

CEFIC LRI Workshop
on AMBIT and READ-ACROSS
21 Jan 2016

Hands on AMBIT functionality



Public, Hands on AMBIT functionality
Dr. Qiang Li, Clariant, LRI Workshop on AMBIT, 21.01.2016



Log in Info

Link:

- <https://apps.ideaconsult.net/ambit3>
- Please use the latest versions of browsers
- Username: ambit3
- Password: Jan2016

Practical exercises

Exact Search

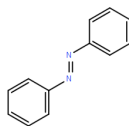
- Search structures using chemical names “Caffeine”, “caffei” (fragment search)
- Search structure using CAS No. 111-96-6 and display substances containing this structure as constituent/impurity
- Search structure and Derek prediction data using SMILES “CC(=O)N(C)C”

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Practical exercises

Similarity and substructure search

- Draw the following structure using the structure editor and search similar structures



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Practical exercises

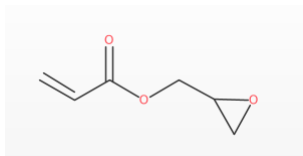
Substance search

- Search substance “Triglyme” and check the available composition and endpoint data
- Search substances which have LD50 values > 5000 (dermal) and are not sensitising

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Practical exercises

- Run Toxtree prediction for the following chemical



- Create an assessment for Category amines, C12-18-alkyldimethyl (e.g. “N,N-dimethylhexadecan-1-amine”, CAS 112-69-6) with regard to genetic toxicity in-vivo and short-term toxicity to fish

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Results

- Search structures using chemical names "Caffeine", "cafein" (fragment search)

Search structures and associated data

Exact structure Similarity Substructure URL ☐ Enable fragment search

Identifiers Datasets

Showing from 1 to 1 in pages of 20 entries

Diagram	CasRN	EC number	IUCLID 5 R	Names	Trade Name	IUPAC name	SI
	58-08-2	200-362-1	ECB5-61	caffeine(1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-1,3,7-trimethyl-3,7-dihydro-1H-purine-2,6-dione)(Caffeine(1,3,7-trimethyl-1,2,3,6-tetrahydropurine, 1,3,7-trimethyl-2,6-dioxopurine, 1,3,7-trimethylxanthine, 1-methyltheobromine, 3,7-dihydro-1,3,7-trimethyl-1H-purine-2,6-dione, 7-methylxanthine)) Alert-Pep; Caffeina; caffeineum; Cafpep; eldiatric c;	Theine(Koffein)(Cafein(1,3,7-Trimethyl-2,6-dioxopurine(3,7-Dihydro-1,3,7-Trimethyl-1H-purine-2,6-dione)(Thein(Guaranine(7-Methyltheophylline(1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-(6C)Caffeinum(Coffein wasserfrei(Mateina)(Cafein(1,3,7-	-	Cn2

Search structures and associated data

Exact structure Similarity Substructure URL ☒ Enable fragment search

Identifiers Datasets

Showing from 1 to 13 in pages of 20 entries

Diagram	CasRN	EC number	IUCLID 5 R	Names	Trade Name	IUPAC name	SI
	569-34-6			8-methoxycaffeine(1H-Purine-2,6-dione, 3,7-dihydro-8-methoxy-1,3,7-trimethyl-)	-	-	CX
	58-08-2			caffeine(1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-1,3,7-trimethyl-3,7-dihydro-1H-purine-2,6-dione)(Caffeine(1,3,7-trimethyl-1,2,3,6-tetrahydropurine, 1,3,7-trimethyl-2,6-dioxopurine, 1,3,7-trimethylxanthine, 1-methyltheobromine, 3,7-dihydro-1,3,7-trimethyl-1H-purine-2,6-dione, 7-methylxanthine))	Theine(Koffein)(Cafein(1,3,7-Trimethyl-2,6-dioxopurine(3,7-Dihydro-1,3,7-Trimethyl-1H-purine-2,6-dione)(Thein(Guaranine(7-Methyltheophylline(1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-	-	Cn2

Results

- Search structure using CAS No. 111-96-6 and display substances containing this structure as constituent/impurity

Exact structure Similarity Substructure URL ☐ Enable fragment search

Identifiers Datasets

Showing from 1 to 1 in pages of 20 entries

Diagram	CasRN	EC number	IUCLID 5 R	Names	Trade Name	IUPAC name	SMILES	Std. InChI key	Std. InChI	REACH registration da
	111-96-6			Glymes, Diethylene glycol dimethyl ether (DEGDME, Diglyme) ICS_MSE_DE71						Taurus / Germany
	111-96-6			bis(2-methoxyethyl)ether						European Chemicals Agency / Helsinki / Finland
	111-96-6			Glymes, Ethylene glycol dimethyl ether (EGDME, Monoglyme) ICS_MSE_DE71						Clariant Produkte (Deutschland) GmbH /

Identifiers Substances

Identifiers	Substances
2 - Glymes, Diethylene glycol dimethyl ether (DEGDME, Diglyme) ICS_MSE_DE71	mono constituent substance
3 - bis(2-methoxyethyl)ether	mono constituent substance
4 - Glymes, Ethylene glycol dimethyl ether (EGDME, Monoglyme) ICS_MSE_DE71	mono constituent substance

constituent

constituent

impurity

- Search structure and Derek prediction data using SMILES “CC(=O)N(C)C”

The screenshot displays the Ambit v0.6c web application interface. The top navigation bar includes the Ambit logo, a search bar, and a list of tabs: Exact structure, Similarity, Substructure, URL, and a button to enable fragment search. The 'CC(O)N(C)C' chemical structure is highlighted in the top right. The main panel features a 'Diagram' tab and a table of datasets. The 'ISUID' tab is selected, showing a table with columns: Name, Value, SameAs, and Source. The 'DX.Oestrogenicity.monkey' dataset is highlighted in the table. The 'DX.Oestrogenicity.monkey' dataset is highlighted in the table.

Similarity and substructure search

- Draw the following structure using the structure editor and search similar structures



The screenshot shows the ChemSpider search interface. At the top, the search bar contains the text "C1=CC=CC=C1N=NC1=CC=CC=C1". Below the search bar, the "Only hits with substance data" checkbox is checked. The search results are displayed in a table with columns for "Structure", "Name", and "Molecular Weight". The first result is "Azobenzene" with a molecular weight of 182.22. The chemical structure of azobenzene is shown in the "Structure" column. Red circles and numbers 1 through 7 highlight specific UI elements: 1. Search button, 2. & 6. Filter/Sort buttons, 3. Search results list, 4. Draw button, 5. Only hits with substance data checkbox, and 7. Chemical structure of azobenzene.

Results

- Search substance "Triglyme" and check the available composition and endpoint data

Search substances by identifiers ☐ Name ☐ UUID ☐ Name (regex) ☐ External identifier

Substances Advanced search Download

Showing from 1 to 1 in pages of 10 substances [Previous](#) [Next](#)

	Substance Name	Substance UUID	Substance Type	Public name	Reference substance UUID	Owner	Info
- 1 -	Glymes, Triethylens glycol dimethyl ether (TEGDME, Triglyme) ICS_MSe_DE71	IUCS-203e228e-...	mono constituent substance	Triglyme	EC85-40dcbe61...	Clariant Produkte (Deutschland) GmbH / Sulzbach am Taunus / Germany	

Search substances by identifiers ☐ IUCS-203e228e-7422-4f76-9068-82033f998d88 ☐ Name ☐ UUID ☐ Name (regex) ☐ External identifier

IUC Substance **Composition** **Eco-Tox (5)** **Env Fate (1)** **P-Chem (7)** **Tox (11)**

Filter...

Triglyme

7.2.1 Acute toxicity - oral (2)

Results

- Search substances which have LD50 values > 5000 (dermal) and are not sensitising

ambit **cefic** Search Assessments Import Enhanced functions Admin Help [\[ambit3\]](#) [Log out](#)

Search substances by endpoint data [Hit list](#)

Update results

- P-Chem
- Eco-Tox
- Env Fate
- Tox
 - 7.2.1, Acute toxicity - oral (5) [1029]
 - 7.2.2, Acute toxicity - inhalation (5) [556]
 - 7.2.3, Acute toxicity - dermal (5) [1292]
 - ☒ **Endpoint name** **Units**
 - LD50
 - Value**
 - Interpretation of the results**
 - 7.3.1, Skin irritation / Corrosion (5) [539]
 - 7.3.2, Eye irritation (5) [430]
 - 7.3.4, Skin sensitisation (5) [671]
 - ☒ **Interpretation of the results**
 - not sensitising

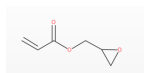
Hit list Download Help

Showing from 1 to 21 in pages of 100 substances [Previous](#) [Next](#)

	Substance Name	Substance UUID	Substance Type	Public name	Reference substance UUID	Owner	Info
- 1 -	4-nitrotoluene (IUC4 DSN 20)	IUC4-79206c66-...	Existing Chemical		IUC4-67bf61c3-...	OECD / Paris / France	IUC4ID4 = DSN 20
- 2 -	triphenyl phosphate (IUC4 DSN 113)	IUC4-567539b9-...	Existing Chemical		IUC4-3987fa71-...	OECD / Paris / France	IUC4ID4 = DSN 113
- 3 -	2-naphthol (IUC4 DSN 121)	IUC4-5df650a3-...	Existing Chemical		IUC4-cf6aba9a-...	OECD / Paris / France	IUC4ID4 = DSN 121
- 4 -	N-tert-butylbenzothiazole-2-sulphenamide (IUC4 DSN 51)	IUC4-0f0e6cac-...	Existing Chemical		IUC4-525ecbfb-...	OECD / Paris / France	IUC4ID4 = DSN 51
- 5 -	N-1,3-dimethylbutyl-N-phenyl-p-phenylenediamine (IUC4 DSN 80)	IUC4-5c2d4279-...	Existing Chemical		IUC4-78b9c014-...	OECD / Paris / France	IUC4ID4 = DSN 80
- 6 -	N,N-dimethylacetamide (IUC4 DSN 13)	IUC4-38cc707-...	Existing Chemical		IUC4-4e4663a6-...	OECD / Paris / France	IUC4ID4 = DSN 13

Results

- Run Toxtree prediction for the following chemical



Enhanced functions ▾ Admin ▾ I

Algorithms ▾
Models ▾
Predictions ▾
Run Toxtree predictions
Build model

Exact structure Similarity Substructure URL

Enable fragment search C=CC(=O)OCC1CO1

Select the search within given dataset

Available structure attributes (1/1)

Attribute	Value
CasRN	106-90-1
EC number	203-440-3
IUCLD 5 Reference substance	ECBS-85789des-b1d3-424d-886c-6a2b35aaf7
Names	2,3-epoxypropyl acrylate; 2-Propenoic acid, oxir.
SMILES	C=CC(=O)OCC1CO1
Std. InChI key	RPQRDASANLAFOM-UHFFFAOYSA-N
Std. InChI	InChI=1S/C9H10O3/c1-2,4/7/9-4-5-3-6-5/2,9/1,1
REACH registration date	30.11.2010
Cramer rules	High (Class III)

Structure diagram

Toxicity prediction modules (14/14)

Cramer rules

Module	Result
Q1 Normal constituent of the body	No
Q2 Contains functional groups associated with enhanced toxicity	No
Q3 Contains elements other than C,H,O,N,divalent S	No
Q5 Simply branched aliphatic hydrocarbon or a common carbohydrate	No
Q6 Benzene derivative with certain substituents	No
7 Heterocyclic	Yes
Q8 Lactone or cyclic diester	No
10 3-membered heterocycle	Yes Class High (Class III)

Extended Cramer rules

Module	Result
Q1 Normal constituent of the body	No
Q2 Contains functional groups associated with enhanced toxicity	No
Q3 Contains elements other than C,H,O,N,divalent S	No
Q43 Possibly harmful divalent sulphur (not detected via Q3)	No
Q5 Simply branched aliphatic hydrocarbon or a common carbohydrate	No
Q6 Benzene derivative with certain substituents	No
Q42 Possibly harmful analogue of benzene	No

Results

- Create an assessment for Category amines, C12-18-alkyldimethyl (e.g. "N,N-dimethylhexadecan-1-amine", CAS 112-69-6) with regard to genetic toxicity in-vivo and short-term toxicity to fish
- Results: see the following assessment in the public server:

Assessment demonstration No.2-DMA	1	D:\docs\assessments	draft	datamanager1	2efef65-080d-442e-9396-1625d1aeca22	XLSX CSV JSON	Remove
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