

LRI Project EEM9.3



INTERNATIONAL
COUNCIL OF
CHEMICAL
ASSOCIATIONS

LONG-RANGE RESEARCH INITIATIVE

LRI Workshop on AMBIT and Read-across

Dr. Volker Koch, Clariant
LRI Workshop on AMBIT
21.01.2016

Introduction

Public

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Computational Toxicology (1)

➤ **Non-testing approaches are used to fill gaps in Human and Environmental Safety Assessment (ECETOC, 2012 TR116) :**

- To avoid animal testing
- Reduce resource costs
- Bridge the gap of laboratory capacity availability

➤ **Read-across and Category formation**

- Are Non-testing methods which are regularly applied to assess the safety of Chemicals and are accepted by most Regulatory Bodies if the approach taken is sufficiently justified and documented
- Is supported by in-silico tools (see ECETOC, 2012, TR 116) using various methodologies like
- QSARs, Expert systems allowing rule-based predictions , Similarity tools etc.

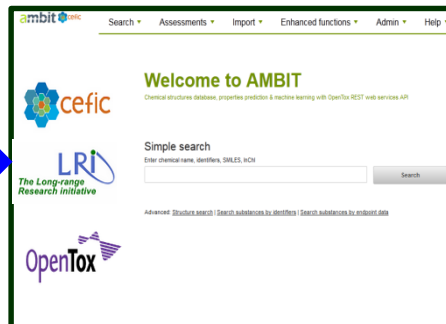
Computational Toxicology (2)

- **LRI AMBIT is an in-silico tool developed continuously since 2005**
- **Goal of the LRI Project EEM9.3 was enhancing the predictive power of AMBIT**
 - **Using large datasets of high quality Substance data**
 - From a IUCLID Database owned by a company itself
 - From ECHA IUCLID Database (non-CBI Disseminated data)
 - From other reliable and quality checked data sources
 - **Implementing workflows for Assessments**
supporting the assessor in setting up a read across/category approach and in establishing a valid justification for the approach taken as requested by authorities
 - **Minimizing overall animal testing and resource costs**
means using available studies for other substances as well if appropriate

Project overview



Data
transfer



Company IUCLID DB
ECHA IUCLID DB
As
Major Data Source

Search for data
possible but
not for structures

CEFIC LRI AMBIT
Chemoinformatics
System

Supporting
Read across
& Category formation

AMBIT FUNCTIONS

Assigning structures

-to constituents, impurities ...

Search structures & Data

- exact, similar, substructure
- combined with data search

Read across/category formation

-Workflows supporting the user

Prediction tools

-Cramer rules, Protein binding etc

Data analysis tools

-Regressions, clustering etc.

Data management

-flexible import/export of data

Data exchange

- manual or automated e.g.
webservices

IUCLID

Data handling, Retrieval & Export

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IUCLID Database

IUCLID Version 4

3.5 Biodegradation

Inoculum: activated sludge, domestic, non-adapted
Concentration: 200 mg/l related to Test substance
Degradation: = 86 % after 28 day
Result: readily biodegradable
Kinetic: 15 day > 10 %
 20 day = 60 %
 25 day = 83 %
Method: other: gemäß OECD-Richtlinie 301 F (1992) (1994) und ISO 9408 (1991) GLP: yes
Year: 1994
Test substance: other TS
Source: Hoechst AG Frankfurt/Main
 Hoechst AG Frankfurt/Main
 Clariant GmbH Frankfurt am Main
Test substance: o-Anisidin; Reinheitsgrad: 99.4 %
Reliability: (1) valid without restriction
 Guideline Studie

Manual Extraction of
substance data to be
used in read
across/category is rather
straightforward

IUCLID Version 5

5.2.1 Biodegradation in water: screening tests

Endpoint study record: KEY_301_1994_HOECHST_93-0133-45

Detail level: Administrative Data Data source Materials and methods
 all fields Results and discussions Overall remarks, attachments Applicant's summary and conclusion

Administrative Data

Purpose flag: key study
 Data waiving:
 Justification for data waiving:
 Study result type: experimental result
 Reliability: 1 (reliable without restriction)
 Rationale for reliability incl. deficiencies: Guideline study performed compliant to GLP.

Data source

Reference type	Author	Year	Title	Bibliographic	Reference	Reference	Reference	Reference	Reference
study report	Teufel & Voelskow	1994	Prüfung der leichten biologischen Abbaubarkeit von o-Anisidin D	unpublished report of Clariant	Hoechst AG, Frankfurt-Höchst, Abt. Umweltschutz, D-65926 Frankfurt am Main	93-0133-45	Clariant	93-0133-45	1994-03-02

Add... Edit... Delete Move up Move down Select Insert

Data access
 data submitter is data owner
Data protection claimed
 yes, but willing to share

% Degradation of test substance

%Degr.	St. dev.	Parameter	Sampling time
86		O2 consumption	28 d
10		O2 consumption	15 d
83		O2 consumption	25 d

Manual Extraction of
substance data to be
used in read
across/category is
cumbersome & time
consuming

Many page scrolls

IUCLID 4 had ca. **850** Database fields

IUCLID 5 has **> 8500** Database fields

IUCLID Substance ID & Composition

➤ IUCLID Substance ID & Composition

- Every Substance in IUCLID is characterized by at least **one Composition**
- A IUCLID Substance composition has
 - **CONSTITUENTS $n \geq 1$, IMPURITIES $n \geq 0$, ADDITIVES $n \geq 0$**
 - **A IUCLID substance itself has NO CHEMICAL STRUCTURE.**
Only constituents, impurities and additives have a structure
 - As a IUCLID composition has at least 1 constituent, at least one structure is assigned. **Very many IUCLID substances are related to more than 1 structure**
 - **When the IUCLID composition is transferred, AMBIT assigns automatically searchable structures to constituents, impurities and additives** (if they are available in the AMBIT structure pool of > 400.000 structures)
- **Most in-silico tools e.g. the OECD Toolbox cannot cope with the composition of a substances and relates one structure to a substance !**

Data retrieval in IUCLID 5 (1)

➤ **Endpoint data in IUCLID can be retrieved**

➤ **“Manually”**

➤ if location is known by the user

➤ **Using the IUCLID Query Tool**

➤ Requires knowledge about the IUCLID data structure (experts only)

➤ **Structures in IUCLID are**

➤ Images which cannot be retrieved

➤ **Smiles codes which can be used for exact structure search only but not for similarity or substructure search**

➤ **Not directly applicable for read across/category formation approaches**

Methods for Data transfer from IUCLID to AMBIT

➤ Manual Transfer

- Using the IUCLID 5 Bulk Export Assistant which is cumbersome requiring a multistep and manual interaction
- Using the IUCLID 5 Batch Export which also requires a limited manual interaction

➤ Automated Transfer using Web services

- IUCLID 5 and AMBIT are IT systems which are running on Web servers
- Web servers can interact via Web services allowing **automated data transfer and update from IUCLID 5** not requiring manual interaction

AMBIT Data import

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Data Import filter for AMBIT

Substances > Import > Retrieve substance(s) from IUCLID5 server

Substance search ?

Name

Study ? : P-Chem ENV
ECO TOX

Reliability ? : 1 2 3 4 5 6

Study purpose ? : K S
WoE D N/A

Robust study ? : Yes No

Result ? : E EP C RAg

Retrieve substance(s) from IUCLID5 server

Select substance by UUID

UUID*

Clear existing study records ☒ Clear existing composition records ☒

Import only high quality study records ☒ (uncheck to import all records)

Purpose flag ☒ + -

- key study
- supporting study
- weight of evidence
- disregarded study
- Not specified

Study result type ☒ + -

- experimental result
- experimental study planned
- estimated by calculation
- read-across based on grouping
- read-across from supporting su

Test material ☒ + -

- yes
- no
- Not specified

Reliability ☒ + -

- 1 (reliable without restriction)
- 2 (reliable with restrictions)
- 3 (not reliable)
- 4 (not assignable)
- other:

Reference type ☒ + -

- study report
- other company data
- publication
- review article or handbook
- secondary source

☒ Select high quality study criteria
+ Select All
- Unselect all

➤ These filter allow to select which data from an IUCLID substance should be imported into AMBIT and work for manual or web based data import from IUCLID

AMBIT Chemoinformatics System

Data & Structure handling
Functions
Communication

Public

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LRI AMBIT Chemoinformatic System



Search ▼

Assessments ▼

Import ▼

Enhanced functions ▼

Admin ▼

Help ▼



Welcome to AMBIT

Chemical structures database, properties prediction & machine learning with OpenTox REST web services API

- **AMBIT Chemoinformatics System** was developed within a CEFIC LRI Project in 2005 and is part of the LRI Toolbox
- Was continuously developed further and is now a state of the art Java web application running on all Operating Systems supporting Java
- Is an **Open Source Application** with the **following functions**
 - **Search for structure(s)** [exact, similar, substructure] and **meta data**
 - **Assessment tools (read across/category formation)**
 - **Prediction tools** e.g. Cramer rules , Protein binding, pKa etc
 - **Data analysis tools** e.g. regression, classification, clustering etc
 - **Data exchange tools:** manual or automated via Opentox API, Webservices etc

AMBIT Search for Structures

Exact, Similarity & Substructure

ambit cefic

Search ▾

Assessments ▾

Import ▾

Enhanced functions ▾

Admin ▾

Help ▾

Search structures and associated data

Exact structure

Similarity

Substructure

URL

☐ Is regular expression

111-96-6

	Diagram	CasRN	IUCLID 5 Reference subs	Similarity	IUPAC name	Names	SMILES
- 1 -		111-96-6	ECB5-19...	-	-	diglyme[Ethane, 1,1'-oxybis(2-methoxy-)]bis(2-methoxyethyl) ether[Ethane, 1,1'-oxybis(2-methoxy-)]diethyleneglycol-dimethylether[111-96-6]1-methoxy-2-(2-methoxyethoxy)ethane	COCOC...

Exact structure

Similarity

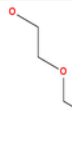
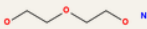
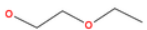
Substructure

URL

Identifiers

Datasets

Showing from 1 to 3 in pages of 20 entries ◀ Previous Next ▶

	Diagram	IUCLID 5 Reference subs	Similarity
- 1 -		-	1
- 2 -		-	1
- 3 -		-	0.92

Exact structure

Similarity

Substructure

URL

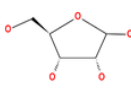
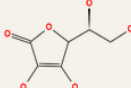
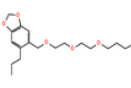
Custom SMARTS

OCCOCCO

Identifiers

Datasets

Showing from 1 to 20 in pages of 20 entries ◀ Previous Next ▶

	Diagram	IUCLID 5 Reference subs	Names	Std. InChI key
- 1 -		-		HMFBZSHGGEWLO-SOOFDHNKSA-N
- 2 -		-		CIWBSHSHKHDKBQ-JLAZNSOCSA-N
- 3 -		-		FIPWRIJSWJWJAI-UHFFFAOYSA-N

AMBIT Search for Structures & Endpoint data



Search ▾

Assessments ▾

Import ▾

Enhanced functions ▾

Admin ▾

Help ▾

Search structures and associated data

Exact structure

Similarity

Substructure

URL

☐ Is regular expression

111-96-6

Diagram	CasRN	IUCLID 5 Reference subs	Similarity	IUPAC name	Names	SMILES
	111-96-6	ECB5-19...	-	-	diglyme Ethane, 1,1'-oxybis 2-methoxy- bis(2-methoxyethyl) ether Ethane, 1,1'-oxybis[2-methoxy- Diethyleneglykol-dimethylether 111-96-6 1-methoxy-2-(2-methoxyethoxy)ethane	COCCO...

1) Find
Structure(s)

2) Find
Substance(s)

Substance Name	Substance UUID	Substance Type	Public name
Glymes_Diethylene glycol dimethyl ether_(DEGDME, Diglyme)_ICS_MSe_DF71	IUC5-a43...	mono constituent substance	Diglyme

3) Display data

IUC Substance	Composition	P-Chem (2)	Env Fate (4)	Eco Tox (8)	Tox (8)
Composition name: Crude Diglyme Composition UUID: L-327712f8-626c-4bd0-b915-621c4b5f87c0 Purity of IUC Substance: 85-99 % (w/w)					
Type	Name	EC No.	CAS No.	Typical concentration	
Constituent	Diglyme, ethane, 1,1'-oxybis 2-methoxy-, bis(2-methoxyethyl) Ether, ethane, 1,1'-oxybis[2-methoxy-, diethyleneglykol-dimethylether, 111-96-6, 1-methoxy-2-(2-methoxyethoxy)ethane	203-924-4	111-96-6	ca. 92 % (w/w)	
Impurity	2-(2-methoxyethoxy)ethanol, diethyleneglycol monomethyl ether, ethanol, 2-(2-methoxyethoxy)-, methyl diglykol, diethyleneglykol monomethylether, 111-77-3	203-906-6	111-77-3	ca. 8 % (w/w)	
Impurity	Unknown Organic Impurities, unknown			<1 % (w/w)	

IUC Substance	Composition	P-Chem (2)	Env Fate (4)	Eco Tox (8)	Tox (8)
Filter...					
Diglyme					
6.1.1 Short-term toxicity to fish (1)					
6.1.3 Short-term toxicity to aquatic invertebrates (2)					
6.1.4 Long-term toxicity to aquatic invertebrates (1)					
6.1.5 Toxicity to aquatic algae and cyanobacteria (2)					
6.1.7 Toxicity to microorganisms (2)					

	64-17-5_Benzoic acid_TRA0002_CLN test substance 2_TST_DE00_REACH P4	IUC5-fae82ecc-67... 	mono constituent substance	Benzoic acid	ECB5-172b9987-8... 	Clariant Produkte (Deutschland) GmbH / Sulzbach am Taunus / Germany	Clariant GHS, Clariant GHS, Clariant GHS, CompTox
Composition name: Benzoic Acid,200-618-2 (98 % (v/v)) Composition UUID: L-ab77c243-e03b-4cf1-8542-2a72ce34194a Purity of IUC Substance: 97-99 % (v/v)							
Type ▲	Name ▼	EC No. ▼	CAS No. ▼	Typical concentration ▼	Concentration ranges ▼		Structure ▼
Constituent	Benzoic Acid,200-618-2	200-618-2	65-85-0	98 % (w)	>97 % (w)	<99 % (w)	Also contained in...
Impurity	Formaldehyde	200-001-8	50-00-0	1 % (w)	>0.5 % (w)	0.7 % (w)	Also contained in...

IUCLID Substance Data in AMBIT

- **IUCLID Data in AMBIT are organized in tab sections allowing easy access by clicking on the tab of interest**

IUC Substance	Composition	P-Chem (6)	Env Fate (1)	Eco Tox (3)	Tox (4)
IUC Substance name:	Velsan SC_Sorbitane Caprylate_60177-36-8_TRA115477_ICs_MSe_Phase II_DE71				
IUC Substance UUID:	IUC5-e49aaecc-76d3-4f9f-b1b7-171fbff19363				
IUC Public name:	Sorbitane Caprylate				
Legal entity:	Clariant Produkte (Deutschland) GmbH / Sulzbach am Taunus / Germany				
Legal entity UUID:	IUC5-8da74af7-c7dd-4e38-8d8e-8fc765d5d15f				
Type substance composition:	UVCB				
IUC Substance Reference Identifier					
CAS:					
EC:	939-179-3				
Chemical name:	octanoic acid, esters with anhydrosorbitol and dianhydrosorbitol				
IUPAC name:	?				
UUID:	IUC5-a5f2fd8d-2e4b-413b-b785-2ec9104165d4				
IUC Flags:	Clariant EHS = TRA115477 CompTox = Ambit Transfer				

IUCLID Substance Data in AMBIT

- **IUCLID Composition Data in AMBIT allow a straightforward overview on constituents, impurities & additives as well as the concentrations associated**

IUC Substance Composition P-Chem (6) Env Fate (1) Eco Tox (3) Tox (4)							
Composition name: Octanoic Acid, Esters With Anhydrosorbitol And Dianhydrosorbitol Composition UUID: L-3b892463-4e89-4898-a5fc-b160cd3c46d8 Purity of IUC Substance: 45-100 % (w/w)							
Type ▲	Name ▼	EC No. ▼	CAS No. ▼	Typical concentration ▼	Concentration ranges ▼		
Constituent	⌘ Octanoic Acid, 124-07-2	204-677-5	124-07-2	0.8 % (w/w)	>=0 % (w/w)	<1 % (w/w)	Also contained in...
Constituent	⌘ Unknown Organic Compounds, unknown			ca. 0.5 % (w/w)	>=0 % (w/w)	<1 % (w/w)	Also contained in...
Constituent	⌘ Anhydrosorbitol, Triesters With Octanoic Acid			4.2 % (w/w)	>0 % (w/w)	<10 % (w/w)	Also contained in...
Constituent	⌘ Sorbitol, Mono- And Di-dehydrated			21.4 % (w/w)	>0 % (w/w)	<25 % (w/w)	Also contained in...
Constituent	⌘ Sorbitol, Mono- And Di-dehydrated, Diesters With Octanoic Acid			24.2 % (w/w)	>0 % (w/w)	<30 % (w/w)	Also contained in...
Constituent	⌘ Sorbitol, Mono- And Di-dehydrated, Monoesters With Octanoic Acid			48.8 % (w/w)	>45 % (w/w)	<100 % (w/w)	Also contained in...

Showing 1 to 6 of 6 entries

IUCLID Substance Data in AMBIT

Data for 44 Endpoints from IUCLID

▼ P-Chem	▼ Env Fate	▼ Eco Tox	▼ Tox
☐ 4.1. Appearance (14) [18]	☐ 5.1.1. Phototransformation in Air (4) [4]	☒ 6.1.1. Short-term toxicity to fish (13) [32]	☒ 7.2.1. Acute toxicity - oral (15) [28]
☐ 4.2. Melting point / freezing point (15) [20]	☒ 5.1.2. Hydrolysis (6) [6]	☒ 6.1.2. Long-term toxicity to fish (4) [4]	☐ 7.2.2. Acute toxicity - inhalation (5) [8]
☐ 4.20. pH (10) [11]	☒ 5.2.1. Biodegradation in water - screening tests (14) [32]	☒ 6.1.3. Short-term toxicity to aquatic invertebrates (15) [24]	☐ 7.2.3. Acute toxicity - dermal (6) [8]
☐ 4.21. Dissociation constant (7) [10]	☐ 5.2.2. Biodegradation in water and sediment: simulation tests (6) [6]	☐ 6.1.4. Long-term toxicity to aquatic invertebrates (6) [8]	☐ 7.3.1. Skin irritation / Corrosion (16) [30]
☐ 4.3. Boiling point (15) [21]	☐ 5.2.3. Biodegradation in Soil (5) [5]	☐ 6.1.5. Toxicity to aquatic algae and cyanobacteria (11) [18]	☐ 7.3.2. Eye irritation (12) [18]
☐ 4.5. Particle size distribution (Granulometry) (2) [2]	☒ 5.3.1. Bioaccumulation: aquatic / sediment (5) [5]	☐ 6.1.7. Toxicity to microorganisms (10) [13]	☒ 7.4.1. Skin sensitisation (6) [9]
☐ 4.6. Vapour pressure (12) [19]	☐ 5.3.2. Bioaccumulation: terrestrial (4) [4]	☐ 6.2. Sediment toxicity (5) [5]	☐ 7.5.1. Repeated dose toxicity - oral (7) [14]
☒ 4.7. Partition coefficient (12) [21]	☐ 5.4.1. Adsorption / Desorption (5) [7]	☐ 6.3.1. Toxicity to soil macroorganisms (6) [7]	☐ 7.5.2. Repeated dose toxicity - inhalation (5) [8]
☒ 4.8. Water solubility (17) [23]	☐ 5.4.2. Henry's Law constant (4) [4]	☐ 6.3.2. Toxicity to terrestrial arthropods (5) [5]	☐ 7.5.3. Repeated dose toxicity - dermal (3) [5]
☐ 4.9. Solubility in organic solvents (10) [11]		☐ 6.3.3. Toxicity to terrestrial plants (6) [6]	☒ 7.6.1. Genetic toxicity in vitro (13) [33]
		☐ 6.3.4. Toxicity to soil microorganisms (5) [5]	☐ 7.6.2. Genetic toxicity in vivo (5) [11]
			☐ 7.7. Carcinogenicity (5) [5]
			☐ 7.8.1. Toxicity to reproduction (7) [10]
			☐ 7.8.2. Developmental toxicity / teratogenicity (8) [15]

IUCLID Substance Data in AMBIT

IUC Substance
Composition
P-Chem (6)
Env Fate (1)
Eco Tox (3)
Tox (4)

Filter...
Expand all
Collapse all

Sorbitane Caprylate

4.1 Appearance (1)
4.2 Melting point / freezing point (1)
4.3 Boiling point (1)
4.6 Vapour pressure (1)
4.7 Partition coefficient (1)

Value ▲	Temperature ⇅	pH ⇅	Guideline ⇅	Owner ⇅	UUID ⇅
= 2.55	= 23 °C	ca. 7	OECD Guideline 107 (Partition Coefficient (n-octanol / water), Shake Flask Method)	Clariant	IUC5-0068a11f-9274-... 📄

Showing 1 study(s) (1 to 1)
Previous
Next

4.8 Water solubility (1)

Value ▲	Temperature ⇅	pH ⇅	Remark ⇅	Guideline ⇅	Owner ⇅	UUID ⇅
= 2.7 g/L	= 20 °C	[5.9, 6.4)	-	OECD Guideline 105 (Water Solubility)	Clariant	IUC5-818b7e62-efea-... 📄

Showing 1 study(s) (1 to 1)
Previous
Next

IUCLID Substance Data in AMBIT

IUC Substance
Composition
P-Chem (6)
Env Fate (1)
Eco Tox (3)
Tox (4)

Filter...
Expand all
Collapse all

Sorbitane Caprylate

5.2.1 Biodegradation in water - screening tests (1)

Test type ▲	Sampling time ▼	Degradation ▼	Degrad. Parameter ▼	result ▼	Guideline ▼	Owner ▼	UUID ▼
aerobic	= 28 d	= 88 %	CO2 evolution	readily biodegradable	OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test)	Clariant Produkte (Deutschland) GmbH, Corporate Product Stewardship on behalf of BU ICS	IUC5-2de7e7a0-1629... 🔒

Showing 1 study(s) (1 to 1)
Previous
Next

IUCLID Substance Data in AMBIT

IUC Substance
Composition
P-Chem (6)
Env Fate (1)
Eco Tox (3)
Tox (4)

Filter...
Expand all
Collapse all

Sorbitane Caprylate

6.1.1 Short-term toxicity to fish (1)

Test Medium	Organism	Meas. Conc.	Exposure	Endpoint		Effect	Based on	Guideline	Owner	UUID
freshwater	Danio rerio	nominal	= 96 h	LC50	> 100 mg/L	mortality	test mat.	OECD Guideline 203 (Fish, Acute Toxicity Test)	Clariant Produkte (Deutschland) GmbH, Corporate Product Stewardship on behalf of BU ICS	IUC5-21...
		nominal	= 96 h	LC0	= 100 mg/L	mortality	test mat.			
		nominal	= 96 h	NOEC	= 100 mg/L	mortality	test mat.			

Showing 1 study(s) (1 to 1) [Previous](#) [Next](#)

6.1.3 Short-term toxicity to aquatic invertebrates (1)

Test Medium	Organism	Meas. Conc.	Exposure	Endpoint		Effect	Based on	Guideline	Owner	UUID
freshwater	Daphnia magna	nominal	= 48 h	EC50	= 40.1 mg/L	mobility	test mat.	OECD Guideline 202 (Daphnia sp. Acute Immobilisation Test)	Clariant Produkte (Deutschland) GmbH, Corporate Product Stewardship on behalf of BU ICS	IUC5-2c...
		nominal	= 48 h	EC10	= 28.2 mg/L	mobility	test mat.			

Showing 1 study(s) (1 to 1) [Previous](#) [Next](#)

6.1.5 Toxicity to aquatic algae and cyanobacteria (1)

IUCLID Substance Data in AMBIT

IUC Substance
Composition
P-Chem (6)
Env Fate (1)
Eco Tox (3)
Tox (4)

Filter...
Expand all
Collapse all

Sorbitane Caprylate

7.2.1 Acute toxicity - oral (1)

Species ▲	Endpoint ▾	Value ▾	Sex ▾	Interpretation of the results ▾	criteria ▾	Guideline ▾	Study year ▾	Owner ▾	UUID ▾
rat	LD50	> 2000 mg/kg bw	female	not classified	EU	OECD Guideline 423 (Acute Oral toxicity - Acute Toxic Class Method)	2009	Clariant	IUC5-aef4cde...

Showing 1 study(s) (1 to 1)
Previous
Next

7.3.1 Skin irritation / Corrosion (1)

Method type ▲	Species ▾	Interpretation of the results ▾	criteria ▾	Guideline ▾	Study year ▾	Owner ▾	UUID ▾
in vivo	rabbit	not irritating	EU	OECD Guideline 404 (Acute Dermal Irritation / Corrosion)	2009	Clariant	IUC5-86bbb5...

Showing 1 study(s) (1 to 1)
Previous
Next

7.3.2 Eye irritation (1)

7.4.1 Skin sensitisation (1)

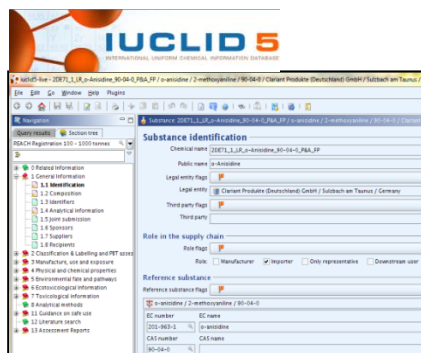
AMBIT Chemoinformatics System

Communication with other Systems

Public

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21.01.2016

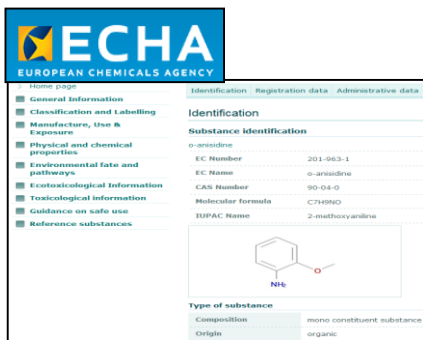
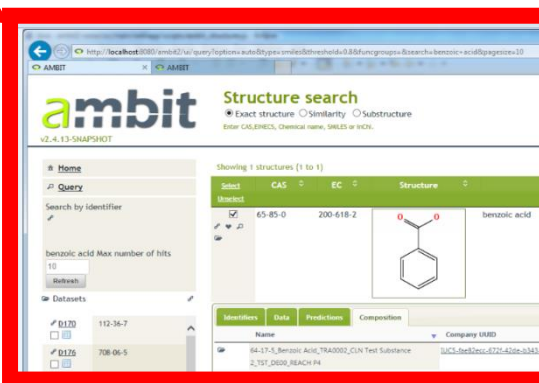
AMBIT Communication



Transfer via
Web service
or manually

**Company
Database**

**Other
Databases**



Transfer
of 14570
Datasets

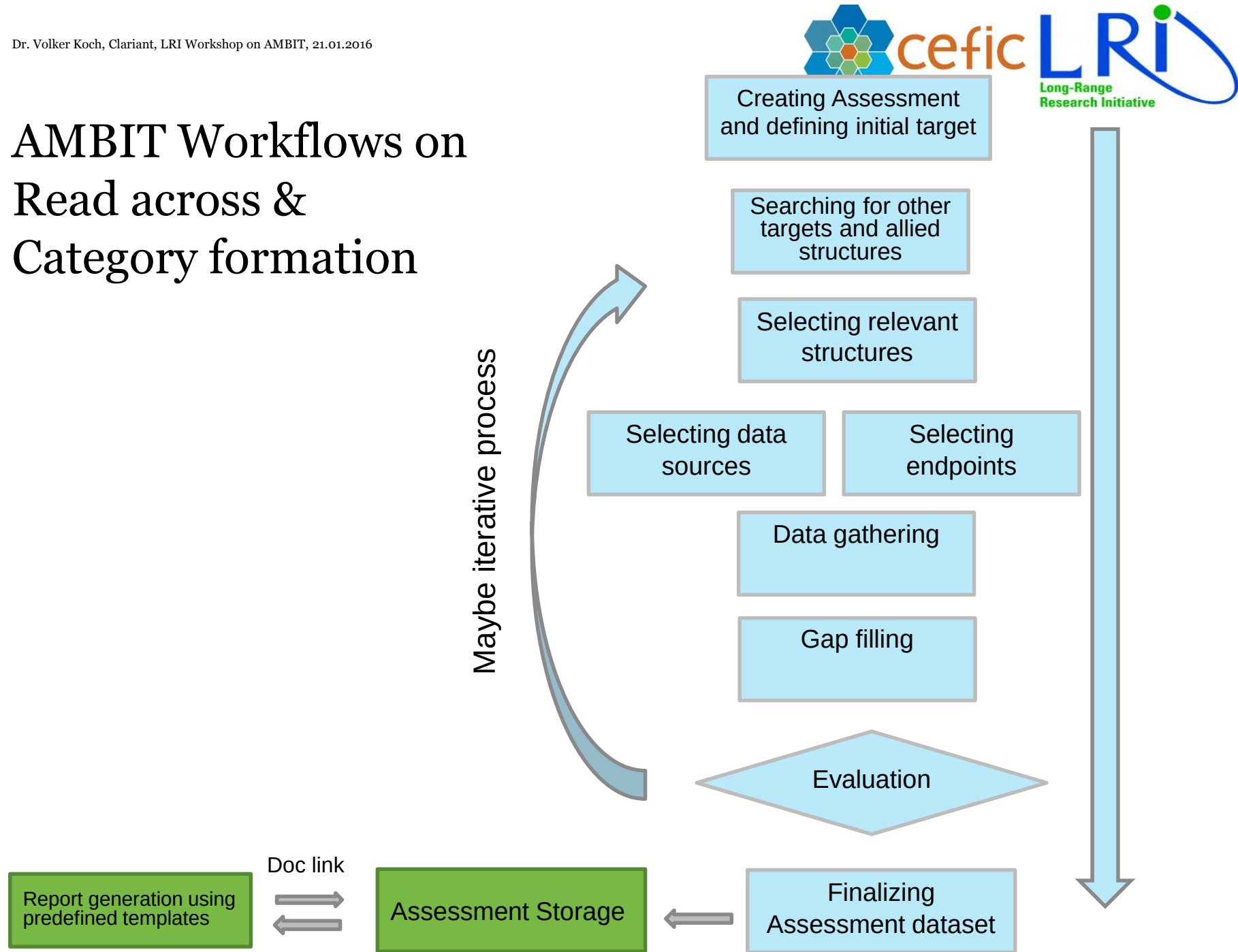
**Other
Tools**

Workflow Read across & Category formation

Public

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21.01.2016

AMBIT Workflows on Read across & Category formation



New Assessment & Identifier

ambit 

Search ▾ Assessments ▾ Import ▾ Enhanced functions

Home > All assessments >

New assessment ▸ Use of empty template

Existing assessments ▸ Use of existing assessment

Assessment identifier | Collection structure | Import | Assessment details | Report

Assessment title ⓘ :	Category justification for Glymes
Owner ⓘ :	user1
Purpose ⓘ :	REACH Registration
Version ⓘ :	1
Version start date ⓘ :	03.08.2015
Version last modified on ⓘ :	03.08.2015
Status ⓘ :	☒ Draft version ☐ Final assessment ☐ Archived version
Assessment code ⓘ :	\\sharepoint\REACH
Assessment Doclink(s) ⓘ :	VK-GLY01
Assessment ID ⓘ :	6b137267-39b8-11e5-aa88-001e68a9cd90
Users with write access ⓘ :	
Users with read access ⓘ :	

Finalize assessment Generate new version

Collect (Search) structures for Assessment

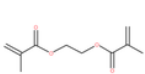
Assessment identifier **Collect structures** Endpoint data used Assessment details Report

Collect structures List collected

Search

Exact structure Similarity **Substructure** URL ☒ Filter by substance Custom SMARTS

Showing from **1** to **18** in pages of entries [Previous](#) [Next](#)

	Diagram	CasRN	EC number	Names	Rationale
T S CM		97-90-5	202-617-2	ethylene dimethacrylate 2-Propenoic acid, 2-methyl-, 1,2-ethanediyl ester Ethylene glycol dimethacrylate	
T S CM		110-71-4	203-794-9	1,2-dimethoxyethane Ethane, 1,2-dimethoxy-	Homologue of Target

T = Target, S = Source, CM = Category member

- Based on the Smiles code of the Target Diglyme a substructure search was carried out limited to those having substance data
- Clicking T, S or CM allows to assign the structure for intended purpose

List collected structures for Assessment

Assessment identifier

Collect structures

Endpoint data used

Assessment details

Report

Collect structures

List collected

Showing from 1 to 3 in pages of 20 entries

Previous

Next

Filter...

	Diagram	CasRN	EC number	Names	Rationale
T S CM		110-71-4	203-794-9	1,2-dimethoxyethane Ethane, 1,2-dimethoxy-	Homologue of Target
T S CM		111-96-6	203-924-4	diglyme Ethane, 1,1'-oxybis 2-methoxy- bis(2-methoxyethyl) ether Ethane, 1,1'-oxybis[2-methoxy- 1-methoxy-2-(2-methoxyethoxy)ethane 1,1'-Oxybis[2-methoxyethane] Diethylene glycol dimethyl ether Ansol Ether 141 2,5,8-Trioxanonane 1,5-Dimethoxy-3-oxapentane Diglyme Dimethyl carbitol 2,2'-oxybis-, dimethyl ether Dimethyl digol	Target
T S CM		112-36-7	203-963-7	bis(2-ethoxyethyl) ether diethylene_glycol_diethyl_ether Ethane, 1,1'-oxybis[2-ethoxy- 1-ethoxy-2-(2-ethoxyethoxy)ethane	Homologue of Target

T = Target, S = Source, CM = Category member

- Based on the Smiles code of the Target Diglyme a substructure search was carried out limited to those having substance data

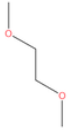
Search Substances

Assessment identifier Collect structures **Endpoint data used** Assessment details Report

Search substance(s) Selection of endpoints

Showing from 1 to 3 in pages of 20 entries ◀ Previous Next ▶

Filter...

	Diagram	CasRN	EC number	Names	Rationale	Tag
- 1 -		110-71-4	203-794-9	1,2-dimethoxyethane Ethane, 1,2-dimethoxy-	Homologue of Target	

Showing from 1 to 3 in pages of 10 substances ◀ Previous Next ▶

Filter...

	Substance Name	Substance UUID	Substance Type	Public name	Reference substance UUID	Owner	Info	Contained in as
☒ - 1 -	Glymes_Ethylene glycol dimethyl ether_(EGDME, Monoglyme)_ICS_MSe_DE71	IUC5-eb8...	mono constituent substance	Monoglyme	ECB5-73...	Clariant Produkte (Deutschland) GmbH / Sulzbach am Taunus / Germany		constituent ⓘ
☐ - 2 -	Glymes_Ethylene glycol dimethyl ether_(EGDME, Monoglyme)_ICS_MSe_DE71	IUC5-eb8...	mono constituent substance	Monoglyme	ECB5-73...	Clariant Produkte (Deutschland) GmbH / Sulzbach am Taunus / Germany		constituent ⓘ
☐ - 3 -	Glymes_Ethylene glycol dimethyl ether_(EGDME, Monoglyme)_ICS_MSe_DE71	IUC5-eb8...	mono constituent substance	Monoglyme	ECB5-73...	Clariant Produkte (Deutschland) GmbH / Sulzbach am Taunus / Germany		constituent ⓘ

- When clicking the Tab “Endpoint data used” associated substances can be display from the list and selected for further use (Subtab “Search substance(s)”)

Search Substances

Assessment identifier

Collect structures

Endpoint data used

Assessment details

Report

Search substance(s)

Selection of endpoints

☐ Show all endpoints

▶ P-Chem

▶ Env Fate

▶ Eco Tox

▼ Tox

Showing 10 endpoint(s) (1 to 10)

☒	7.2.1. Acute toxicity - oral
☒	7.2.2. Acute toxicity - inhalation
☒	7.2.3. Acute toxicity - dermal
☒	7.3.1. Skin irritation / Corrosion
☒	7.3.2. Eye irritation
☒	7.5.2. Repeated dose toxicity - inhalation
☒	7.6.1. Genetic toxicity in vitro
☒	7.6.2. Genetic toxicity in vivo
☒	7.8.2. Developmental toxicity / teratogenicity
☐	7.999.9. Supporting information

- When clicking the Tab “Endpoint data used” and subsequently Subtab “Selection of endpoints” a list of IUCLID Endpoints are displayed for selection by check marking

Working matrix (Composition section)

	CAS	Substance Name	IUCLID	Data source	Tag	Diagram	Constituent Name	Content	Contained As
- 1 - 		Tetraglyme	1UCS-541... 	Clariant Produkte (Deutschland) GmbH / Sulzbach am Taunus / Germany	 S  0		112-49-2	2.4 % (w/w)	impurity 
					 T  0		143-24-5	>99 % (w/w)	constituent 
					 T  0			50.4 % (w/w)	constituent 
- 2 - 		Triglyme	1UCS-203... 	Clariant Produkte (Deutschland) GmbH / Sulzbach am Taunus / Germany	 S  0		112-49-2	ca.90 % (w/w)	constituent 
					 S  0			>=99 % (w/w)	constituent 
- 3 - 		Monoglyme	1UCS-585... 	Clariant Produkte (Deutschland) GmbH / Sulzbach am Taunus / Germany	 S  0		1,2-dimethoxyethane	ca.97.5 % (w/w)	constituent 
					 S  0			>=99.9 % (w/w)	constituent 
					 S  0			ca.97 % (w/w)	constituent 
					 S  0		111-95-5	ca.0.5 % (w/w)	impurity 
					 S  0		112-49-2	ca.0.5 % (w/w)	impurity 
- 4 - 		Diglyme	1UCS-543... 	Clariant Produkte (Deutschland) GmbH / Sulzbach am Taunus / Germany	 S  0		111-95-5	ca.92 % (w/w)	constituent 
					 S  0			>=99.9 % (w/w)	constituent 

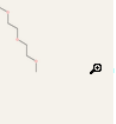
Working matrix (Endpoint section)

Assessment identifier
Collect structures
Endpoint data used
Assessment details
Report

Initial matrix
Working matrix
Final matrix
Save

Identifiers
P-CHEM
ENV FATE
ECOTOX
TOX
Export

Showing from 1 to 4 in pages of 20 entries Previous Next Filter...

	CasRN	Substance Name	ISUUUID	Data source	Tag	Diagram	6.1.1. Short-term toxicity to fish	6.1.3. Short-term toxicity to aquatic invertebrates	6.1.4. Long-term toxicity to aquatic invertebrates
- 1 - T S CM ▼		SiA_EC211-076-1_1,2-Diethoxyethane_en	IUC5-87c...	Example Company 1 / Example city / Finland	-		+	+	+
- 2 - T S CM ▲ ▼		bis(2-methoxyethyl)ether	IUC5-fb67...	European Chemicals Agency / Helsinki / Finland	T i		+	+	+
- 3 - T S CM ▲ ▼		Diglyme	IUC5-a43...	Clariant Produkte (Deutschland) GmbH / Sulzbach am Taunus / Germany	T i T i	 	• NOEC = 2000_mg/L (Exposure = 96.0 h) i • LC0 > 2000_mg/L (Exposure = 96.0 h) i • +	• EC0 > 1000_mg/L (Exposure = 48.0 h) i • NOEC = 1000_mg/L (Exposure = 48.0 h) i • EC50 = 943_mg/L (Exposure = 48.0 h) i • +	• NOEC = 320_mg/L i • +

EXCEL Export of Working Matrix

matrix.xlsx [Read-Only] - Excel

FILE CLARANT HOME INSERT PAGE LAYOUT FORMULAS DATA REVIEW VIEW

Calibri 11 A A

Wrap Text

General

AutoSum

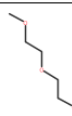
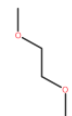
Fill

Sort & Find & Filter

Volker Koch

B6

Monoglyme

	A	B	C	D	E	AB	AC	AI	AJ
1	Tag	Substance name	CAS No.	Structure	Contained as	6.1.5. Toxicity to aquatic algae and cyanobacteria	6.1.7. Toxicity to microorganisms	7.2.1. Acute toxicity - oral	7.2.2. Acute toxicity - inha
2					constituent				
3	3	Diglyme			constituent	EC10 >= 1000.0 mg/L (growth rate ,Exposure=72.0 h) EC50 >= 1000.0 mg/L (biomass ,Exposure=72.0 h) NOEC >= 1000.0 mg/L (growth rate ,Exposure=72.0 h) NOEC = 5000.0 mg/L (growth rate ,Exposure=72.0 h) EC50 >= 1000.0 mg/L (growth rate ,Exposure=72.0 h) EC10 >= 1000.0 mg/L (biomass ,Exposure=72.0 h) NOEC >= 1000.0 mg/L (biomass ,Exposure=72.0 h) EC50 >= 10000.0 mg/L (growth rate ,Exposure=72.0 h)	EC10 >= 1000.0 mg/L (Effect=respiration rate ,Exposure=3.0 h) EC20 = 1067.0 mg/L (Effect=respiration rate ,Exposure=3.0 h)	LD50 = 4760.0 mg/kg bw (rat)	LC0 = 11.0 mg/L air (rat)
4					constituent				
5	5	Monoglyme			constituent				
6									

- AMBIT has several reporting functions, one is the export of the Working matrix into EXCEL for easier handling and printing

Assessment report

ambit cefic

Search ▾ Assessments ▾ Import ▾ Enhanced functions ▾ Admin ▾ Help ▾

Home > All assessments > This assessment > Report

Assessment identifier

Report

Create Word file

Ambit Assessment Report

Category justification for Glymes

Author: Unknown
Company: datamanager1
Date: 26.05.2015
Assessment code: 64e268d4-1252-4b5d-b121-71df4ba79df8
Purpose: REACH Registration

1. Assessment Identifiers

Assessment title:	Category justification for Glymes
Owner:	Unknown
Purpose:	REACH Registration
Version:	1
Status:	draft
Version start date:	26.05.2015
Version last modified on:	26.05.2015
Published:	draft
Assessment code:	\\sharepoint\REACH
Assessment DocLink:	VK-GLY01
Assessment ID:	64e268d4-1252-4b5d-b121-71df4ba79df8

The original assessment in Ambit can be found via "Assessment ID".

2. List of structures for assessment

In the assessment, similar structures were selected from exact structure, substructure and/or similarity searches, or were added manually. The rationale for the selection is given in the table.

- AMBIT has several reporting functions, one is creating an assessment report in Word

Project information

Public

Dr. Volker Koch, Clariant
LRI Workshop on AMBIT
21.01.2016

Project information

- **Project idea** **Volker Koch, Clariant**
- **LRI Manager** **Bruno Hubesch**
- **Contractors** **Nina Jeliaskova, Ideaconsult Ltd**
Egon Willighagen, Maastricht University
- **Clariant Team for System design** **Udo Jensch, Toxicologist**
Volker Koch, Ecotoxicologist
Qiang Li, Toxicologist
Joachim Schneider-Reigl, Ecotoxicologist
- **Project end** **December 8, 2015**

Acknowledgement



CEFIC LRI would like to thank ECHA for providing the non-confidential IUCLID data which are accessible on the ECHA Website.



Information on Chemicals

Datasets on 14570 Substances have been provided on January 12, 2016 by ECHA in Computer readable format allowing the import into AMBIT