Workshop on CEFIC LRI Project EEM9.4
LRI AMBIT with IUCLID6 support and extended search capabilities

Hands on AMBIT2 functionality

Log in Info

- **Link:** https://ambitlri.ideaconsult.net
- Username: workshop
- Password: ambit2
- Please use the latest versions of browsers

Practical exercises

Exact Search

- Search structures using chemical names “Caffeine”, “caffei” (fragment search)

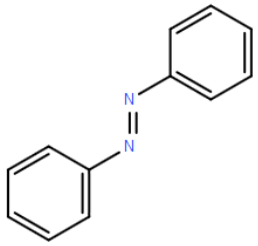
- Search structure using CAS No. 111-96-6 and display substances containing this structure as constituent/impurity

- Search structure in OpenFoodToxData database using SMILES “CCOC(=O)N”

Practical exercises

Similarity and substructure search

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



Practical exercises

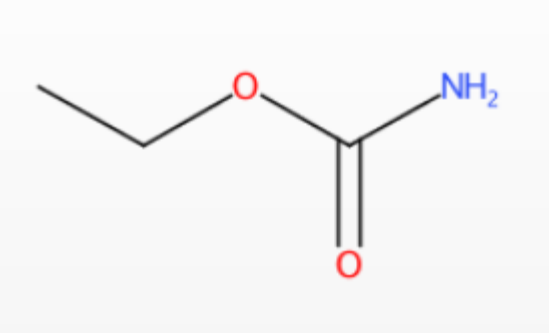
Substance search

– Search substance “Triglyme” and check the available composition and endpoint data

– Search substances which have LD50 values > 5000 (oral) and are not mutagenic (in-vitro)

Practical exercises

– Run VEGA Models and Toxtree prediction for the following chemical

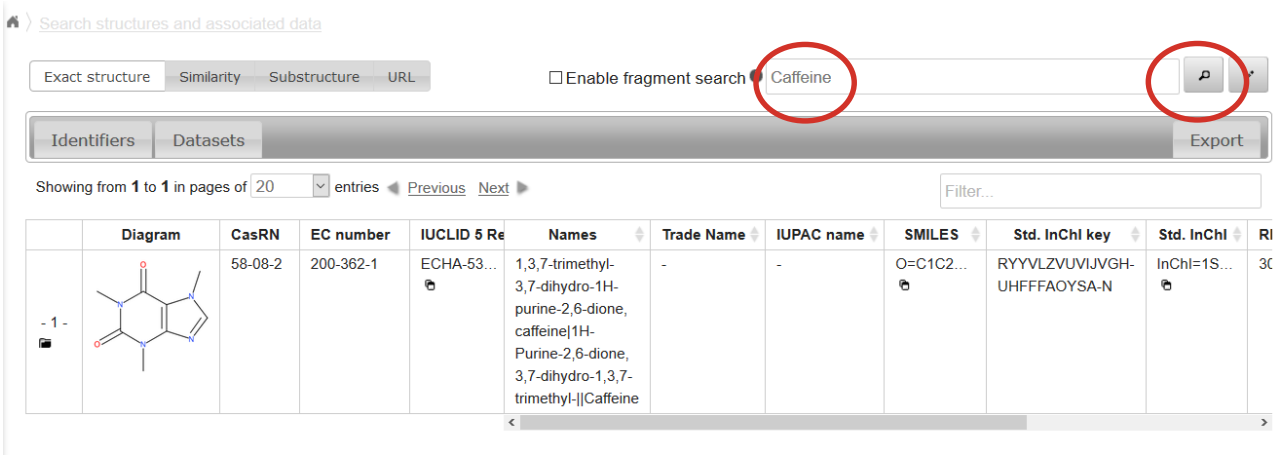


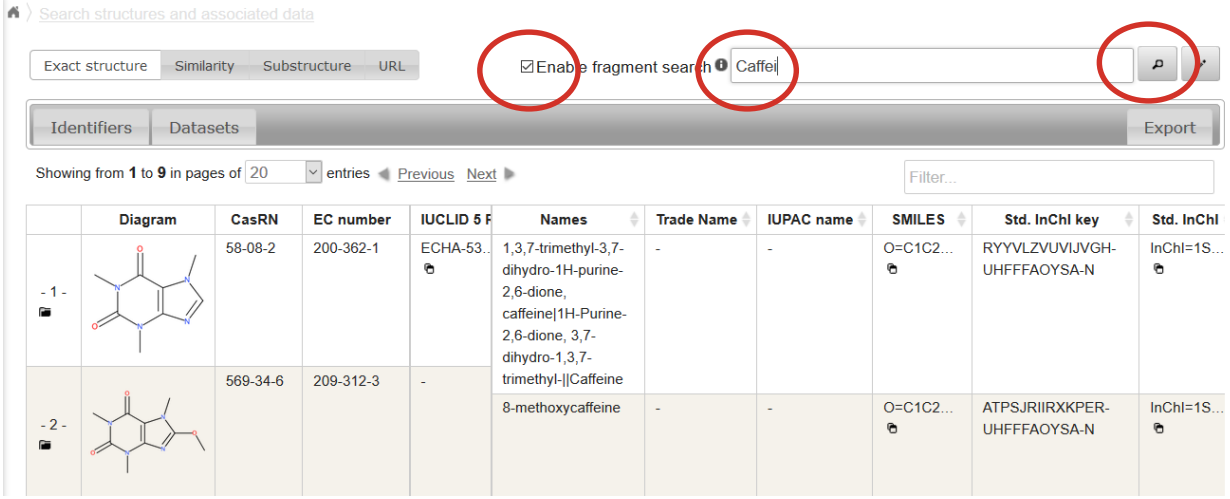
– Create an assessment for Category amines, C12-18-alkyldimethyl (e.g. “N,N-dimethylhexadecan-1-amine”, CAS 112-69-6) with regard to genetic toxicity in-vivo and short-term toxicity to fish

Results

Results

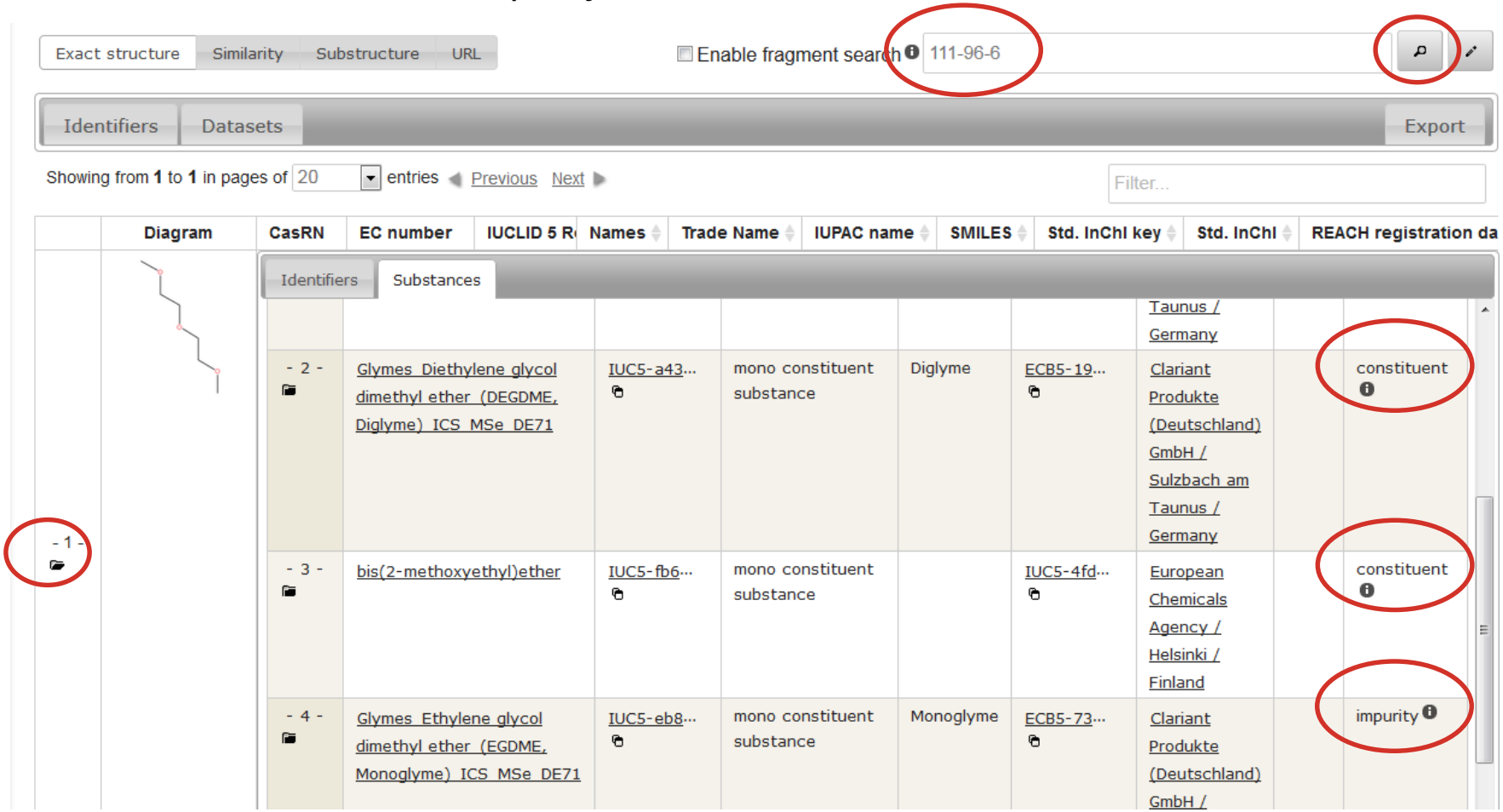
– Search structures using chemical names “Caffeine”, “caffei” (fragment search)





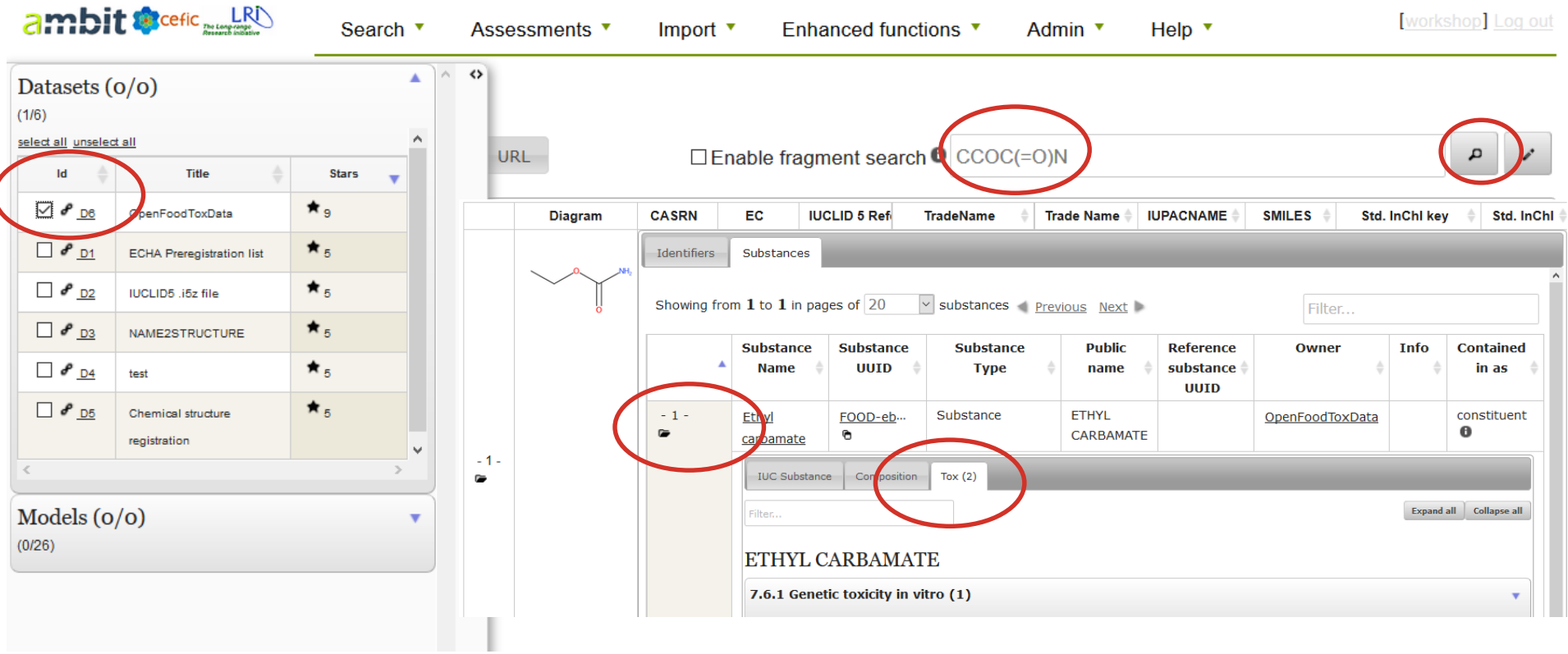
Results

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



Results

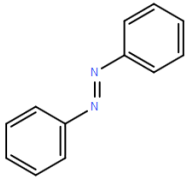
– Search structure in OpenFoodToxData database using SMILES “CCOC(=O)N”

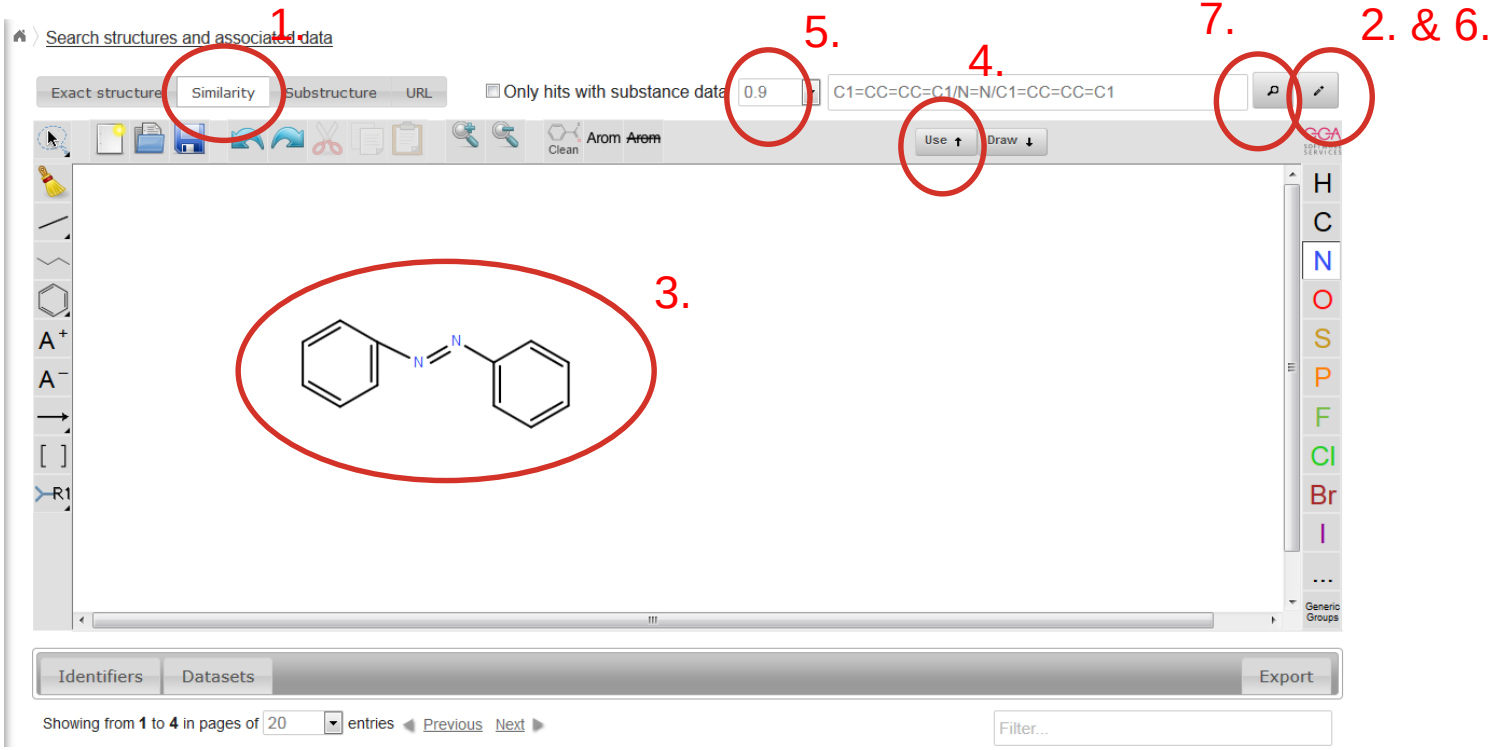


Results

Similarity and substructure search

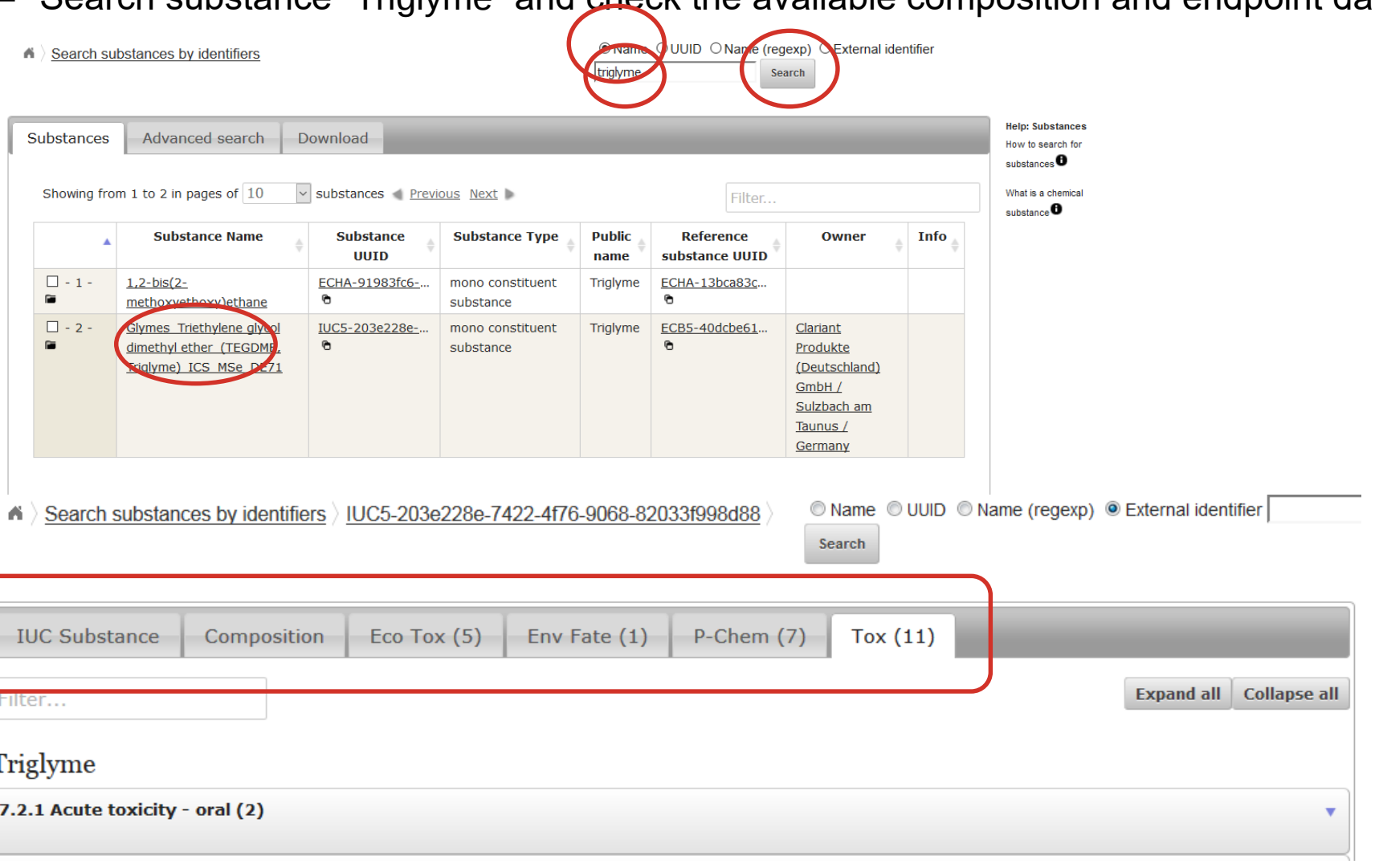
– Draw the following structure using the structure editor and search similar structures





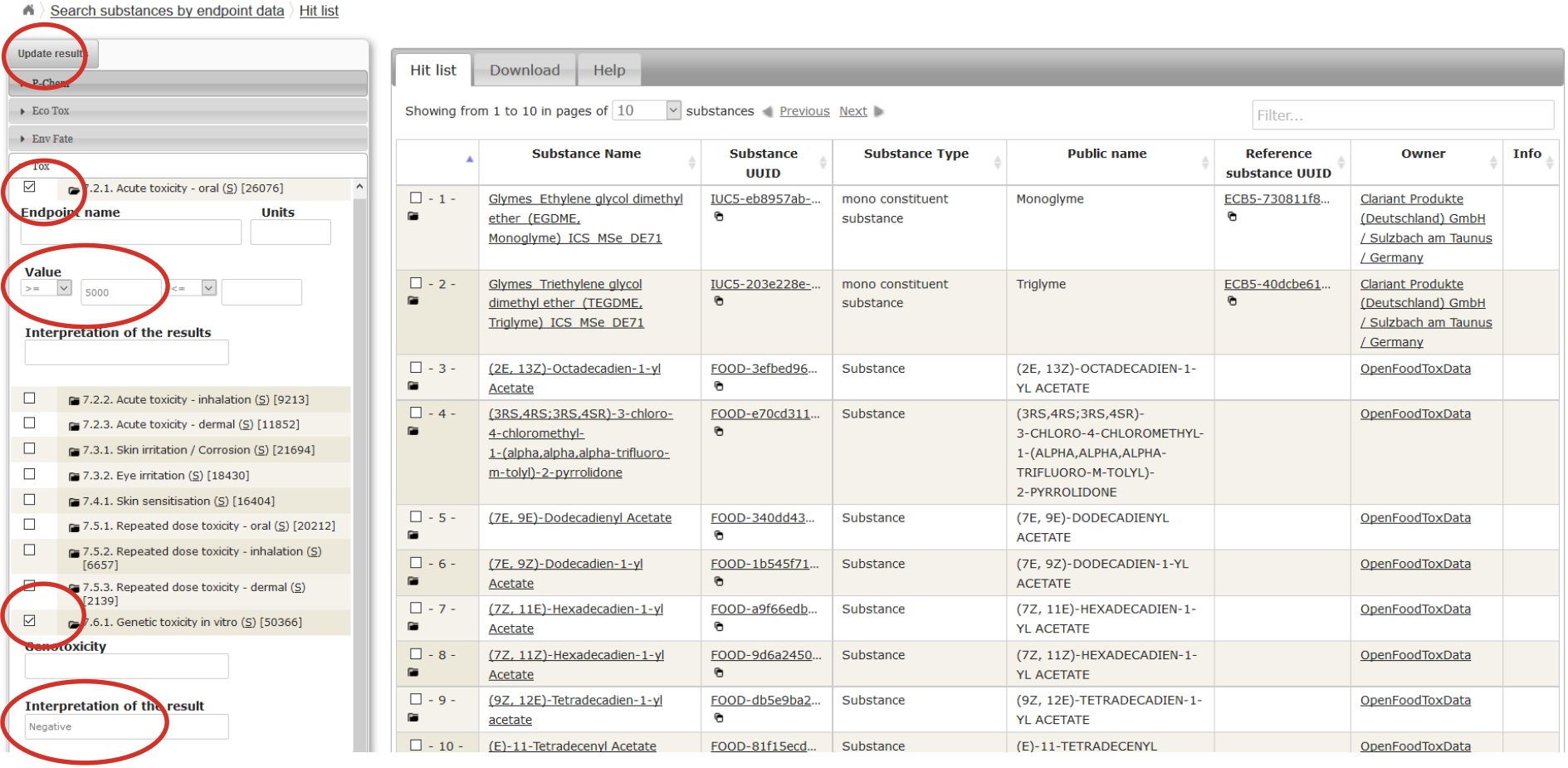
Results

– Search substance “Triglyme” and check the available composition and endpoint data



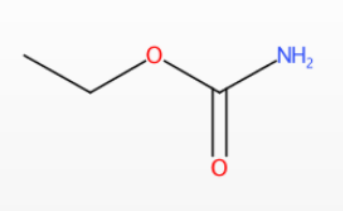
Results

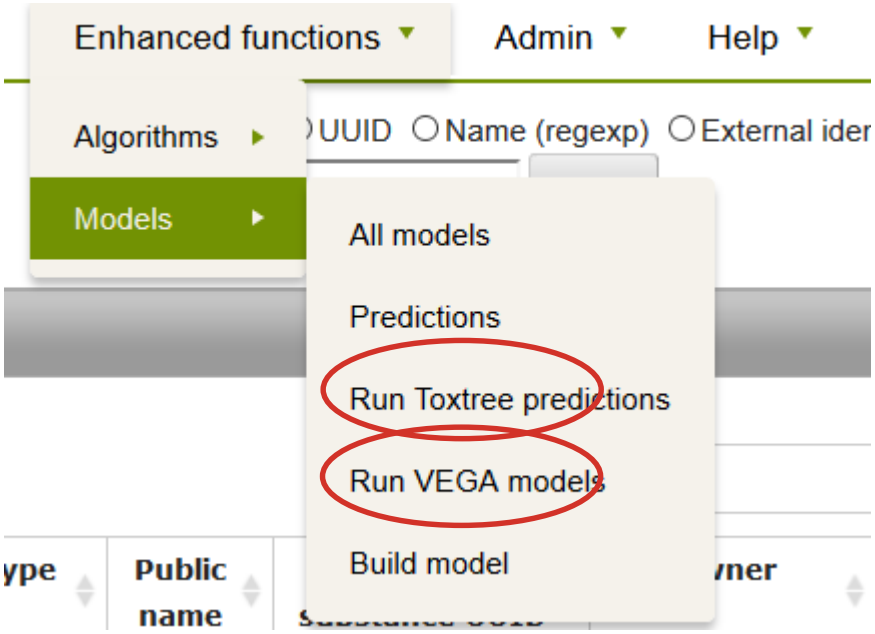
– Search substances which have LD50 values > 5000 (oral) and are not mutagenic



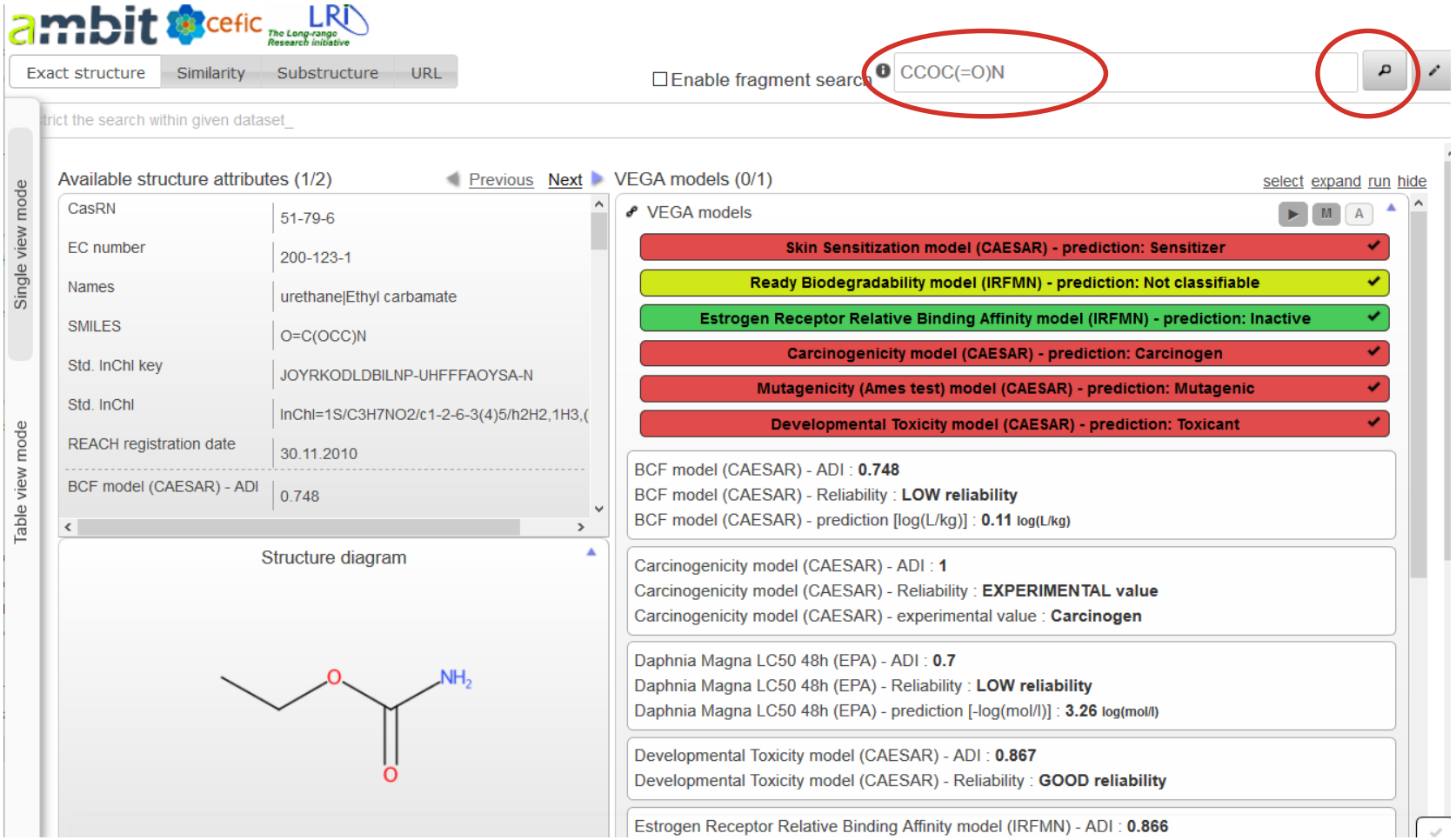
Results

– Run VEGA Models and Toxtree prediction for the following chemical

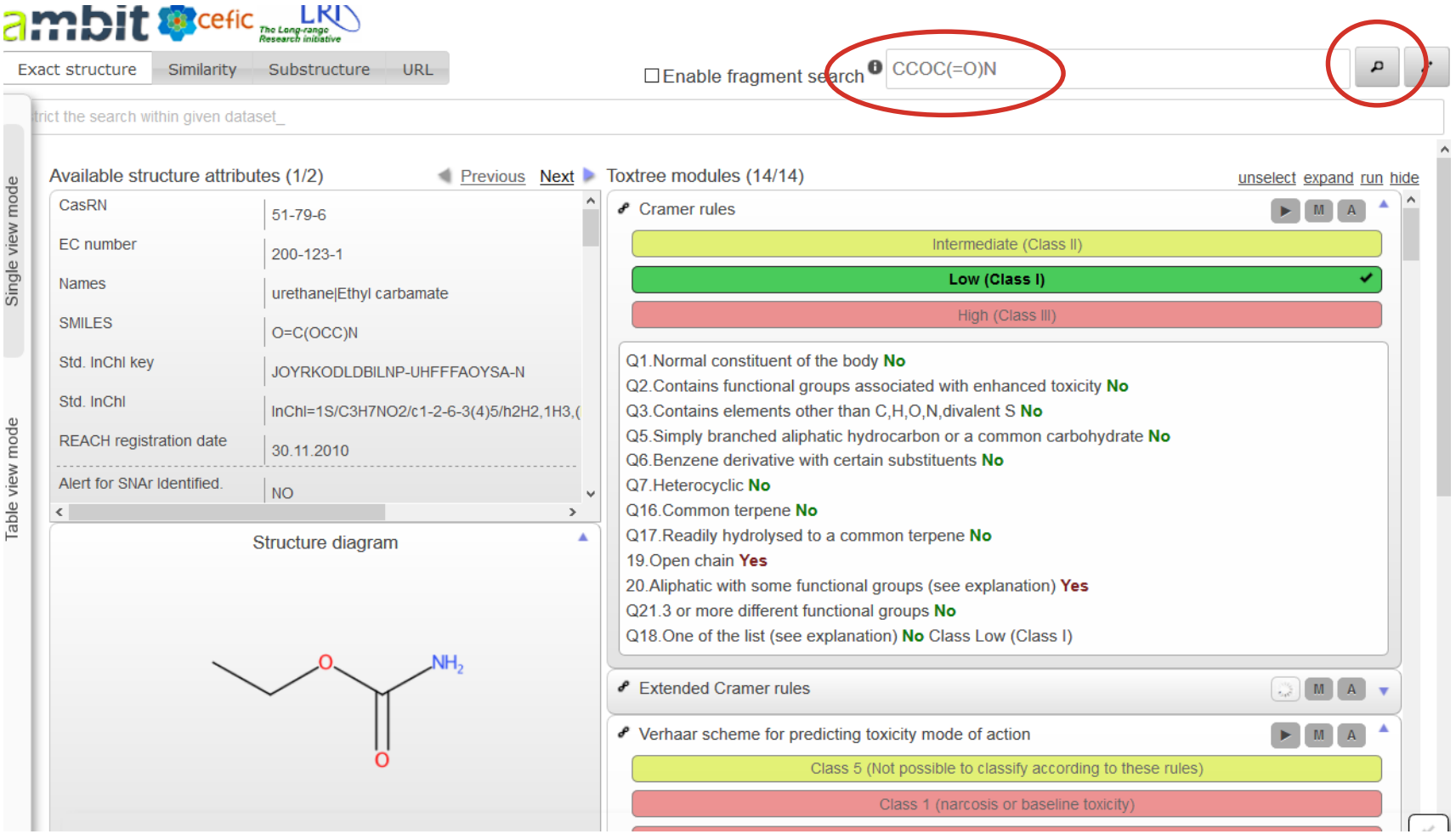




VEGA models Prediction



Toxtree Prediction



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:

Title	Name	Code	Status	Owner
	Assessment demonstration No.2-DMA v2	Glymes20160121	draft	workshop