiers according to the criteria below

Sort by: Trade name

Dossier type:

- Registration dossier
- C&L notification
- PPORD notification
- DU report
- DU notification

[Legal notice](#) [Help](#) [Contact](#)



Do I always have to use IUCLID?

- NO!
- Certain types of “dossiers”, (i.e. C&L notifications, Downstream users reports or notifications, PPORD dossiers, application for authorisation, etc...) are much simpler than the registration dossier
- in particular they contain **no (robust) study summaries**
- For those dossiers, **web-applications** will be made available on the Agency web site (i.e. no need to use IUCLID)


C&L notification example

Create Classification & labelling

General information Classification(1 to 6) Classification(6 to 12) Classification(13 to 15) Labelling

[Return to previous step \[General information \]](#)

Please provide here following classifications for your substance: explosiveness, oxidising properties, flammability, the toxicity and acute toxicity - irreversible damage after single exposure.

Fields marked with an asterisk (*) are mandatory. Hovering over a  sign displays help information.

The level of confidentiality chosen in previous page is applicable to the entire classification and labelling.

Classification: 1 to 6

Explosiveness

* Classified: If an entry is not classified the reason must be specified.

* Reason for no classification: Inconclusive

* Classification:
E; R2
E; R3

Oxidising properties

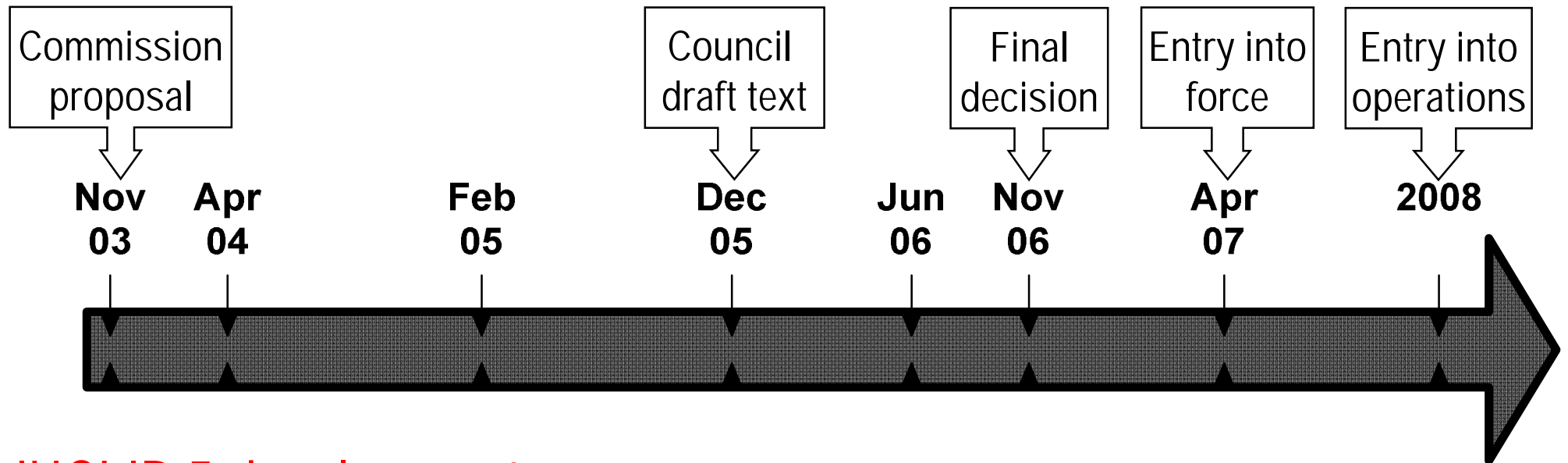
* Classified:

* Reason for no classification: Inconclusive

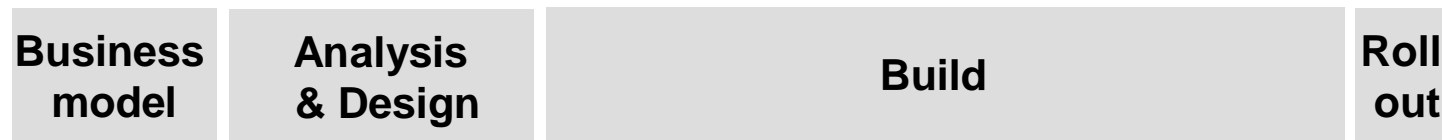
* Classification:
O;R7

Timeline

Legal framework



IUCLID 5 development



- <http://ecb.jrc.it/REACH-IT-INFORMATICS/>

REACH-IT & Informatics	
ECB Home	Documents IUCLID 4 IUCLID 5 REACH-IT
Assessment of Chemicals	<p>Managing information on chemical substances and their hazards requires complex informatics development and IT and ECICS, and also "Global Portals" for Chemicals Information, use of Web Technologies and support to new</p> <p>This is managed under Action no 1314 - Support to REACH and Informatics.</p> <p>Contact Person - Action Leader: Christel MUSSET</p>
Biocides	
Existing Chemicals	
Export-Import	
New Chemicals	
QSARs	Overview
REACH	Working closely with DG ENTR and DG ENV, Action 1314 "Support to REACH and Informatics" will assist in the execution. In particular, support is given to the IT related tasks concerning preparation of the new Agency so that it can begin its capabilities in understanding and structuring the complexities of chemicals information and applying this to the detailed f
Classification & Labelling	provide the detailed content information in designing these IT systems, whilst the responsibility for implementation will larg
Testing Methods	The REACH implementation activities provide a unique competence to underpin the JRC scientific role regarding chemi
REACH-IT & Informatics	the Chemicals community (Member States, Industry and International partners) regarding global cooperation, harmonis
ESIS	formats, data sharing and improved access to information. The generation of hazard data and its global availability (free (
INFOCAP	Forum on Chemical Safety (Forum IV, Bangkok, November 2003). OECD and relevant stakeholders were invited to t
Contacts	developing .chemical. economies of Asia.
Documents	1. REACH-IT
Legislation	At the heart of the future European Chemical Agency's operations will be the REACH-IT system. The goal is to have
Links	substances, and for a selected sample of these to provide a work flow system for evaluation and authorisation processe
Newsletter	JRC is undertaking the role of Technical Manager of the analysis and design of this system, supported by DG ENTR a
Search	work. This system provides the capability necessary for the Chemicals Agency to undertake its work and provides the ne
	and Agency staff to execute their tasks.