Good Read-across Practices Workshop: Making it Work for You!

CEFIC LRI AMBIT Tool Supporting Read-across

Dr. Volker Koch, Clariant
CAAT EUTOXRISK LRI Workshop
26.02.2016

Public

Introduction

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Computational Toxicology (1)

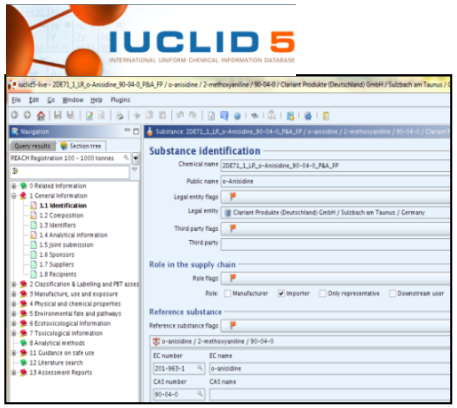
- **Non-testing approaches are used to fill gaps in Human and Environmental Safety Assessment (ECETOC, 2012 TR116) :**
  - To avoid animal testing
  - Reduce resource costs
  - Bridge the gap of laboratory capacity availability

- **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.

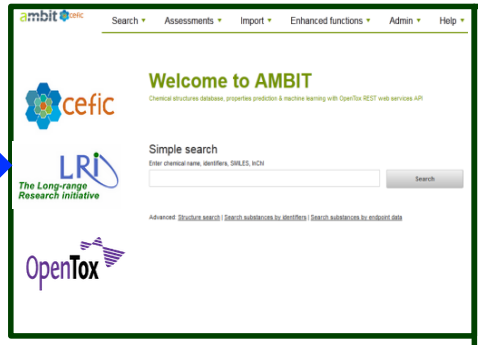
Computational Toxicology (2)

- **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

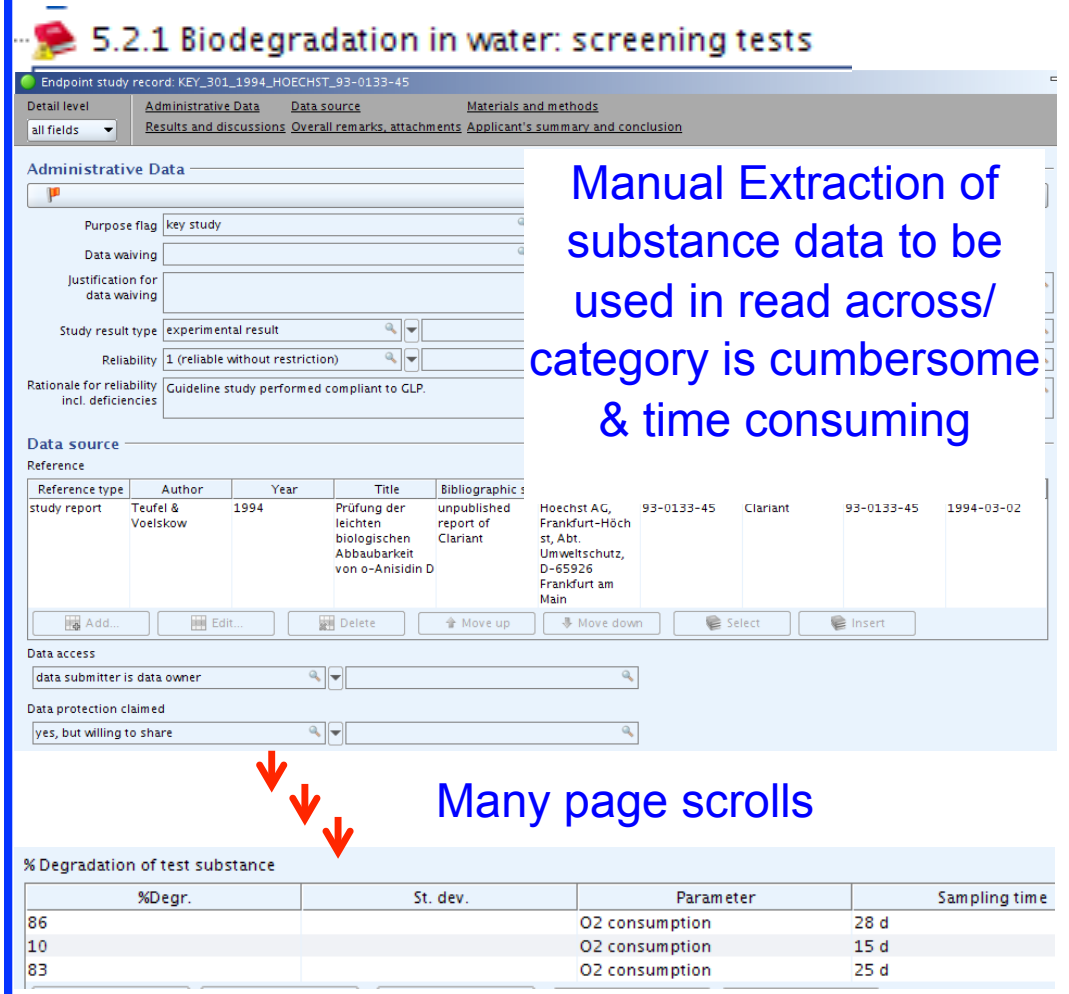
3.5 Biodegradation

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)
Year:	1994 GLP: yes
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 **4** had ca**. 850** Database fields

IUCLID Version 5



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

Many page scrolls

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>= 1, IMPURITIES n>=0, ADDITIVES n>=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 !**

IUCLID 5 Data retrieval & Transfer

- **Endpoint data in IUCLID can be retrieved**
  - **"Manually"**
  - **Using the IUCLID Query Tool**
    - Requires knowledge about the IUCLID data structure (experts only)
- **Structures in IUCLID are mostly**
  - Images which cannot be retrieved and not be used for structures searches
- **Manual Data Transfer**
  - Using the IUCLID 5 Bulk Export Assistant which is cumbersome requiring a multistep and 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 IUCLD 5 not requiring manual interaction

AMBIT
Data import

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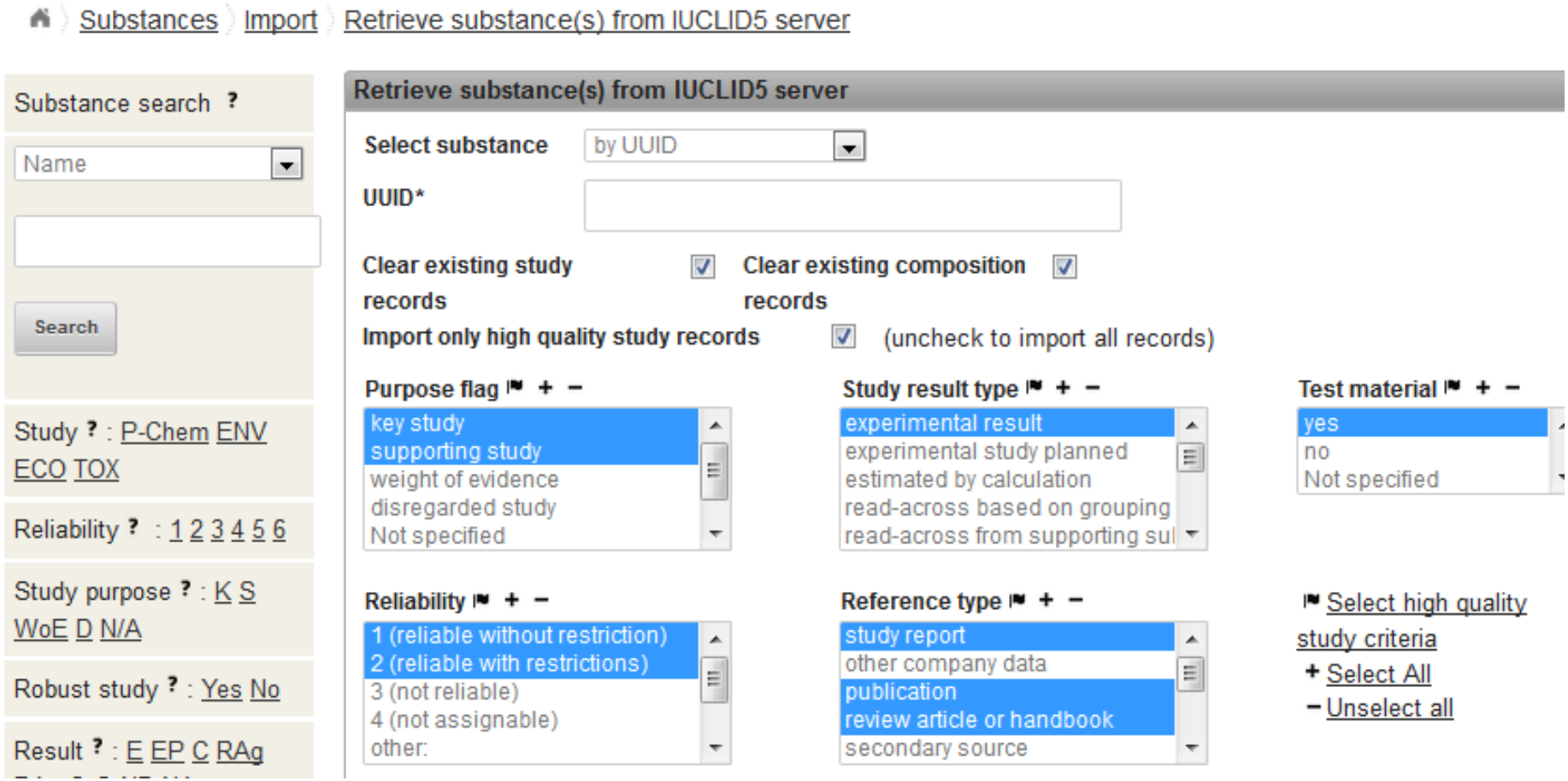
Data Import filter for AMBIT



➢ 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

- **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

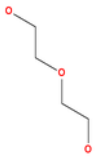
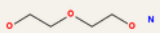
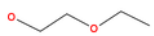
Is regular expression 111-96-6

	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-|Diethylenglykol-dimethylether|111-96-6|1-methoxy-2-(2-methoxyethoxy)ethane	COCCO...

Exact structure | Similarity | Substructure | URL

Identifiers | Datasets

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

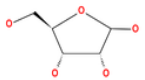
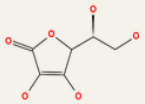
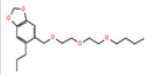
	Diagram	IUCLID 5 Reference subs	Similarity
- 1 -		-	1
- 2 -		-	1
- 3 -		-	0.92

Exact structure | Similarity | Substructure | URL

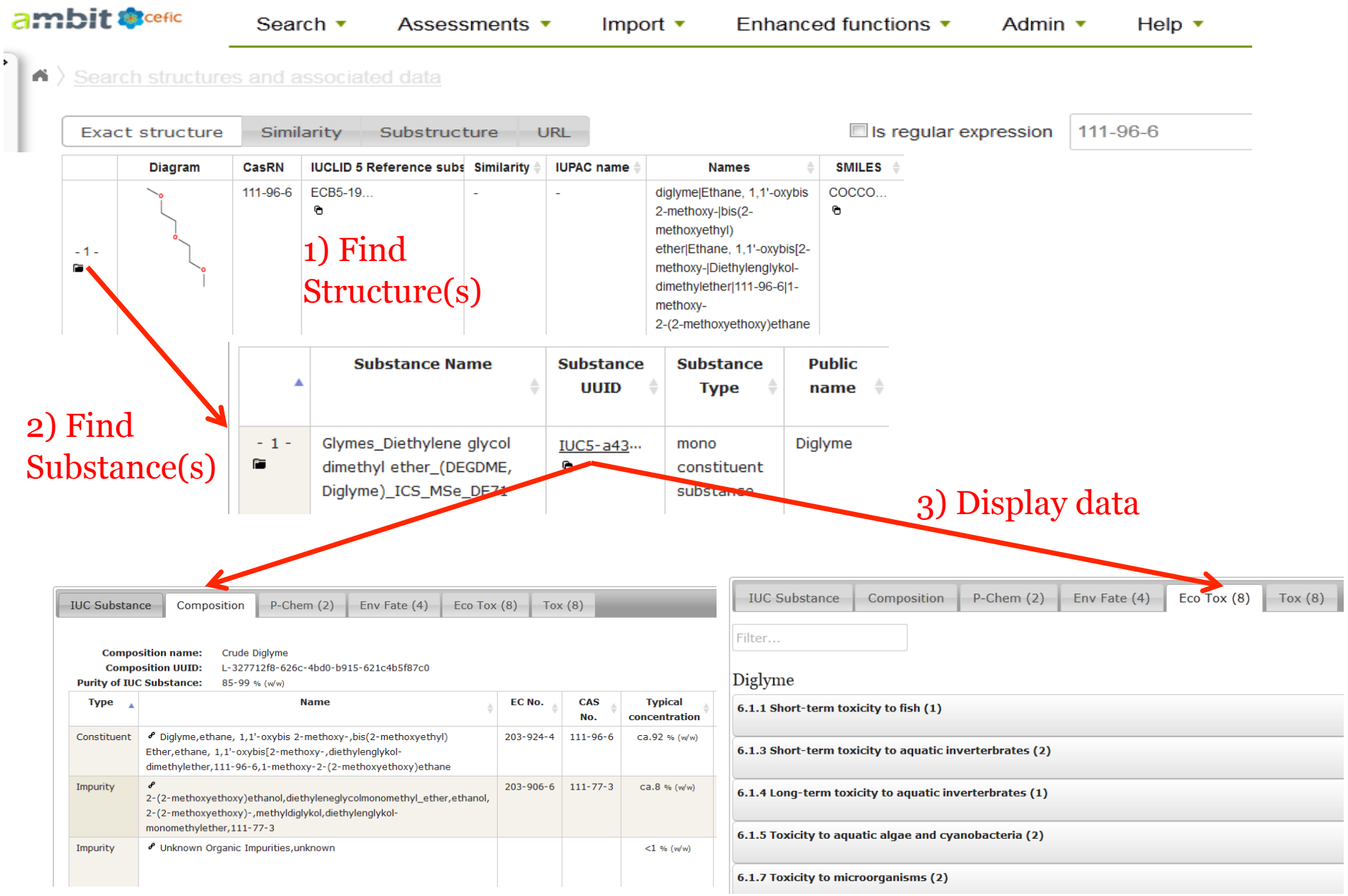
Custom SMARTS OCCOCCO

Identifiers | Datasets

Showing from **1** to **20** in pages of 20 entries Previous Next

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

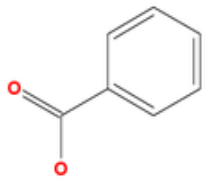
AMBIT Search for Structures & Endpoint data



Structures of Constituents, Impurities, Additives

- 4 -	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**

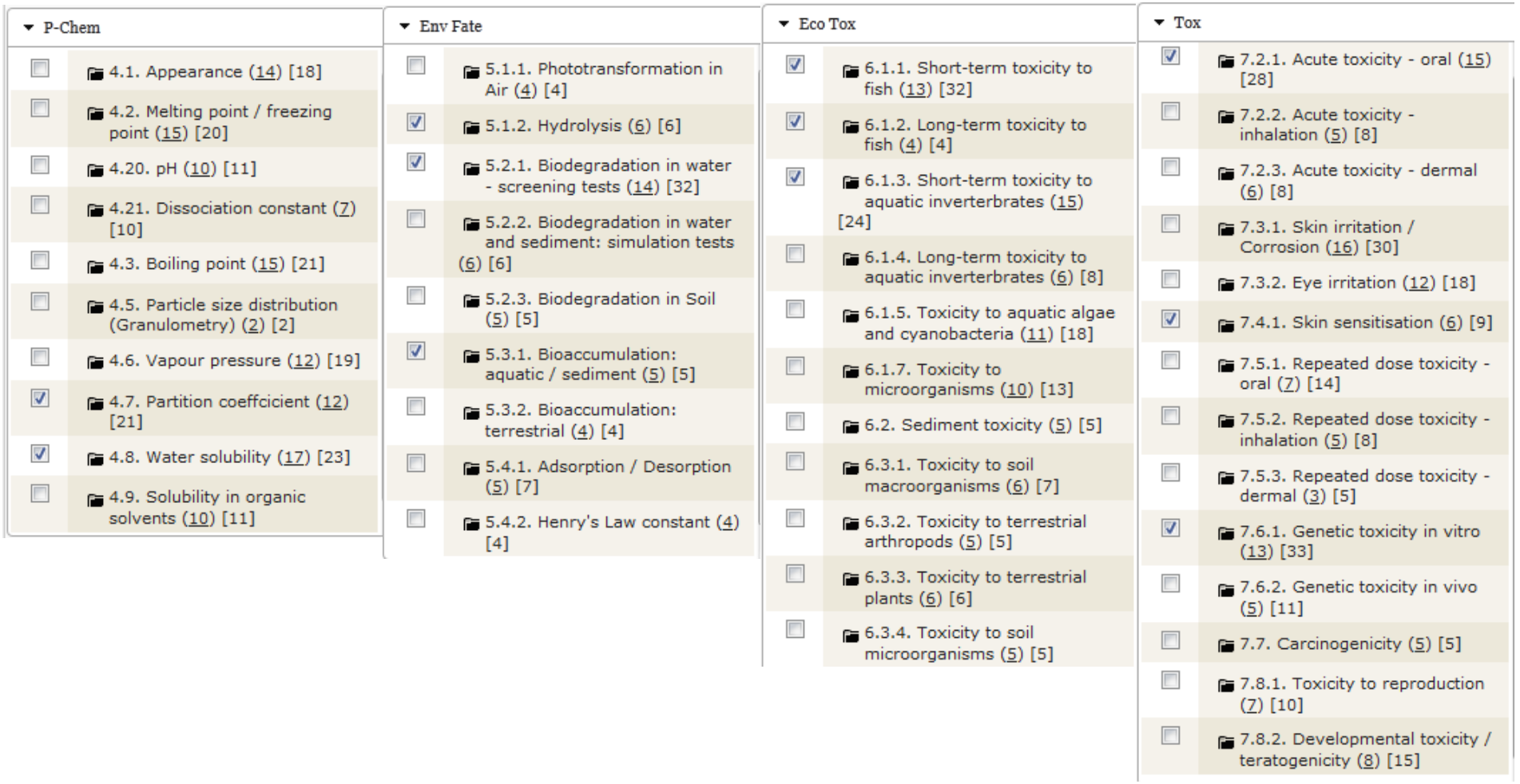
IUC Substance | Composition | P-Chem (6) | Env Fate (1) | Eco Tox (3) | Tox (4)

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 43 Endpoints from IUCLID



P-Chem

- [ ] 4.1. Appearance (14) [18]
- [ ] 4.2. Melting point / freezing point (15) [20]
- [ ] 4.20. pH (10) [11]
- [ ] 4.21. Dissociation constant (7) [10]
- [ ] 4.3. Boiling point (15) [21]
- [ ] 4.5. Particle size distribution (Granulometry) (2) [2]
- [ ] 4.6. Vapour pressure (12) [19]
- [x] 4.7. Partition coeffciient (12) [21]
- [x] 4.8. Water solubility (17) [23]
- [ ] 4.9. Solubility in organic solvents (10) [11]

Env Fate

- [ ] 5.1.1. Phototransformation in Air (4) [4]
- [x] 5.1.2. Hydrolysis (6) [6]
- [x] 5.2.1. Biodegradation in water - screening tests (14) [32]
- [ ] 5.2.2. Biodegradation in water and sediment: simulation tests (6) [6]
- [ ] 5.2.3. Biodegradation in Soil (5) [5]
- [x] 5.3.1. Bioaccumulation: aquatic / sediment (5) [5]
- [ ] 5.3.2. Bioaccumulation: terrestrial (4) [4]
- [ ] 5.4.1. Adsorption / Desorption (5) [7]
- [ ] 5.4.2. Henry's Law constant (4) [4]

Eco Tox

- [x] 6.1.1. Short-term toxicity to fish (13) [32]
- [x] 6.1.2. Long-term toxicity to fish (4) [4]
- [x] 6.1.3. Short-term toxicity to aquatic inverterbrates (15) [24]
- [ ] 6.1.4. Long-term toxicity to aquatic inverterbrates (6) [8]
- [ ] 6.1.5. Toxicity to aquatic algae and cyanobacteria (11) [18]
- [ ] 6.1.7. Toxicity to microorganisms (10) [13]
- [ ] 6.2. Sediment toxicity (5) [5]
- [ ] 6.3.1. Toxicity to soil macroorganisms (6) [7]
- [ ] 6.3.2. Toxicity to terrestrial arthropods (5) [5]
- [ ] 6.3.3. Toxicity to terrestrial plants (6) [6]
- [ ] 6.3.4. Toxicity to soil microorganisms (5) [5]

Tox

- [x] 7.2.1. Acute toxicity - oral (15) [28]
- [ ] 7.2.2. Acute toxicity - inhalation (5) [8]
- [ ] 7.2.3. Acute toxicity - dermal (6) [8]
- [ ] 7.3.1. Skin irritation / Corrosion (16) [30]
- [ ] 7.3.2. Eye irritation (12) [18]
- [x] 7.4.1. Skin sensitisation (6) [9]
- [ ] 7.5.1. Repeated dose toxicity - oral (7) [14]
- [ ] 7.5.2. Repeated dose toxicity - inhalation (5) [8]
- [ ] 7.5.3. Repeated dose toxicity - dermal (3) [5]
- [x] 7.6.1. Genetic toxicity in vitro (13) [33]
- [ ] 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

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

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

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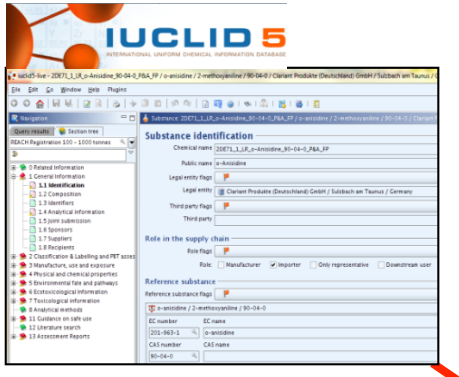
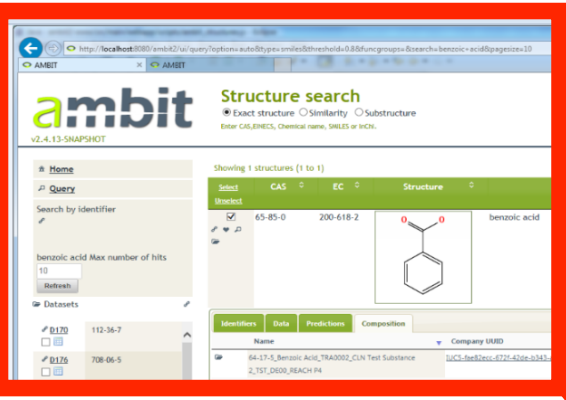
AMBIT Communication



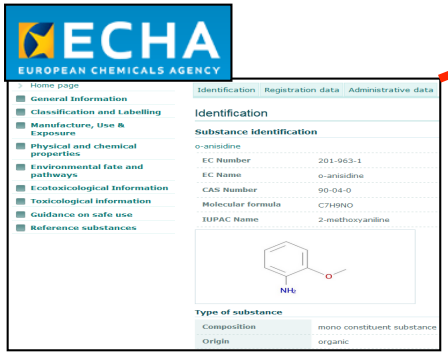
Company Database

Transfer via Web service or manually



Other Databases

Other Tools



Transfer of **14570** Datasets

Workflow
Read across & Category formation

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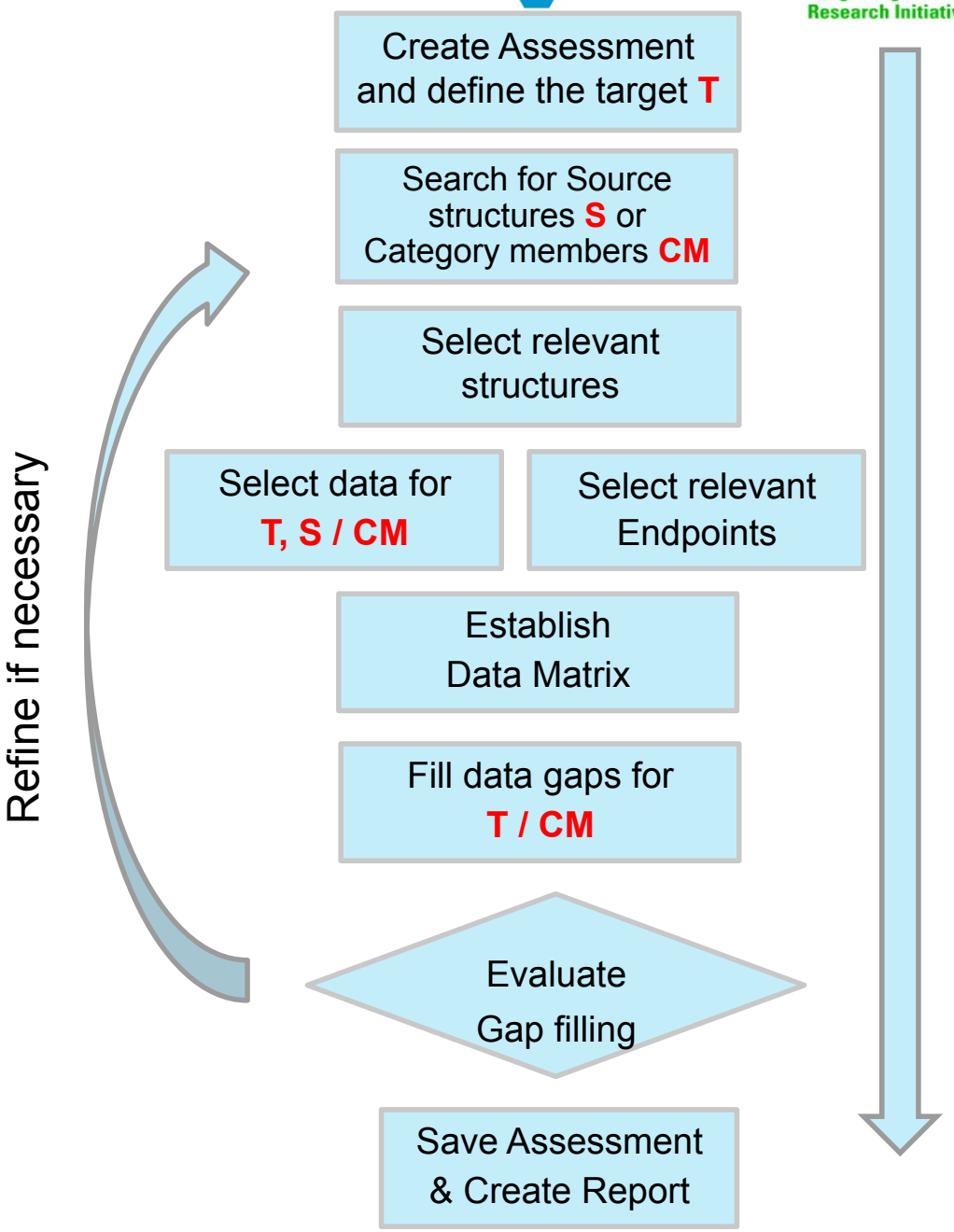
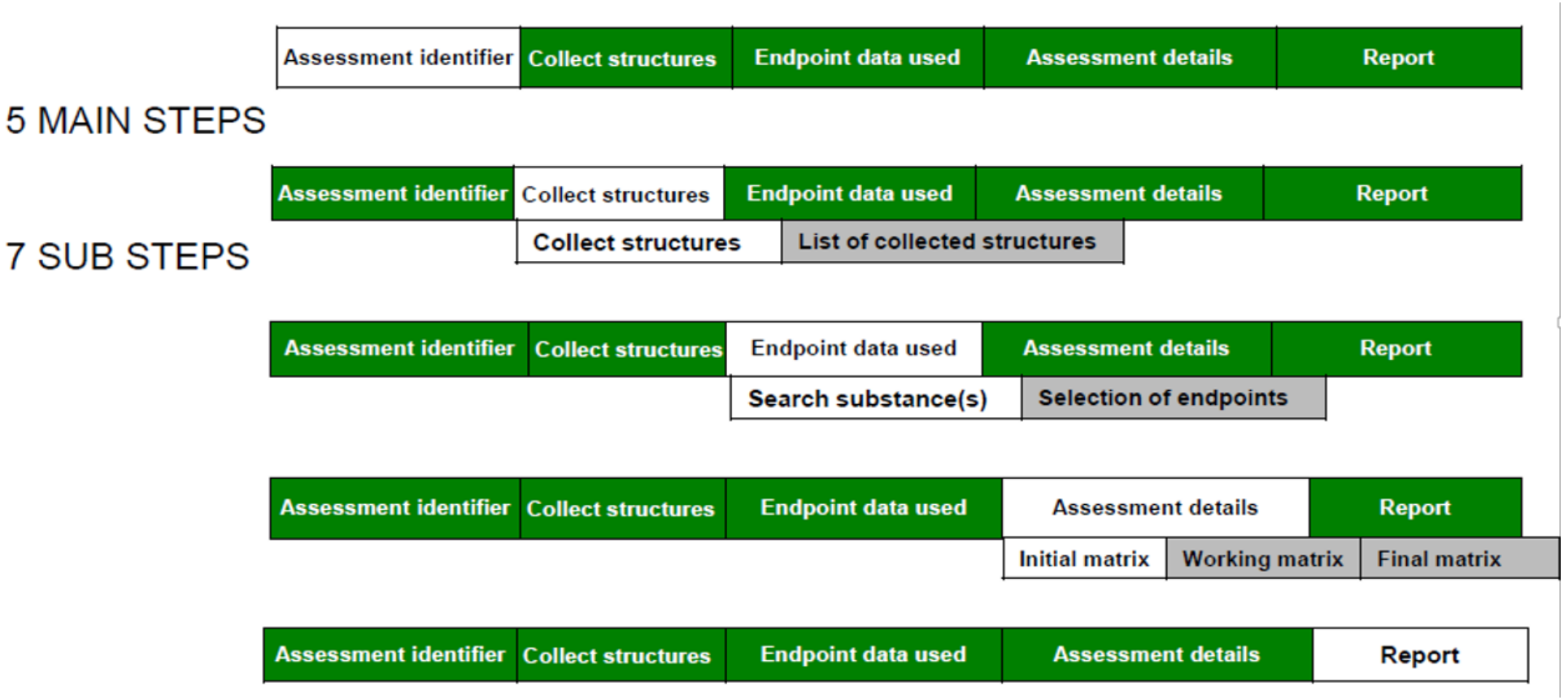
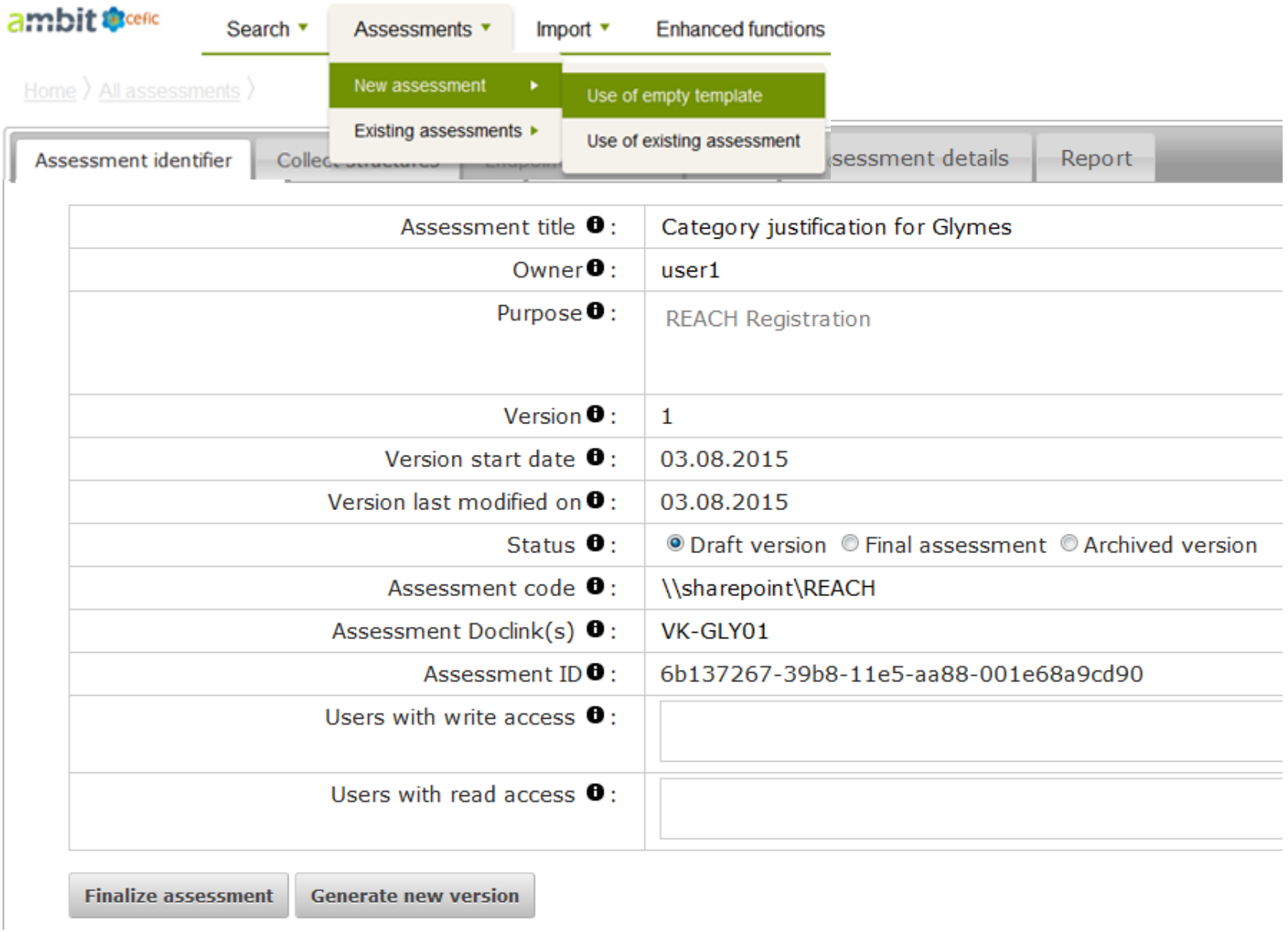
AMBIT Workflows on Read across & Category formation



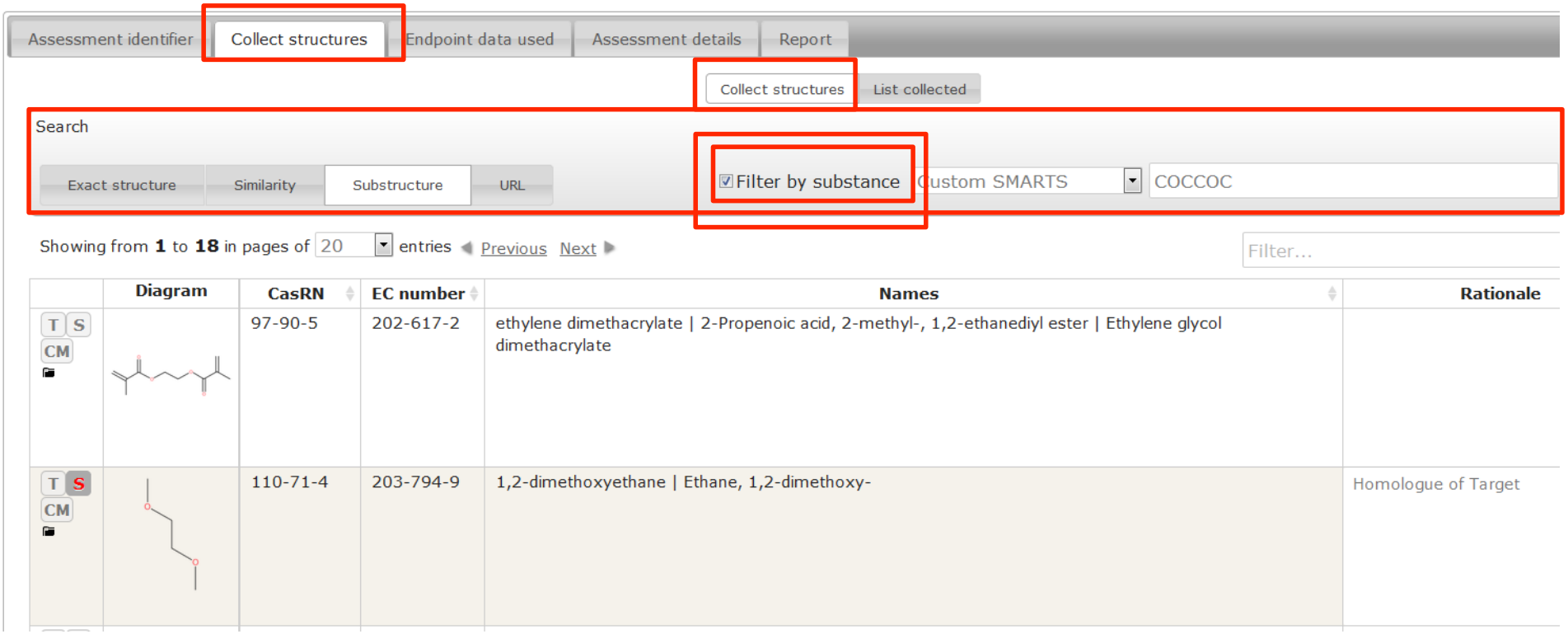
Assessment Workflow in AMBIT Using a Tab Structure



New Assessment & Identifier



Collect (Search) structures for Assessment



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

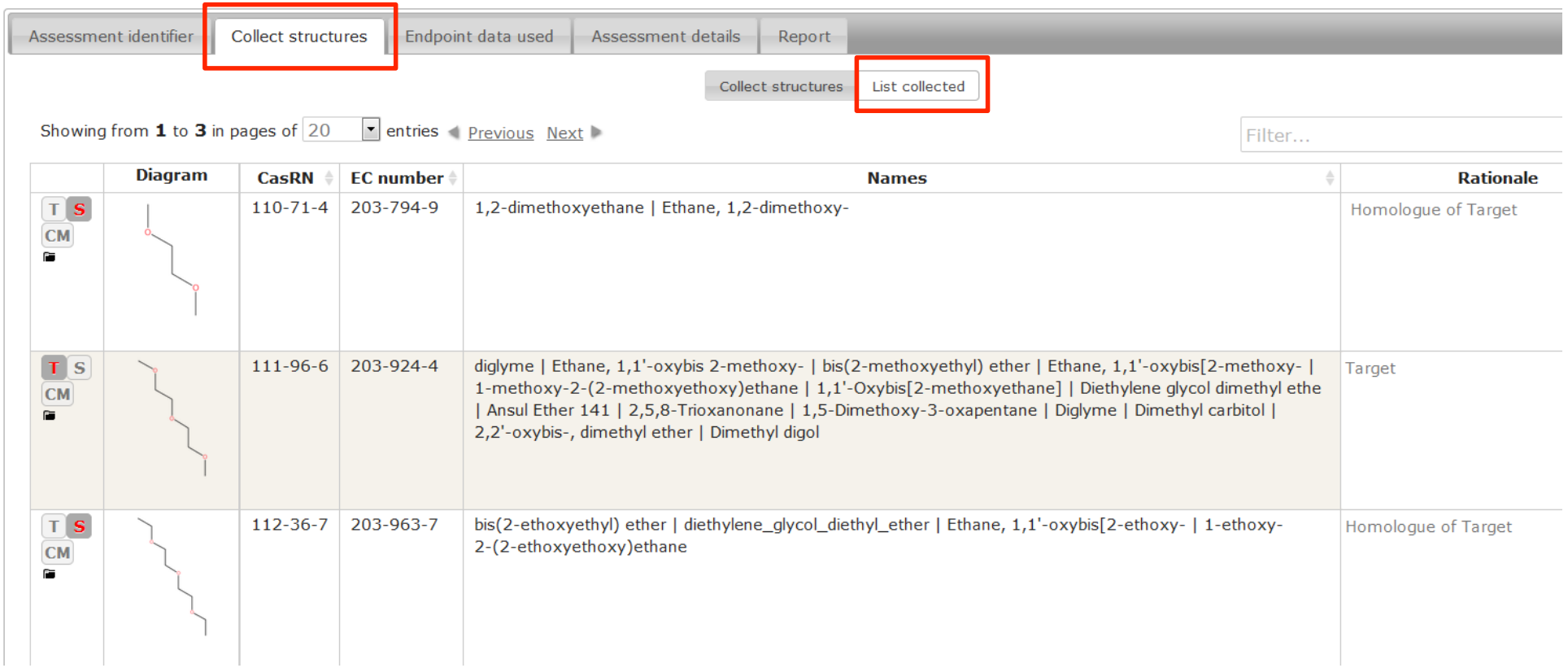
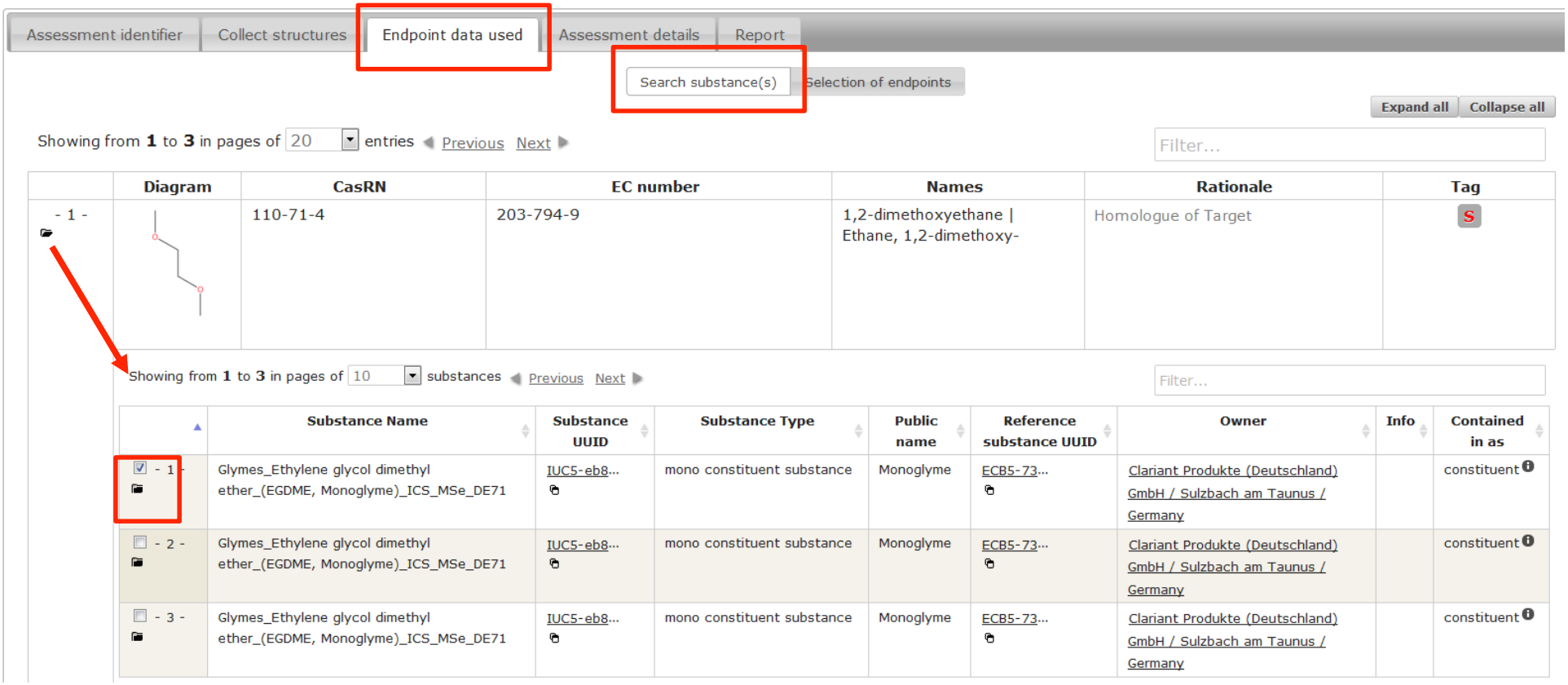


	Diagram	CasRN	EC number	Names	Rationale
T S CM		110-71-4	203-794-9	1,2-dimethoxyethane | Ethane, 1,2-dimethoxy-	Homologue of Target
T S CM		111-96-6	203-924-4	diglyme | Ethane, 1,1'-oxybis 2-methoxy- | bis(2-methoxyethyl) ether | Ethane, 1,1'-oxybis[2-methoxy- | 1-methoxy-2-(2-methoxyethoxy)ethane | 1,1'-Oxybis[2-methoxyethane] | Diethylene glycol dimethyl ethe | Ansul 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

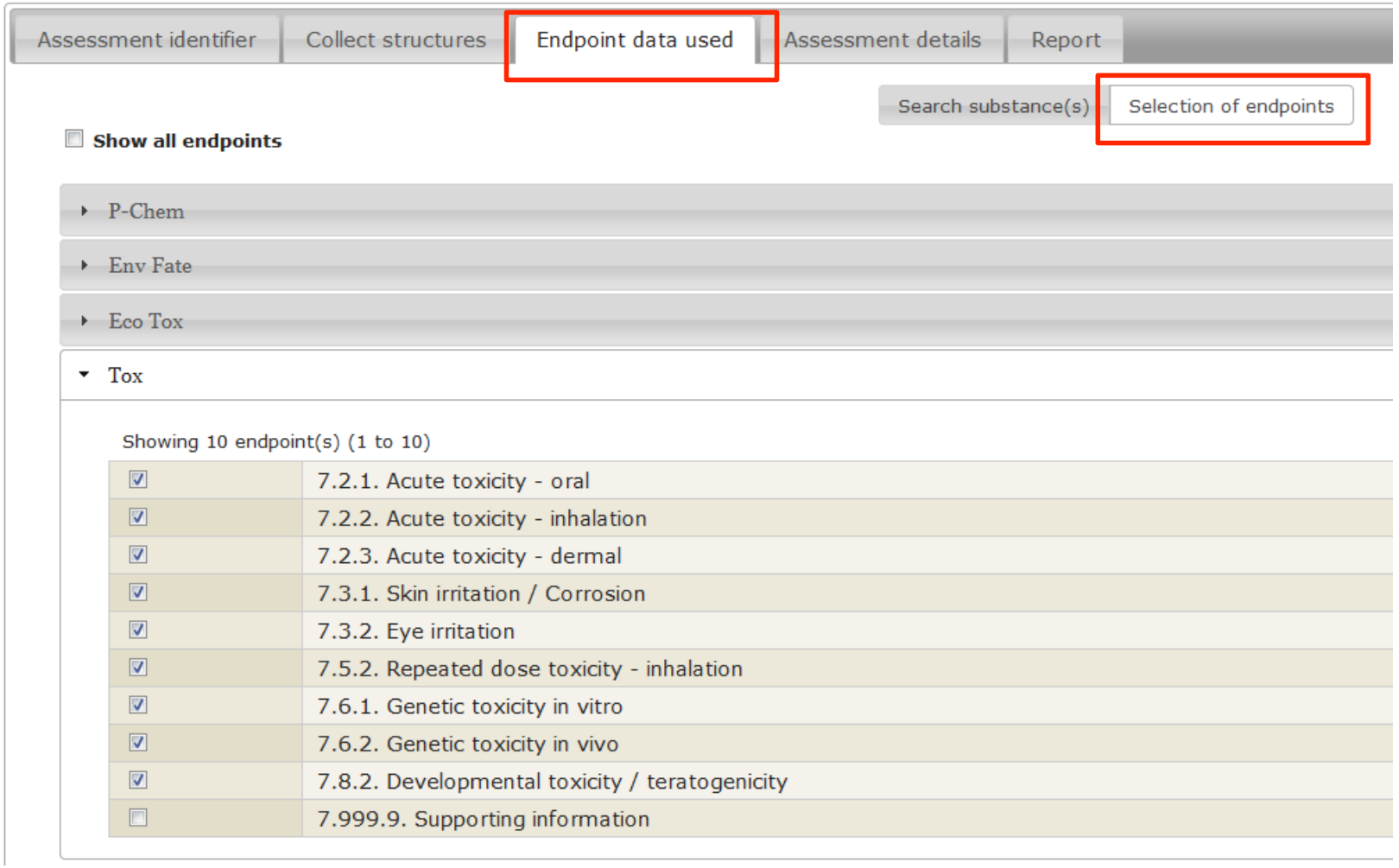
- Based on the Smiles code of the Target Diglyme a substructure search was carried out limited to those having substance data

Search Substances associated to the Structures



- 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

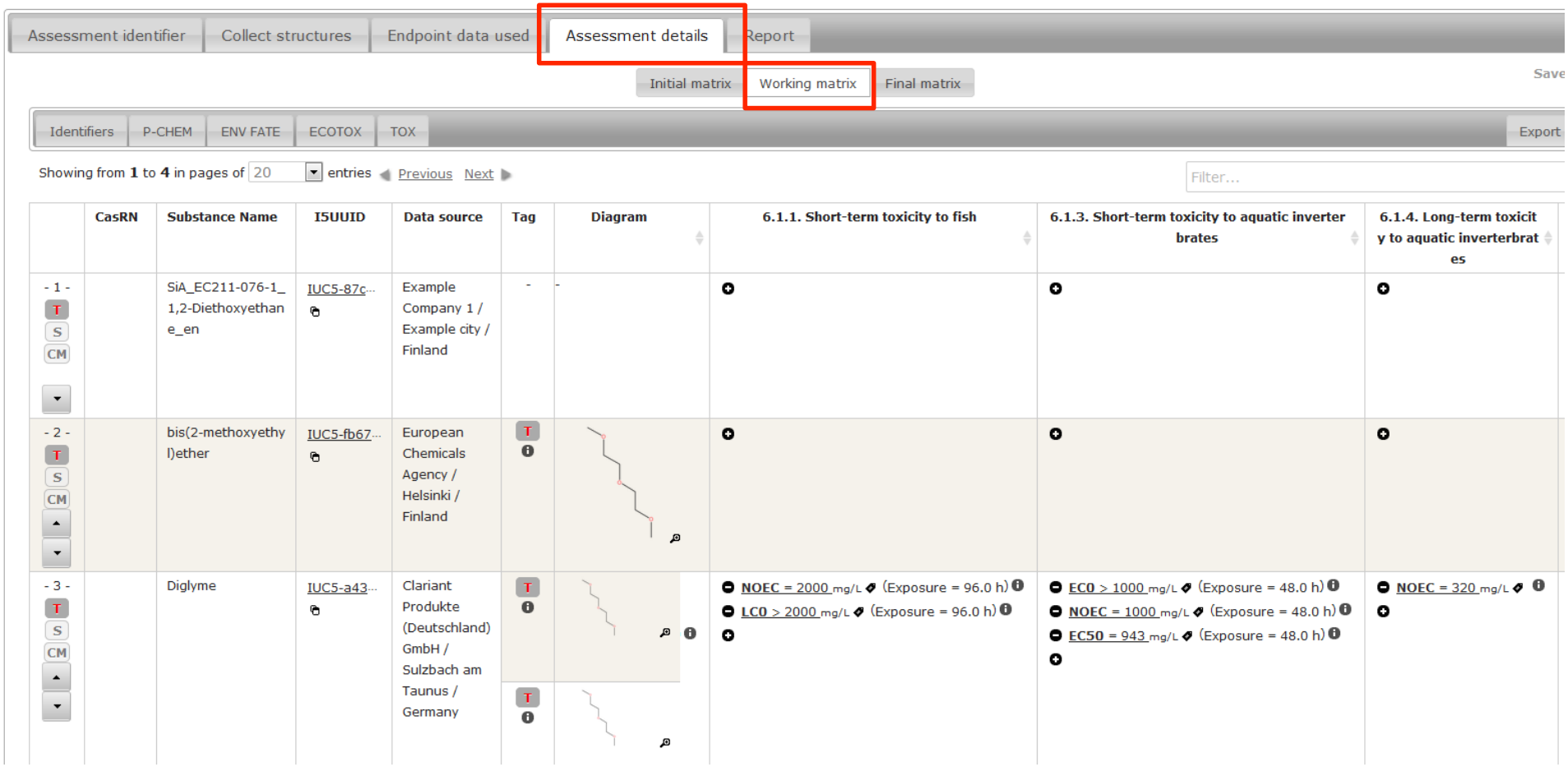


- When clicking the Tab “Endpoint data used” and subsequently Subtab “Selection of endpoints” a list of IUCLID Endpoints are displayed for selection by check marking

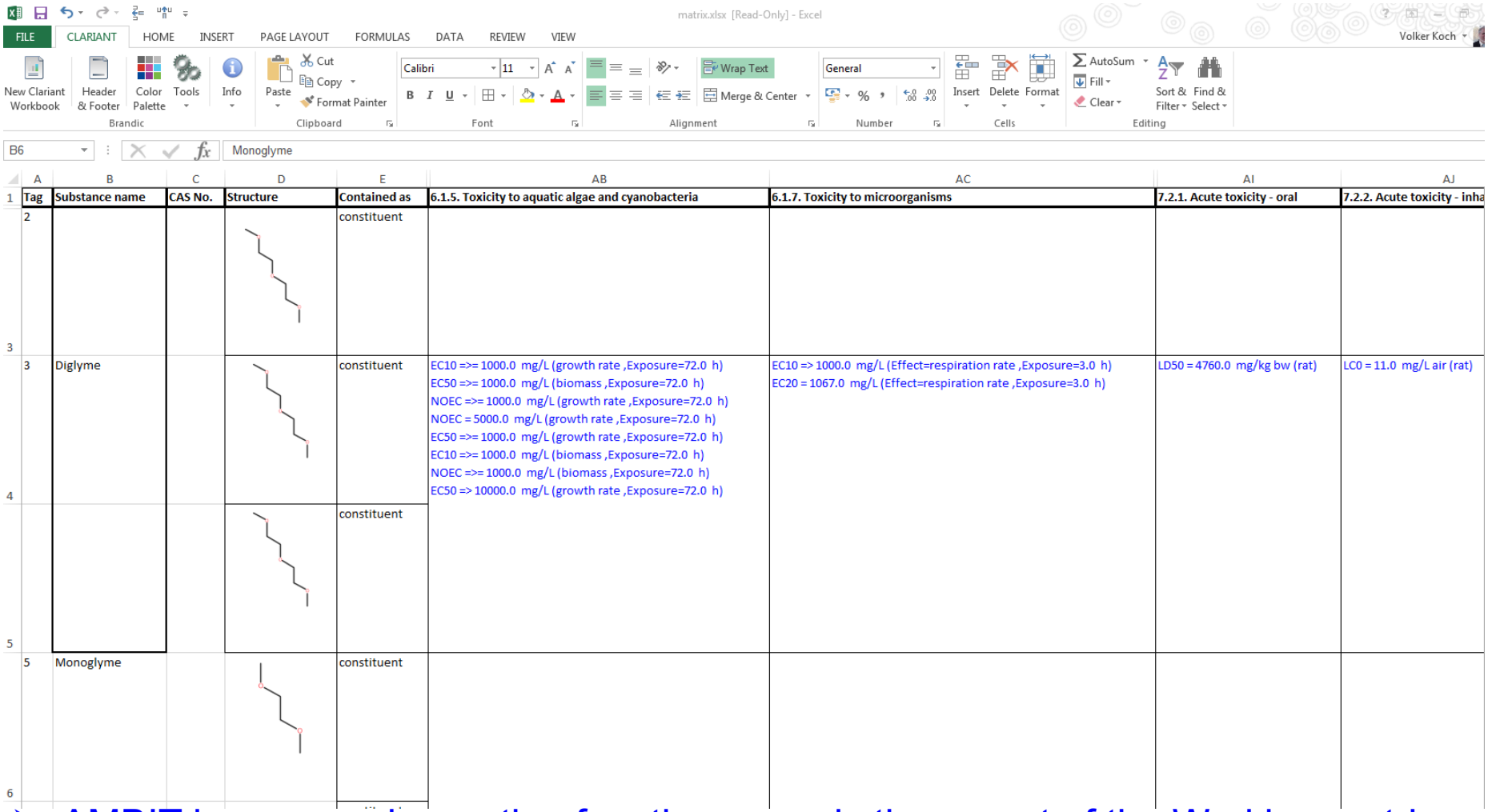
Working matrix (Composition section)

	CAS	Substance Name	ISUUID	Data source	Tag	Diagram	Constituent Name	Content	Contained As
- 1 -		Tetraglyme	IUC5-541...	Clariant Produkte (Deutschland) GmbH / Sulzbach am Taunus / Germany	S		112-49-2	2.4 % (w/w)	impurity
					T		143-24-8	>99 % (w/w)	constituent
					T			80.4 % (w/w)	constituent
- 2 -		Triglyme	IUC5-203...	Clariant Produkte (Deutschland) GmbH / Sulzbach am Taunus / Germany	S		112-49-2	ca.90 % (w/w)	constituent
					S			>=99 % (w/w)	constituent
- 3 -		Monoglyme	IUC5-cb8...	Clariant Produkte (Deutschland) GmbH / Sulzbach am Taunus / Germany	S		1,2-dimethoxyethane	ca.97.8 % (w/w)	constituent
					S			>=99.9 % (w/w)	constituent
					S			ca.97 % (w/w)	constituent
					S		111-96-6	ca.0.5 % (w/w)	impurity
					S		112-49-2	ca.0.5 % (w/w)	impurity
- 4 -		Diglyme	IUC5-a43...	Clariant Produkte (Deutschland) GmbH / Sulzbach am Taunus / Germany	S		111-96-6	ca.92 % (w/w)	constituent
					S			>=99.9 % (w/w)	constituent

Working matrix (Endpoint section)



EXCEL Export of Working Matrix



matrix.xlsx [Read-Only] - Excel

FILE | CLARIANT | HOME | INSERT | PAGE LAYOUT | FORMULAS | DATA | REVIEW | VIEW

Volker Koch

New Clariant Workbook | Header & Footer | Color Palette | Tools | Info | Brandic

Paste | Cut | Copy | Format Painter | Clipboard

Calibri | 11 | Font

Wrap Text | Merge & Center | Alignment

General | Number

Insert | Delete | Format | Cells

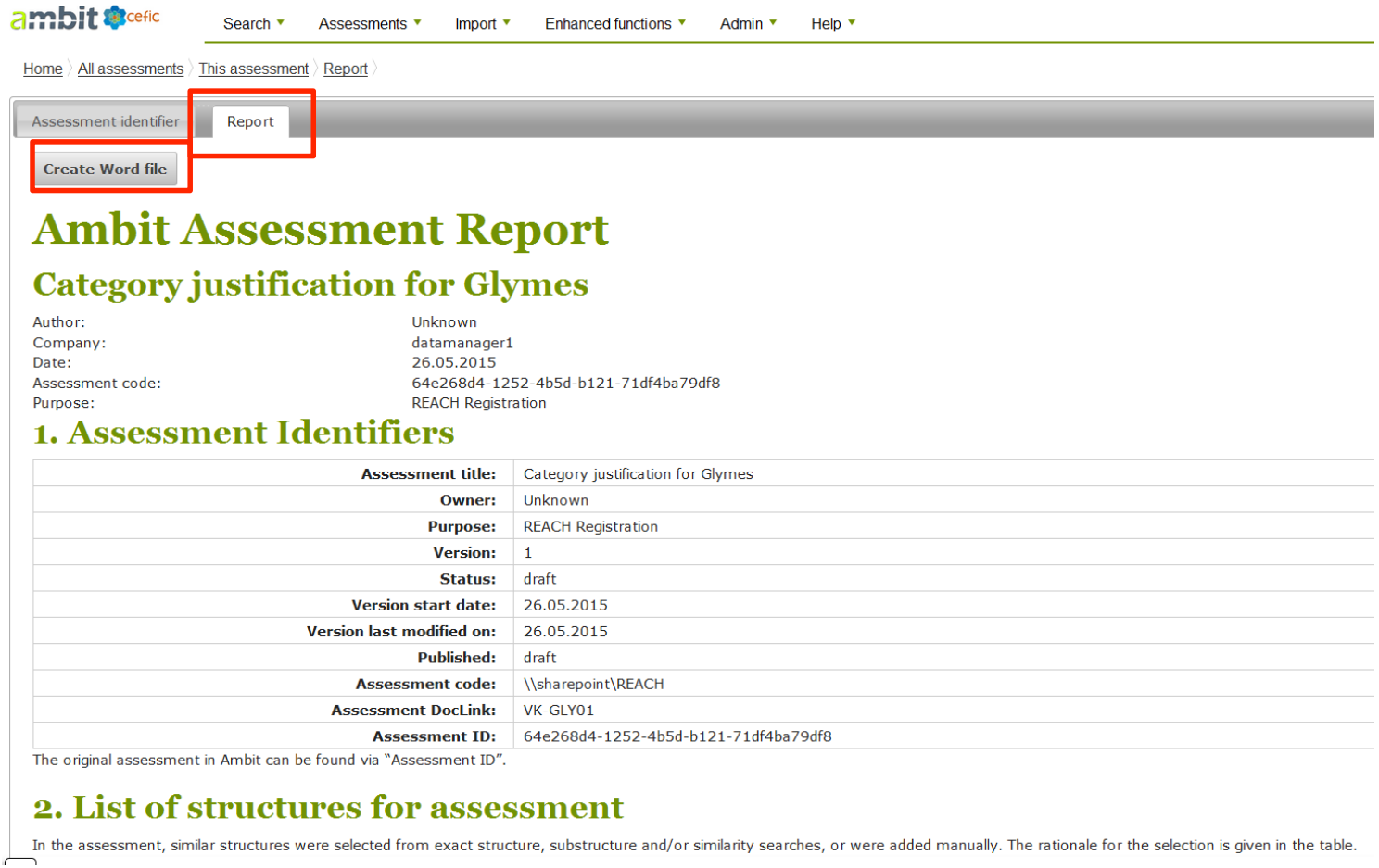
AutoSum | Fill | Clear | Sort & Filter | Find & Select | Editing

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									
4	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)
5					constituent				
6	5	Monoglyme			constituent				

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

Assessment report



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

Project information

Public

Dr. Volker Koch, Clariant
CAAT EUTOXRISK LRI Workshop
26.02.2016

Project information

➢ Project idea	Volker Koch, Clariant
➢ LRI Manager	Bruno Hubesch
➢ Contractors	Nina Jeliazkova, 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 finalized	December 8, 2015

➢ **DETAILED INFORMATION SEE LRI WEBSITE**

LRI Workshop on AMBIT and READ-ACROSS 21 Jan 2016

➢ http://cefic-lri.org/events/lri-workshop-on-ambit-and-read-across/

Legal Disclaimer for Use of ECHA Data within AMBIT

The LRI AMBIT –IUCLID tool is loaded with non-confidential REACH data supplied by ECHA.

The legal notice from the ECHA dissemination website http://echa.europa.eu/web/guest/legal-notice#registration (hardcopy supplied) applies to the AMBIT users.

In addition, Cefic disclaims any liability of whatsoever nature either direct or indirect regarding the use of the AMBIT-IUCLID tool or information / data contained in it.

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