EU Life CONCERT REACH Gateway - course

09/06/2023, QSAR2023

Nelly Giuseppa Raitano

CONCERTREACH
CONCERTING EXPERIMENTAL DATA AND IN SILICO MODELS FOR REACH
LIFE17 GIE/IT/000461

THE PROJECT

September — June

2018 | 2019 | 2020 | 2021 | 2022 | 2023

ISTITUTO DI RICERCHE FARMACOLOGICHE MARIO NEGRI · IRCCS

Istituto di Ricerche Farmacologiche Mario Negri, Italy
Research institute, **Coordinator**

Associated Beneficiaries

big chem · DTU · knoell worldwide registration · kode from data to knowledge · Sviluppo chimica spa

Support

IOEA Consult

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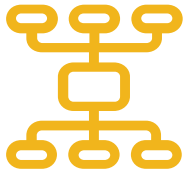
THE PROJECT
Sept 2018 - June 2023

Evaluate the **potential impact** of CS in the EU by exp + *in silico*

A big network of systems offering non-testing methods (NTM) useful both for authorities and industries.



ISTITUTO DI RICERCHE FARMACOLOGICHE MARIO NEGRI · IRCCS

big chem

DTU

knoell worldwide registration

kode from data to knowledge

Sviluppo chimica spa

Results

The network offers **more than 450 *in silico* tools**

42 new *in silico* models

A **new tool** for **grouping**

Updated version of **read-across tools**, freely available and user-friendly

New strategy integrating the results of read-across and *in silico* models (**weight-of-evidence**).

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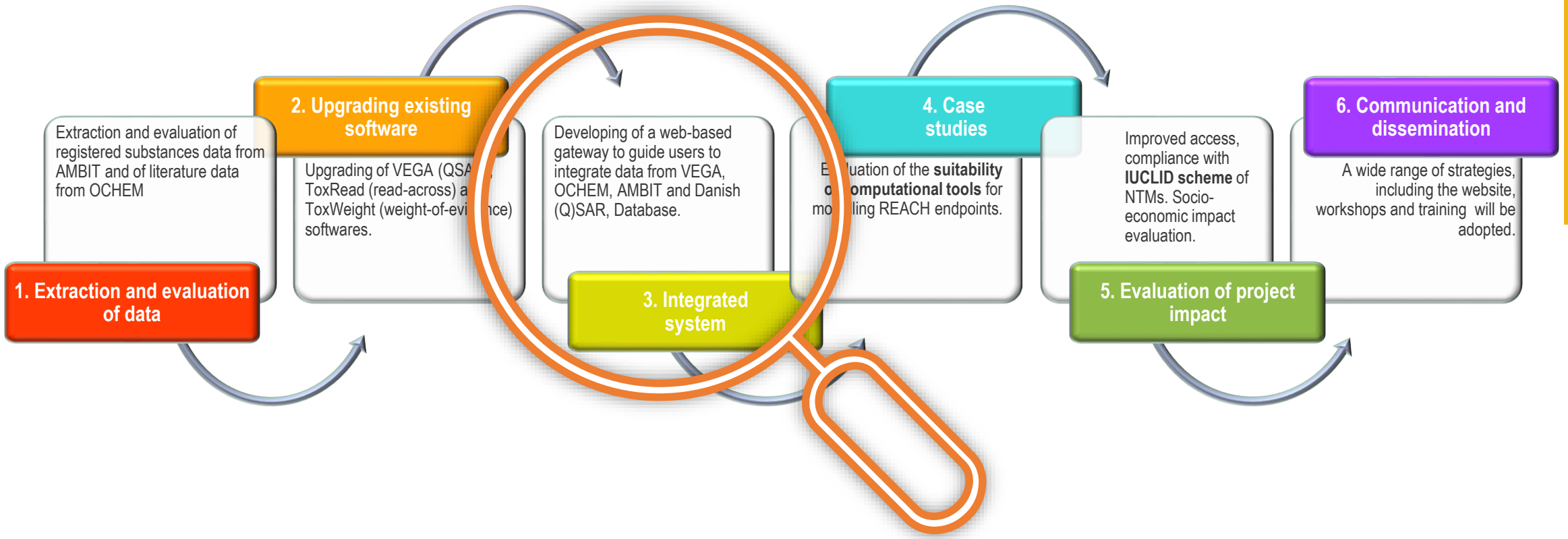
PROJECT ACTIVITIES



THE TOOLS

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The network is composed of **VEGA**, the **Danish (Q)SAR Database**, **OCHEM** for the *in-silico models*, and for the read across workflow and data from the registered substances, of **ToxRead** and **AMBIT**.

THE TOOLS

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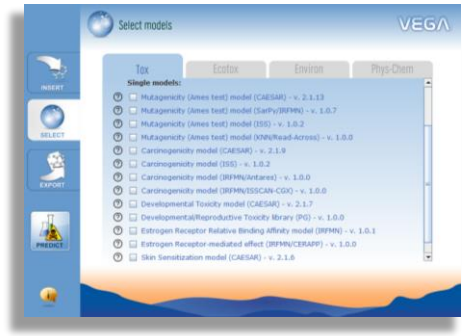
110 (Q)SAR freely available models for regulatory purposes.

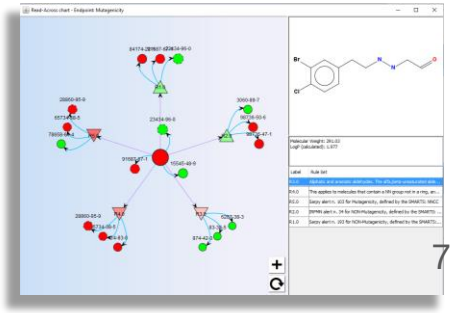
VEGA

Different areas:
-Human toxicity
-Eco-toxicity
-Environmental
-Physico-chemical
-Toxicokinetics



Reproducible **read-across evaluation** for 25 endpoints showing **similar compounds** and **SAs** in common between chemicals.

TOXREAD



THE TOOLS

DQ DATABASE

Estimates for **more than 650,000 substances** obtained with **more than 200 (Q)SARs** from free and commercial platforms.

DQ MODELS

New portal to access some of the models of the database directly, also for new substances.

Downloadable QPRF report is generated.

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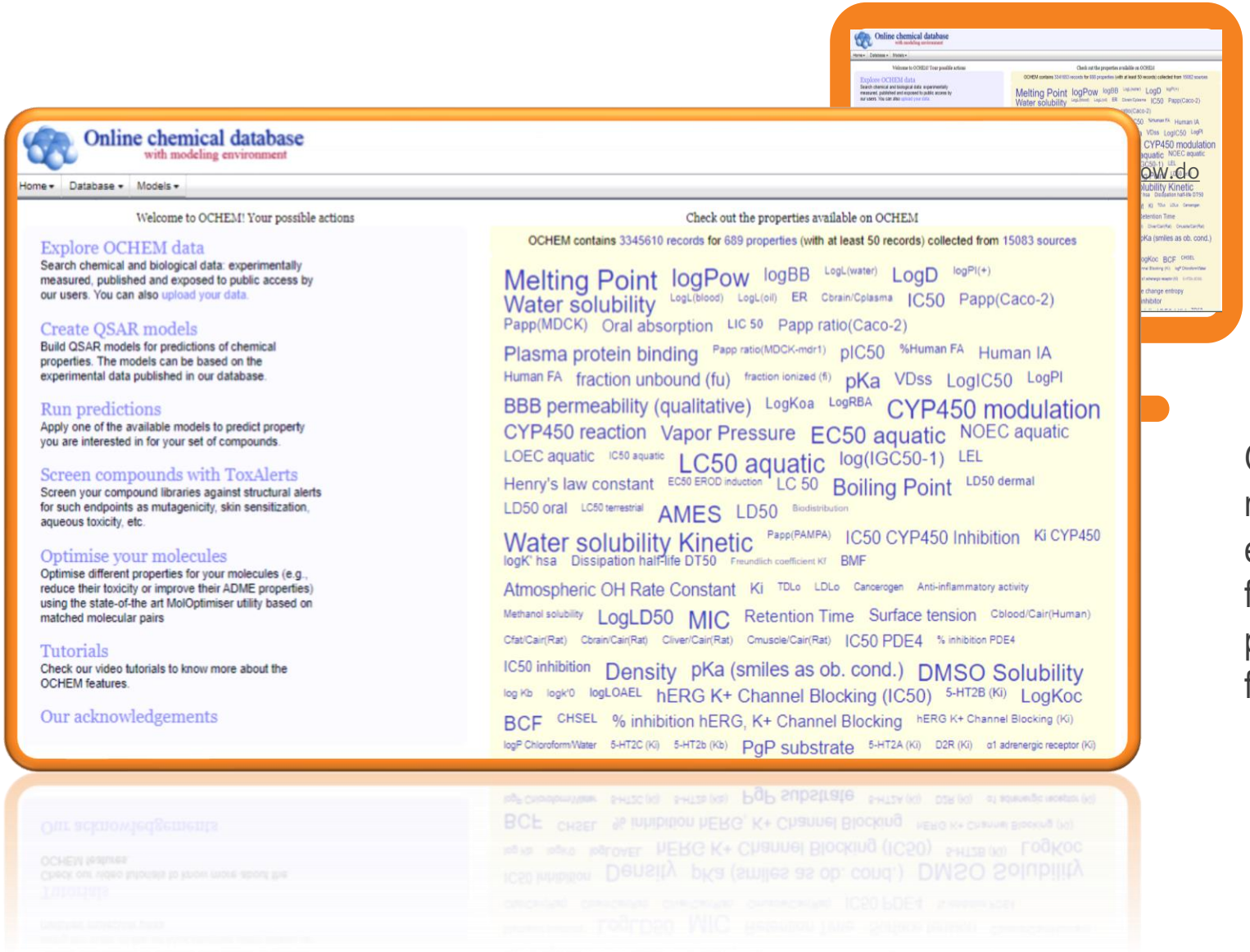
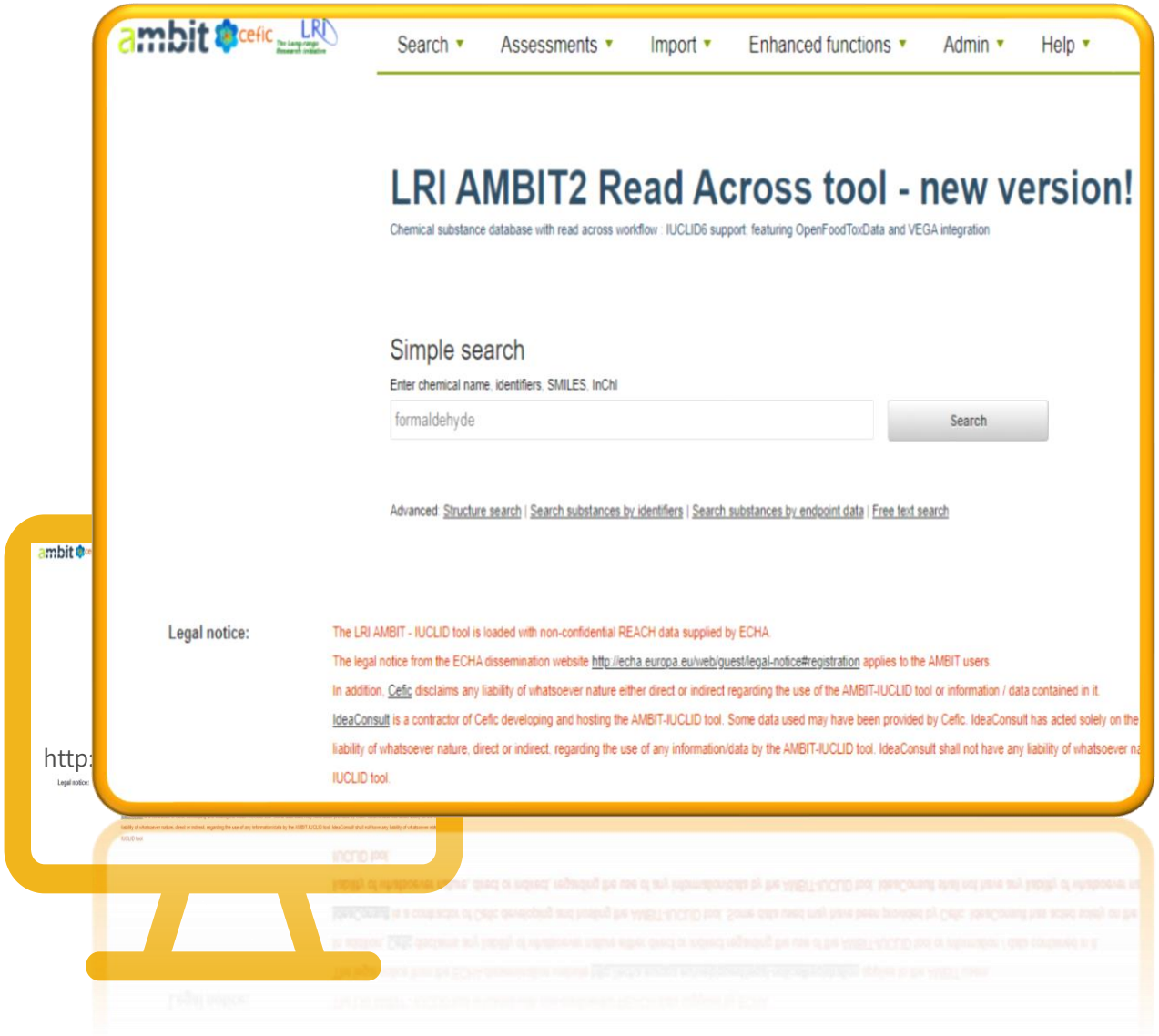


The OCHEM package offers a **database of molecules** and their **ADMET properties.**

OCHEM contains more than **1 million** experimental records for about 499 properties collected from 12428 sources

THE TOOLS

The AMBIT system consists of a database including more than **450.000 chemical** structures and REACH data on **14.570 substances**



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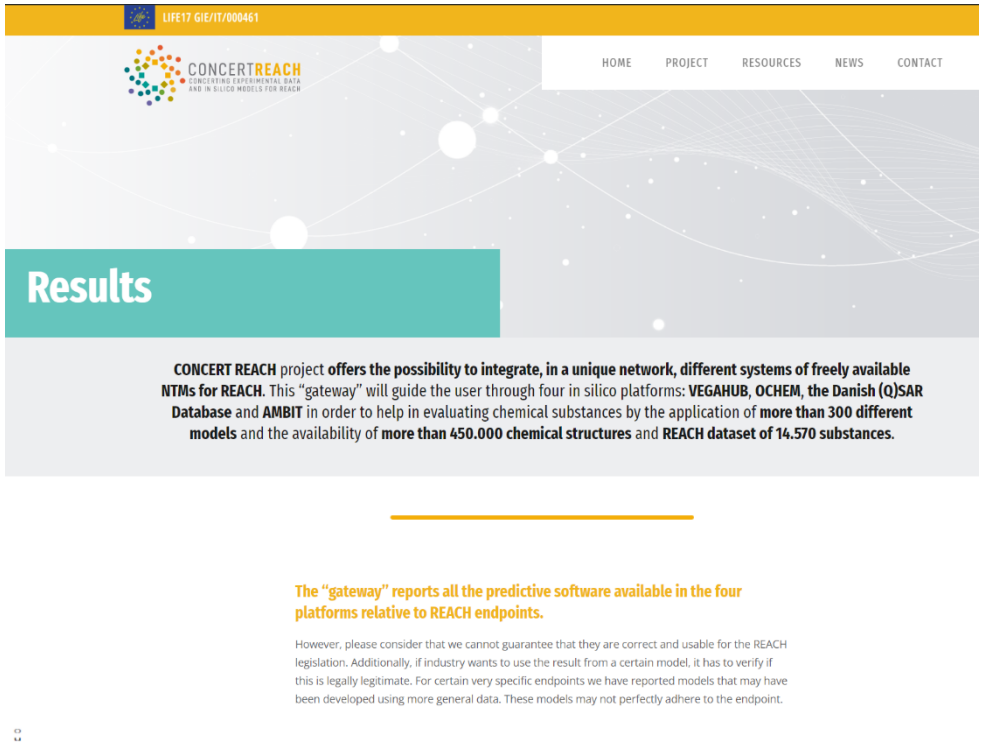
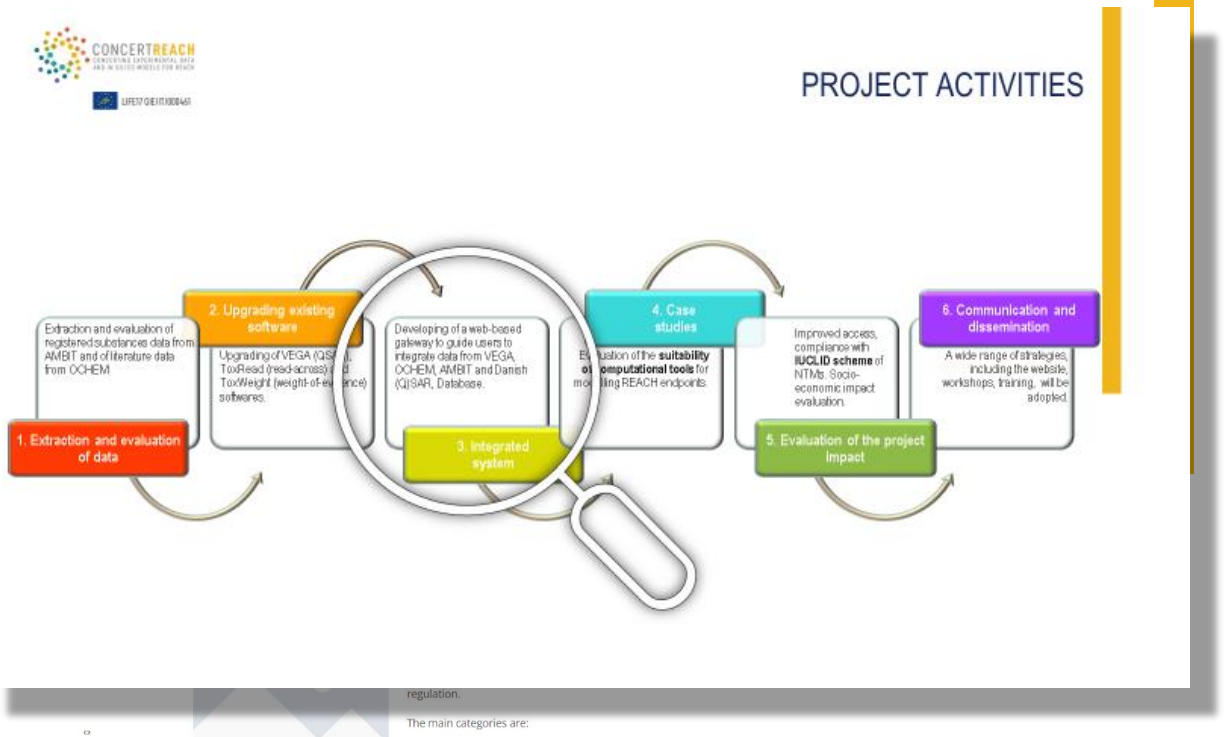
The GATEWAY





https://www.life-concertreach.eu/results/

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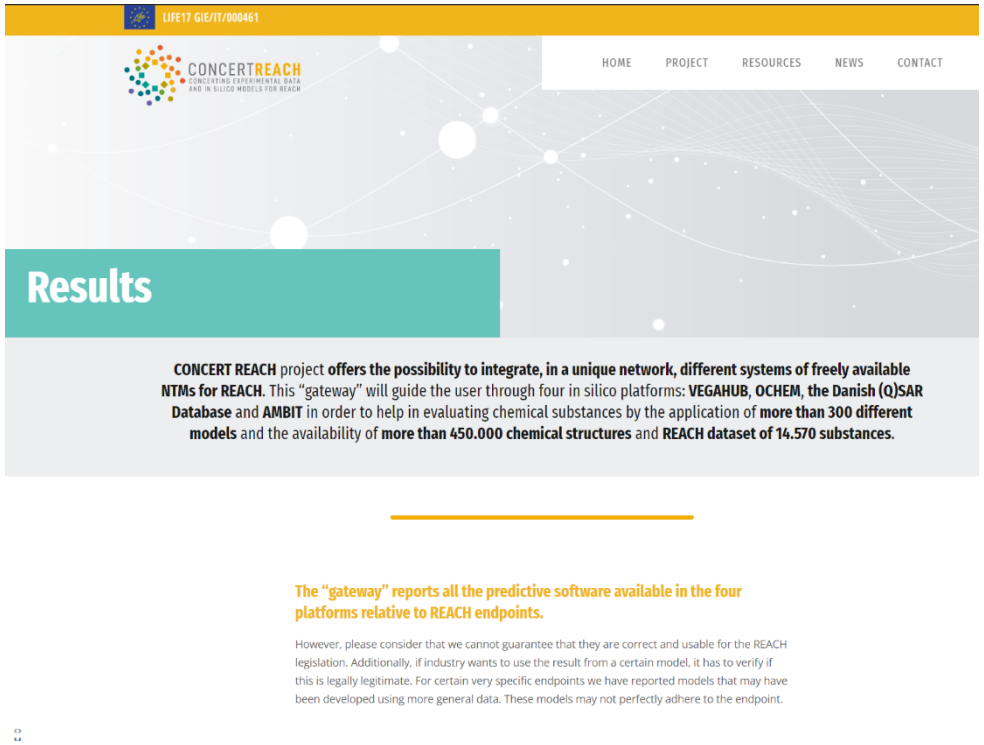
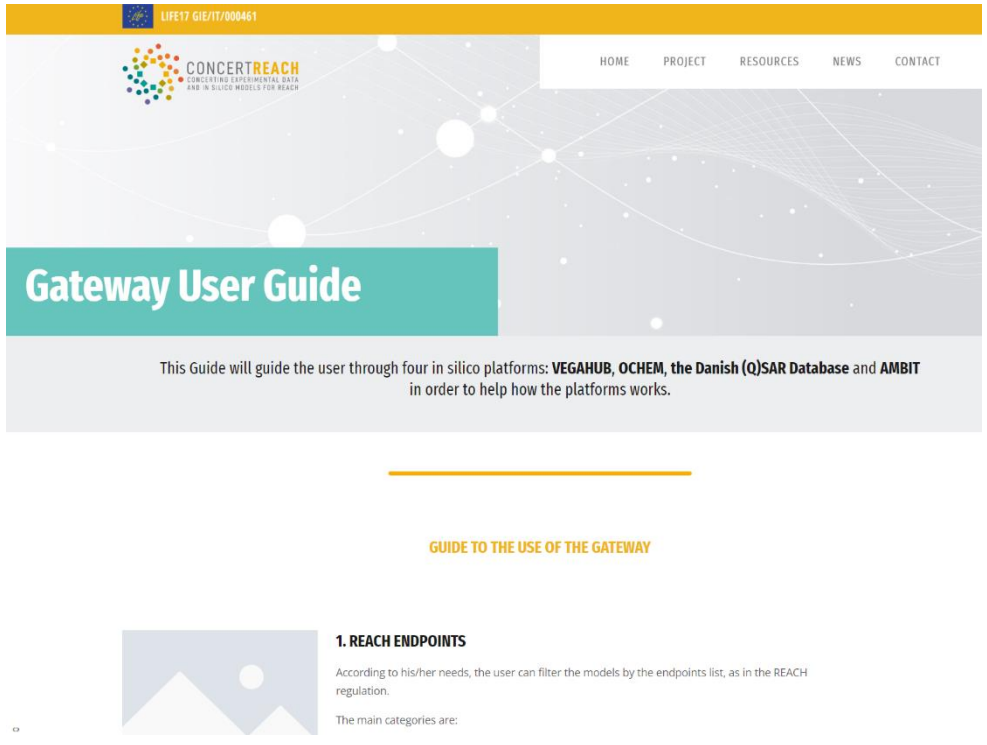
The GATEWAY





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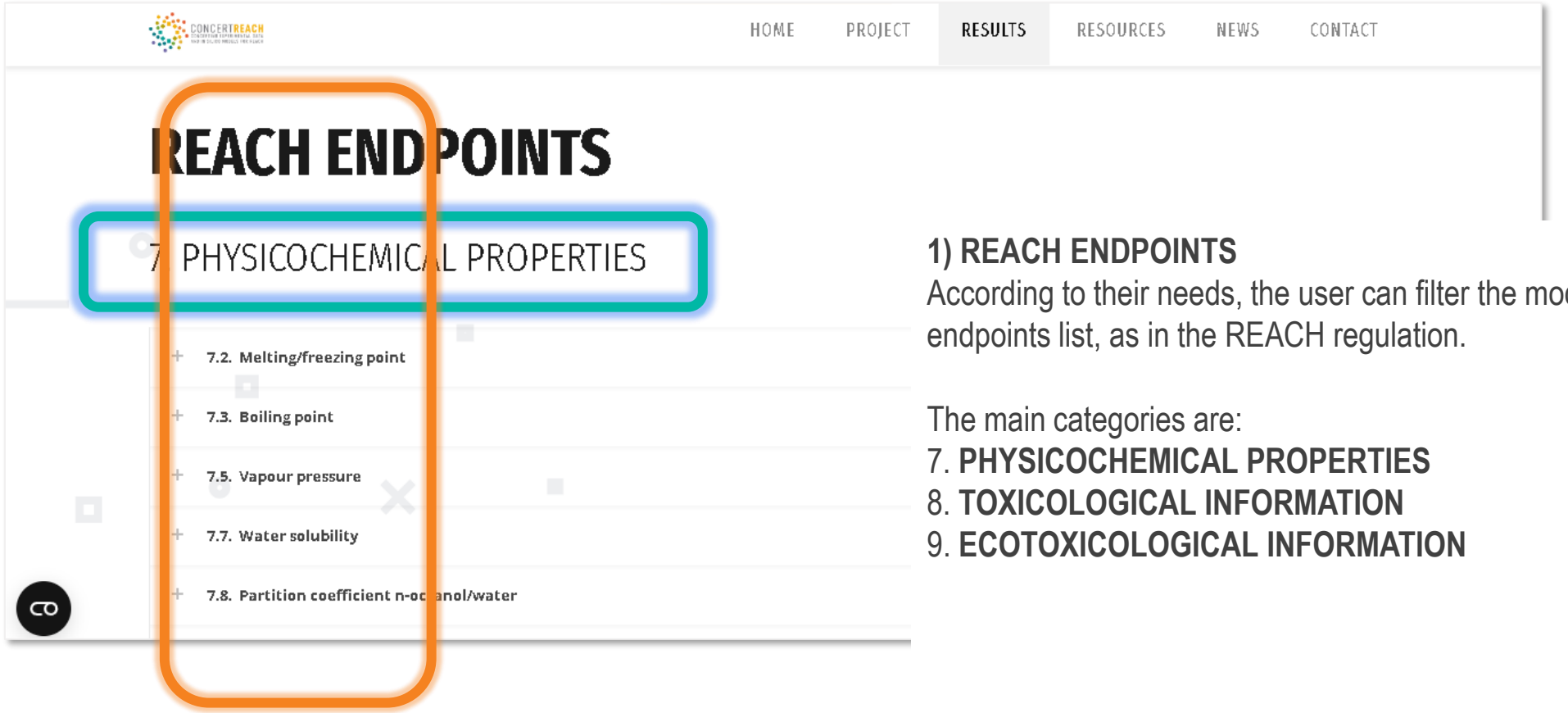
The GATEWAY



1) REACH ENDPOINTS

According to their needs, the user can filter the models by the endpoints list, as in the REACH regulation.

The main categories are:

7. **PHYSICOCHEMICAL PROPERTIES**
8. **TOXICOLOGICAL INFORMATION**
9. **ECOTOXICOLOGICAL INFORMATION**

2) SELECTION OF THE SUITABLE MODEL

https://www.life-concertreach.eu/results/

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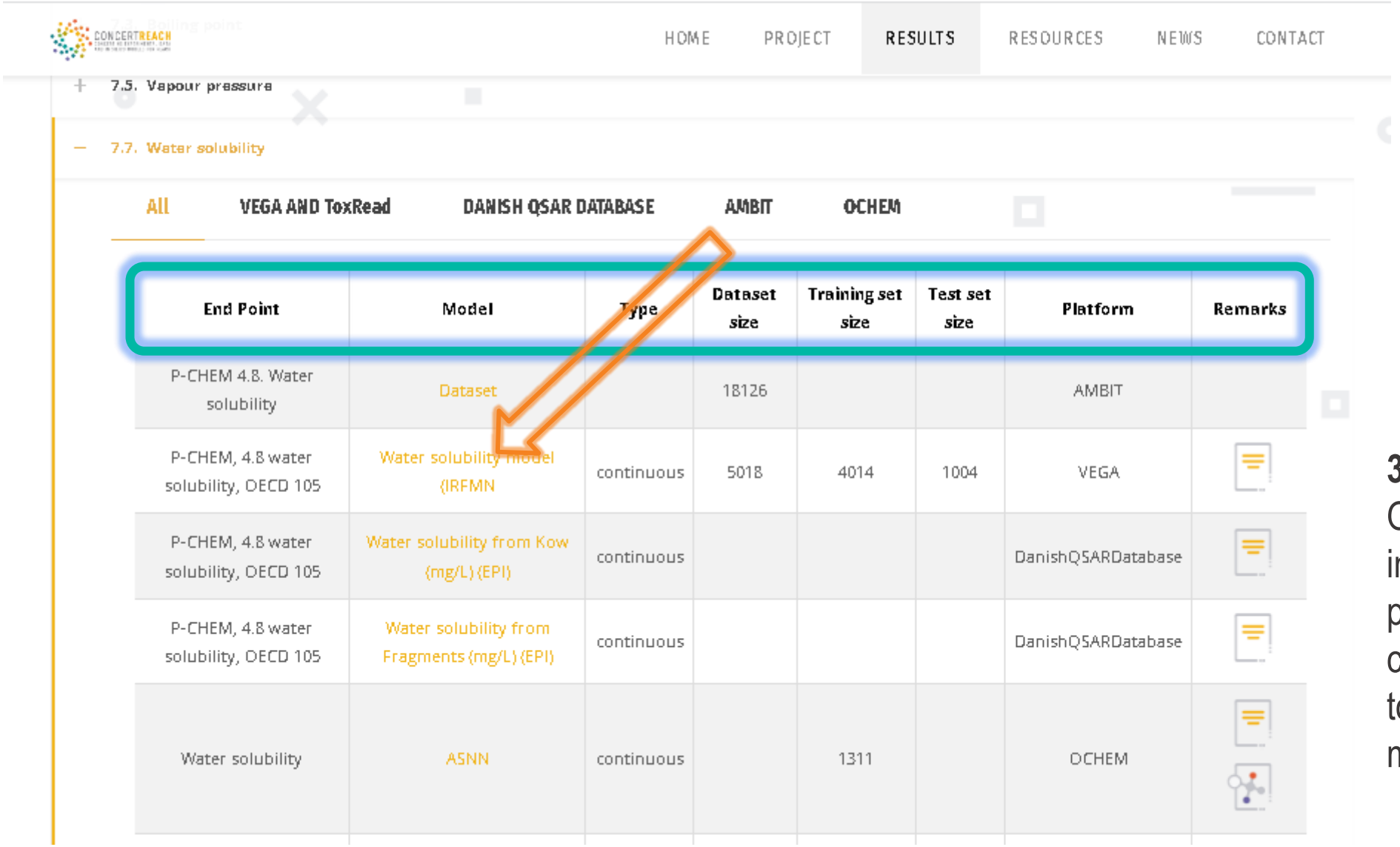
The GATEWAY



End Point	Model	Type	Dataset size	Training set size	Test set size	Platform	Remarks
P-CHEM 4.8. Water solubility	Dataset		18126			AMBIT	
P-CHEM, 4.8 water solubility, OECD 105	Water solubility model (IRFMN	continuous	5018	4014	1004	VEGA	
P-CHEM, 4.8 water solubility, OECD 105	Water solubility from Kow (mg/L) (EPI)	continuous				DanishQSARDatabase	
P-CHEM, 4.8 water solubility, OECD 105	Water solubility from Fragments (mg/L) (EPI)	continuous				DanishQSARDatabase	
Water solubility	ASNN	continuous		1311		OCHEM	

3) PREDICTING

Once selected the model of interest, click on the link present in the “model” column; you will be redirected to the access page of the models.

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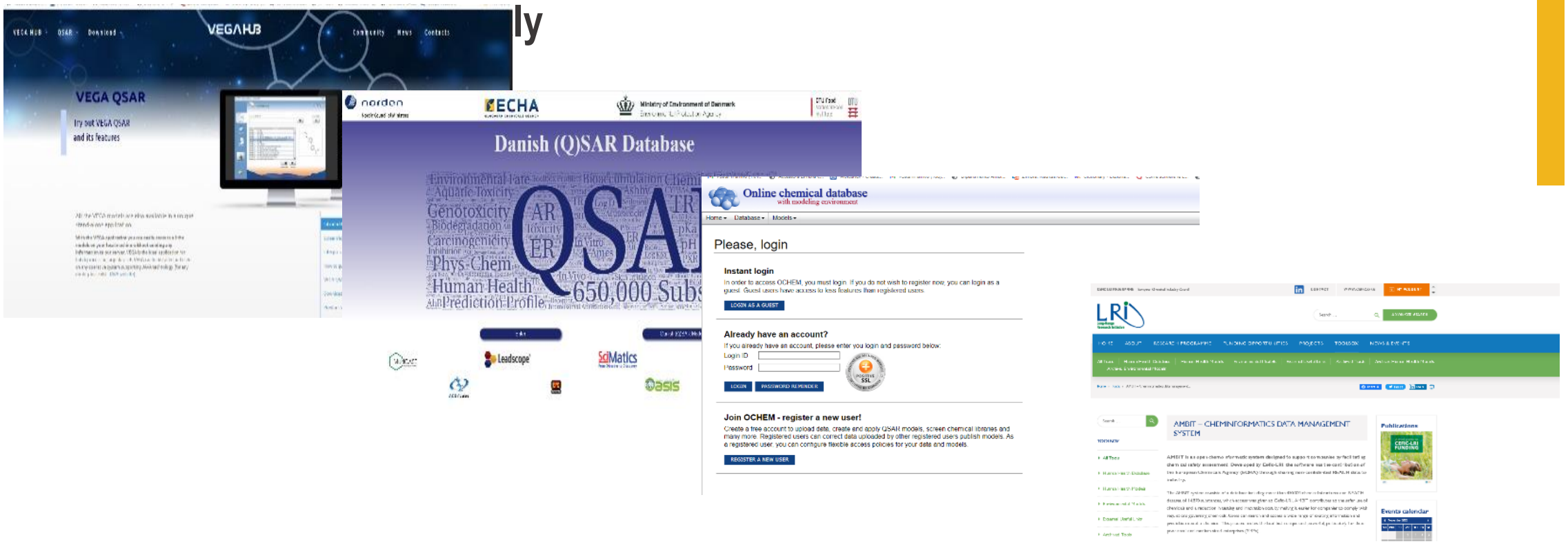
https://www.life-concertreach.eu/results/

3) PREDICTING

Once selected the model of interest, click on the link present in the “model” column; you will be redirected to the access page of the models.



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https://www.life-concertreach.eu/results/

4) INTERPRETATION OF THE RESULTS

The user can consult all the available documentation of the *in silico* tools in the dedicated section.

ELSEVIER

Environment International

Volume 131, October 2019, 105060

Review article

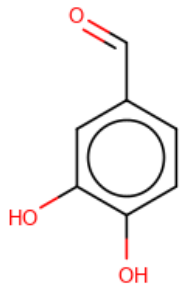
Integrating *in silico* models and read-across methods for predicting toxicity of chemicals: A step-wise strategy

Emilio Benfenati [a], Qasim Chaudhry [b], Giuseppina Gini [c], Jean Lou Dorne [d]

Show more

https://www.sciencedirect.com/science/article/pii/S0160412019312681?via%3Dihub

Target molecule
Tools
Assessment

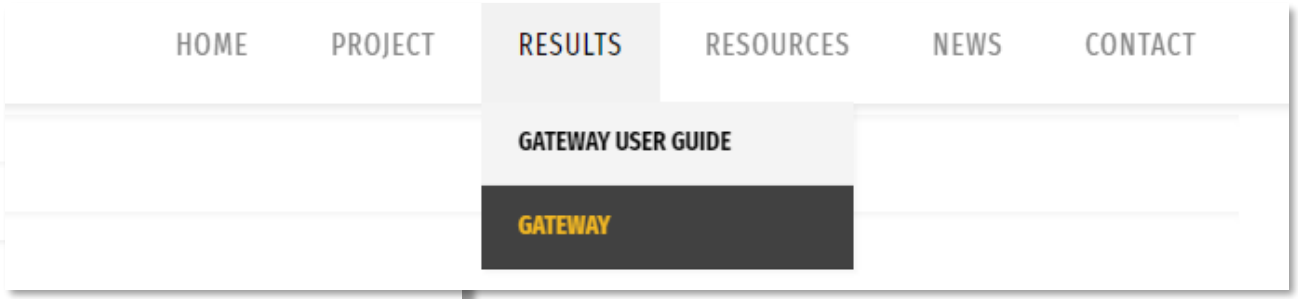


3,4-Dihydroxybenzaldehyde
O=Cc1ccc(O)c(O)c1
Genetic toxicity in vitro.
Ames test

- Checking the availability of the tools for the endpoint in the gateway
- Running the models

OUTPUTS
INTERPRETATION

Checking the availability of the tools for in vitro gene mutation in bacteria in the CONCERT REACH gateway



8.4.1. In vitro gene mutation study in bacteria

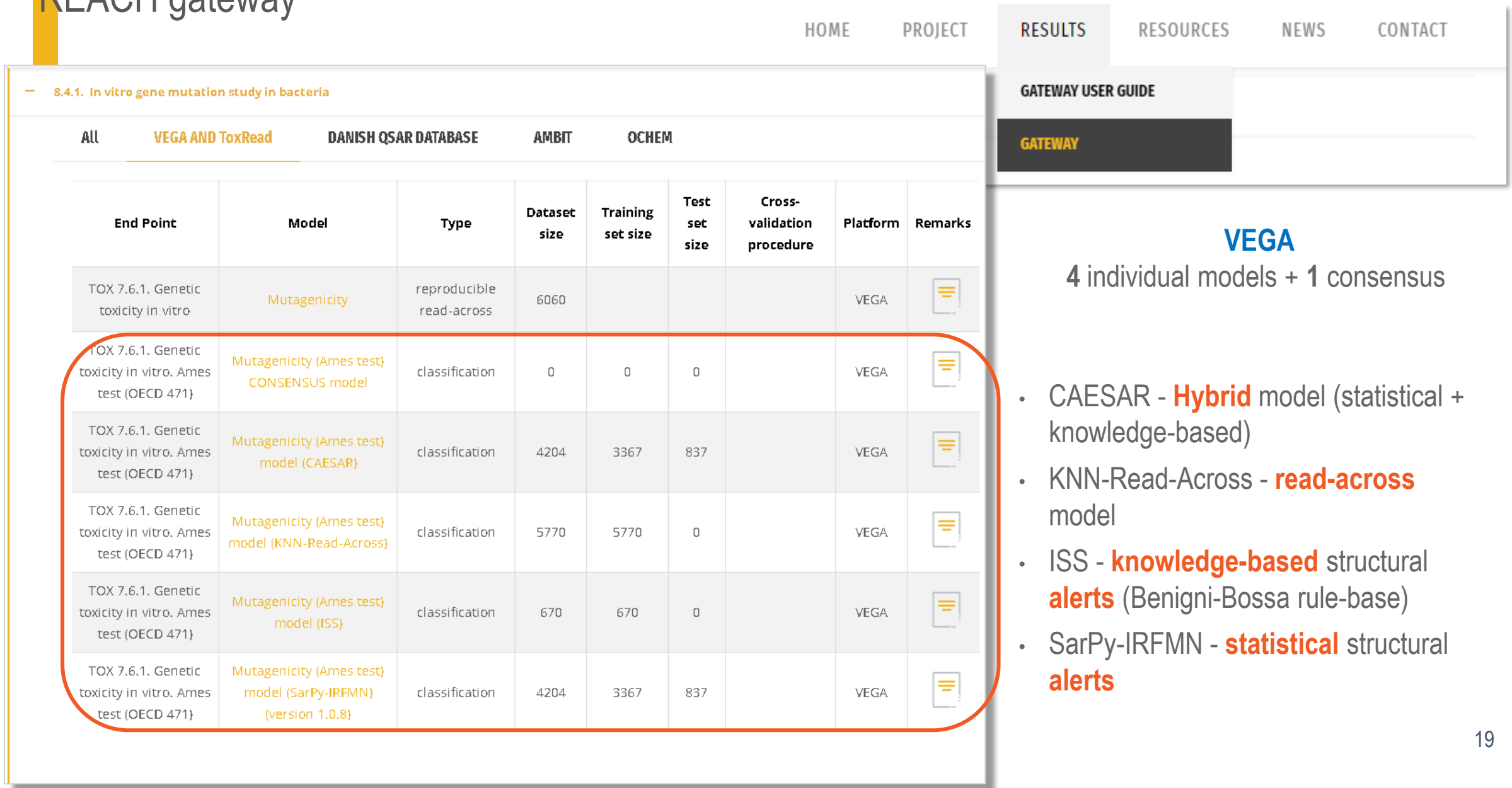
All | VEGA AND ToxRead | DANISH QSAR DATABASE | AMBIT | OCHEM

End Point	Model	Type	Dataset size	Training set size	Test set size	Cross-validation procedure	Platform	Remarks
TOX 7.6.1. Genetic toxicity in vitro. Ames test (OECD 471)	Mutagenicity (Ames test) CONSENSUS model	classification	0	0	0		VEGA	
TOX 7.6.1. Genetic toxicity in vitro. Ames test (OECD 471)	Mutagenicity (Ames test) model (CAESAR)	classification	4204	3367	837		VEGA	
TOX 7.6.1. Genetic toxicity in vitro. Ames test (OECD 471)	Mutagenicity (Ames test) model (KNN-Read-Across)	classification	5770	5770	0		VEGA	

Currently **23 Models** from **VEGA**, **Danish (Q)SAR Database** and **OCHEM**
(Statistical&knwoledge-based)
1 module of **ToxRead**
(read-across)
1 dataset of AMBIT

Direct link to the documentation:
QMRF, papers or guides

Checking the availability of the tools for in vitro gene mutation in bacteria in the CONCERT REACH gateway



End Point	Model	Type	Dataset size	Training set size	Test set size	Cross-validation procedure	Platform	Remarks
TOX 7.6.1. Genetic toxicity in vitro	Mutagenicity	reproducible read-across	6060				VEGA	
TOX 7.6.1. Genetic toxicity in vitro. Ames test (OECD 471)	Mutagenicity (Ames test) CONSENSUS model	classification	0	0	0		VEGA	
TOX 7.6.1. Genetic toxicity in vitro. Ames test (OECD 471)	Mutagenicity (Ames test) model (CAESAR)	classification	4204	3367	837		VEGA	
TOX 7.6.1. Genetic toxicity in vitro. Ames test (OECD 471)	Mutagenicity (Ames test) model (KNN-Read-Across)	classification	5770	5770	0		VEGA	
TOX 7.6.1. Genetic toxicity in vitro. Ames test (OECD 471)	Mutagenicity (Ames test) model (ISS)	classification	670	670	0		VEGA	
TOX 7.6.1. Genetic toxicity in vitro. Ames test (OECD 471)	Mutagenicity (Ames test) model (SarPy-IRFMN) (version 1.0.8)	classification	4204	3367	837		VEGA	

VEGA

4 individual models + **1** consensus

- CAESAR - **Hybrid** model (statistical + knowledge-based)
- KNN-Read-Across - **read-across** model
- ISS - **knowledge-based** structural **alerts** (Benigni-Bossa rule-base)
- SarPy-IRFMN - **statistical** structural **alerts**

Checking the availability of the tools for in vitro gene mutation in bacteria in the CONCERT REACH gateway

8.4.1. In vitro gene mutation study in bacteria

All | VEGA AND ToxRead | DANISH QSAR DATABASE | AMBIT | OCHEM

End Point	Model	Type	Dataset size	Training set size	Test set size	Cross-validation procedure	Platform	Remarks
TOX 7.6.1. Genetic toxicity in vitro	Mutagenicity	reproducible read-across	6060				VEGA	
TOX 7.6.1. Genetic toxicity in vitro. Ames test (OECD 471)	Mutagenicity (Ames test) CONSENSUS model	classification	0	0	0		VEGA	
TOX 7.6.1. Genetic toxicity in vitro. Ames test (OECD 471)	Mutagenicity (Ames test) model (CAESAR)	classification	4204	3367	837		VEGA	
TOX 7.6.1. Genetic toxicity in vitro. Ames test (OECD 471)	Mutagenicity (Ames test) model (KNN-Read-Across)	classification	5770	5770	0		VEGA	
TOX 7.6.1. Genetic toxicity in vitro. Ames test (OECD 471)	Mutagenicity (Ames test) model (ISS)	classification	670	670	0		VEGA	
TOX 7.6.1. Genetic toxicity in vitro. Ames test (OECD 471)	Mutagenicity (Ames test) model (SarPy-IRFMN) (version 1.0.8)	classification	4204	3367	837		VEGA	

ToxRead - 1 module

Dataset = 6060 substances and their public data

4 different rulesets:

- ISS (**knowledge-based** structural **alerts**)
- SARpy (**statistical** structural **alerts)**
- CSR4 (**statistical** structural **alerts)**
- IRFMN (**knowledge-based** structural **alerts**)

Checking the availability of the tools for in vitro gene mutation in bacteria in the CONCERT REACH gateway

HOME | PROJECT | RESULTS | RESOURCES | NEWS | CONTACT

GATEWAY USER GUIDE

GATEWAY

8.4.1. In vitro gene mutation study in bacteria

All | VEGA AND ToxRead | DANISH QSAR DATABASE | AMBIT | OCHEM

End Point	Model	Type	Dataset size	Training set size	Test set size	Cross-validation procedure	Platform	Remarks
Ames test (OECD 471)	Bacterial reverse mutation test (Ames test in S. typhimurium in vitro) (CASE Ultra)	classification		4102		5 times 2-fold external crossvalidation	DanishQSARDatabase	
Ames test (OECD 471)	Bacterial reverse mutation test (Ames test in S. typhimurium in vitro) (Leadscope)	classification		4102		5 times 2-fold external crossvalidation	DanishQSARDatabase	
Ames test (OECD 471)	Bacterial reverse mutation test (Ames test in S. typhimurium in vitro) (SciQSAR)	classification		4102		5 times 2-fold external crossvalidation	DanishQSARDatabase	
Ames test (OECD 471)	Direct acting Ames mutagens (without S9) – ONLY use for Ames POS_IN (CASE Ultra)	classification		388		5 times 2-fold external crossvalidation	DanishQSARDatabase	
Ames test (OECD 471)	Direct acting Ames mutagens (without S9) – ONLY use for Ames POS_IN (Leadscope)	classification		388		5 times 2-fold external crossvalidation	DanishQSARDatabase	
Ames test (OECD 471)	Direct acting Ames mutagens (without S9) – ONLY use for Ames POS_IN (SciQSAR)	classification		388		5 times 2-fold external crossvalidation	DanishQSARDatabase	
Ames test	Base pair Ames mutagens -					5 times 2-fold		

Danish (Q)SAR Database

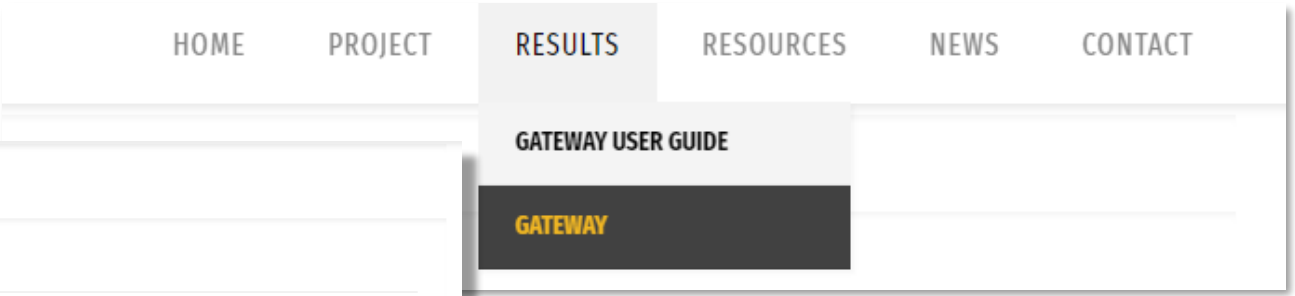
15 statistical models and **2** knowledge-based alert profilers

- Bacterial reverse mutation test (Ames test in S. typhimurium in vitro)
- Direct acting Ames mutagens (without S9)
- Base pair Ames mutagens
- Frame shift Ames mutagens
- Potent Ames mutagens, reversions ≥ 10 times controls

Profilers (OECD QSAR Toolbox V.4.2)

- DNA alerts for AMES by OASIS, alerts in parent only
- In vitro mutagenicity (Ames test) alerts by ISS, alerts in parent only

Checking the availability of the tools for in vitro gene mutation in bacteria in the CONCERT REACH gateway



8.4.1. In vitro gene mutation study in bacteria

All | VEGA AND ToxRead | DANISH QSAR DATABASE | AMBIT | OCHEM

End Point	Model	Type	Dataset size	Training set size	Test set size	Cross-validation procedure	Platform	Remarks
Ames test (OECD 471)	ASNN	Classification		4361	2181		OCHEM	

OCHEM

1 statistical model & ToxAlert match

All | VEGA AND ToxRead | DANISH QSAR DATABASE | AMBIT | OCHEM

End Point	Model	Type	Dataset size	Training set size	Test set size	Cross-validation procedure	Platform	Remarks
TOX 7.6.1. Genetic toxicity in vitro	Dataset		50366				AMBIT	

AMBIT

1 dataset

Models for in vitro gene mutation in bacteria

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How to select the appropriate model(s) for my substance?

A priori selection is generally **not possible**

- However, **experience in using the models** might suggest which could give more reliable results for certain types of substances (e.g., industrial chemicals, active substances, etc.)
- Information on **compliance** of the target molecule **with the applicability domain of the model**
- **Comparison with similar molecules** with available experimental results
- **It is generally required to use multiple and different models for evaluating the same endpoint**

The Gateway makes all those requirements available

Expert analysis of the results and supporting information is needed

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TABLE OF CONTENTS

01

Welcome to the VEGA HUB

Offering a family of tools to evaluate chemical hazard: VEGA, ToxRead, SWAN, VERA, ToxWeight, ToxDelta, and JANUS.

VEGA is the QSAR software with tens of models for individual properties.

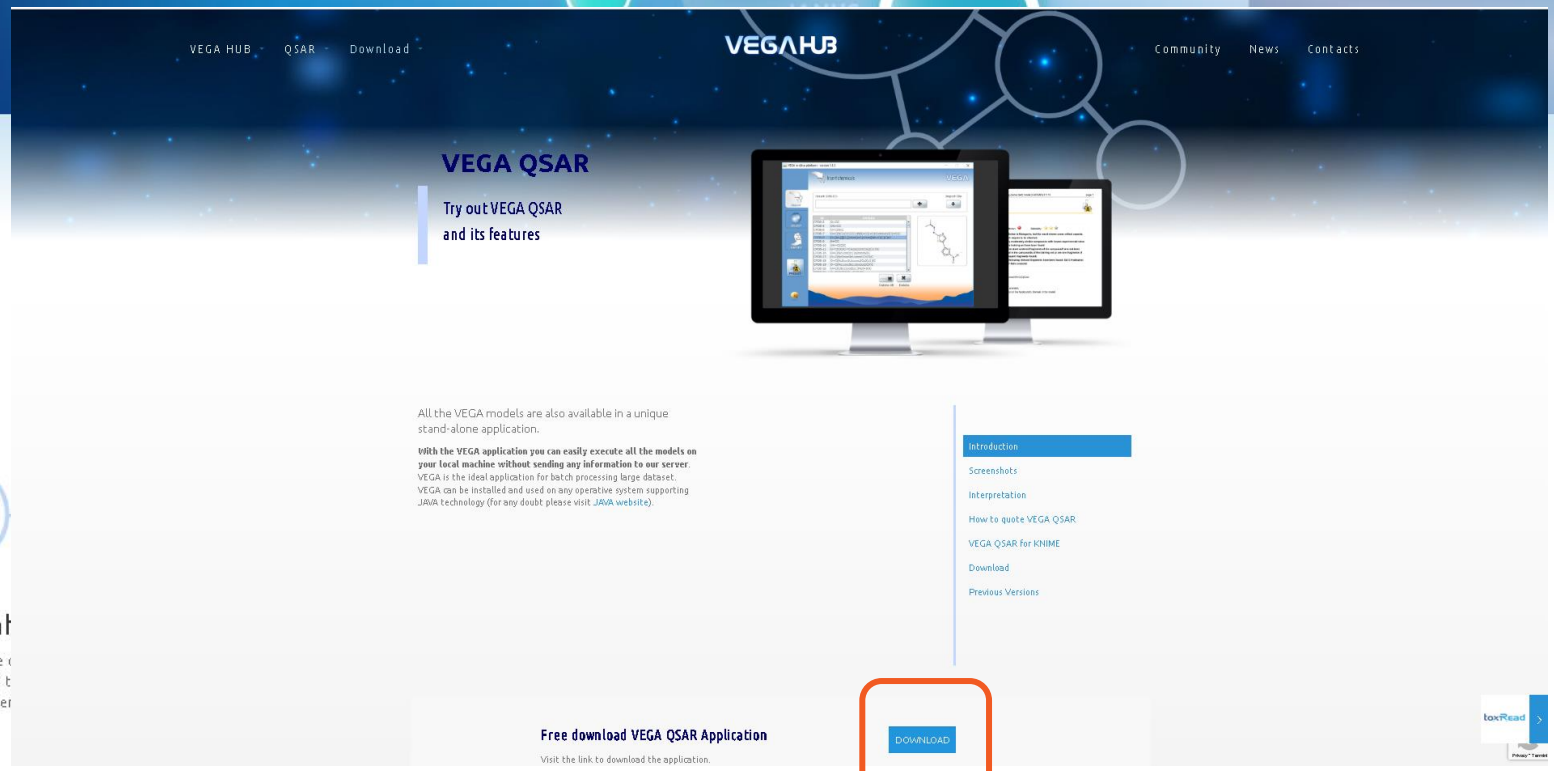
Do you need assistance for a property prediction ?

CONTACT US

VEGA HUB · QSAR · Download

Models and Tools

Assistance



We want to enh

We want to enhance the
of the in silico methods t
the properties of cher
substances.

https://www.vegahub.eu/download/

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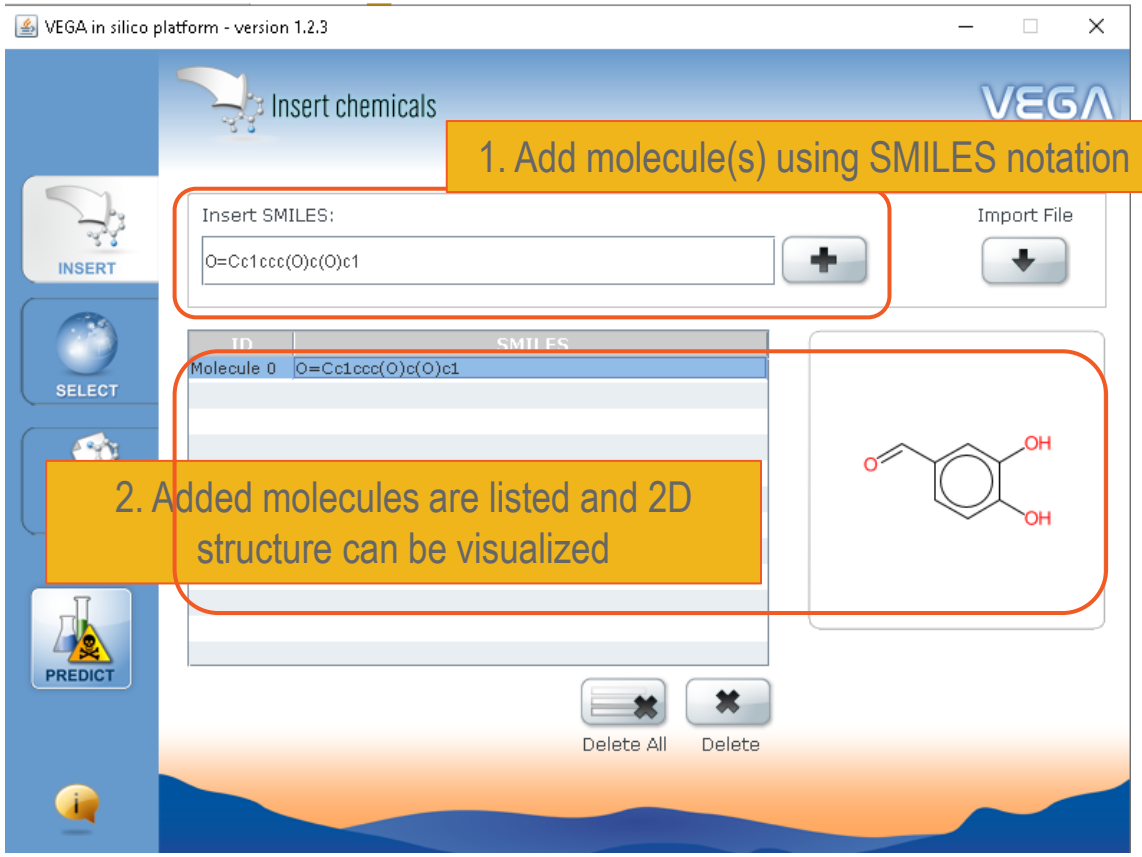
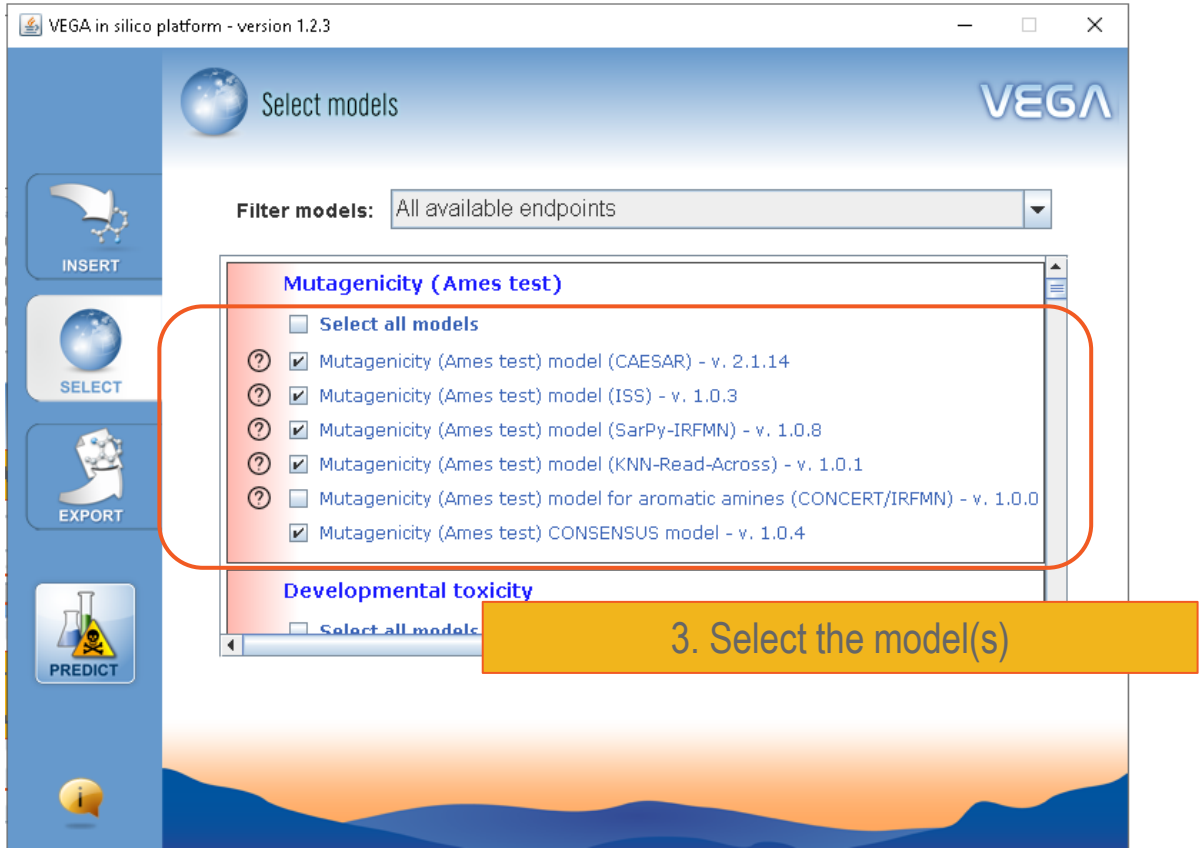
VEGA: running predictions





VEGA: running predictions

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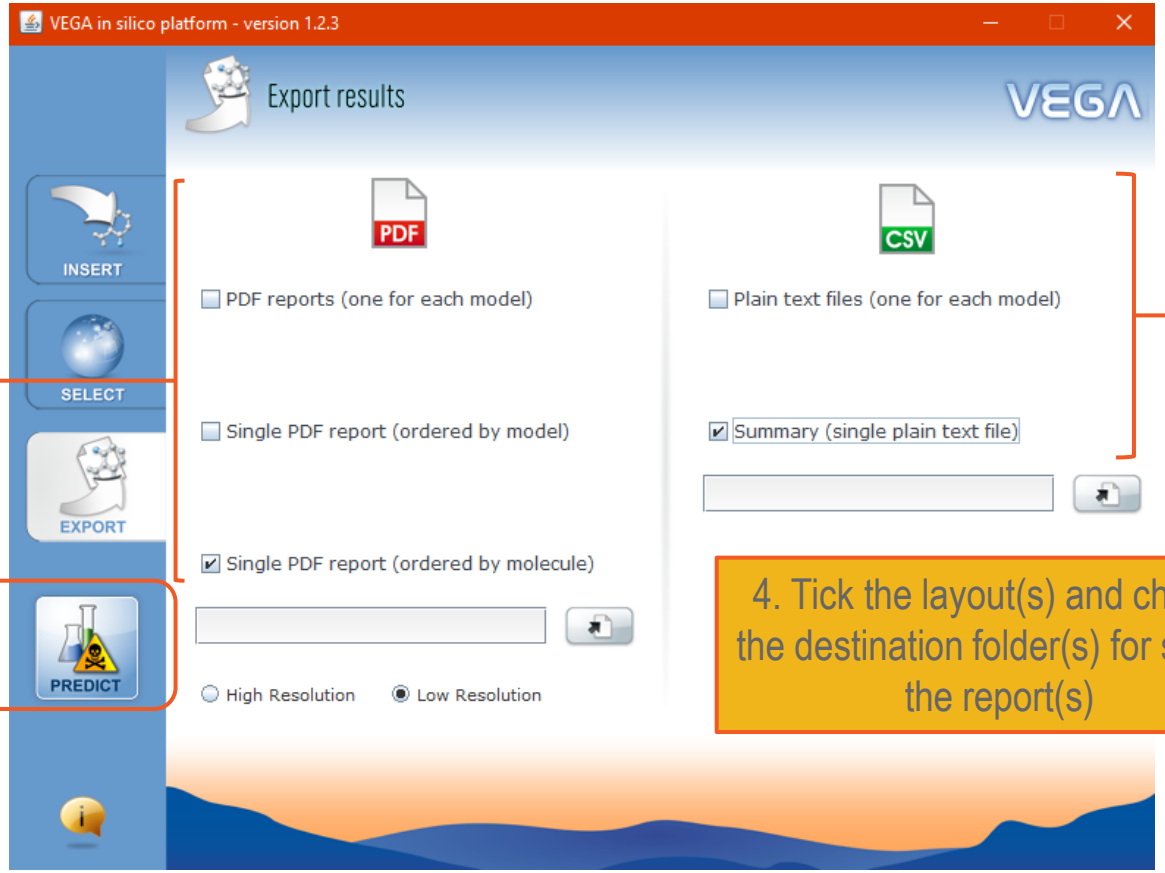
Full PDF reports:

- prediction(s) results
- applicability domain
- experimental data of the target (if any)
- most similar substances
- other supporting info (if any)

5. Click on «Predict»



4. Tick the layout(s) and choose the destination folder(s) for saving the report(s)

Simplified text reports

(useful for excel import)

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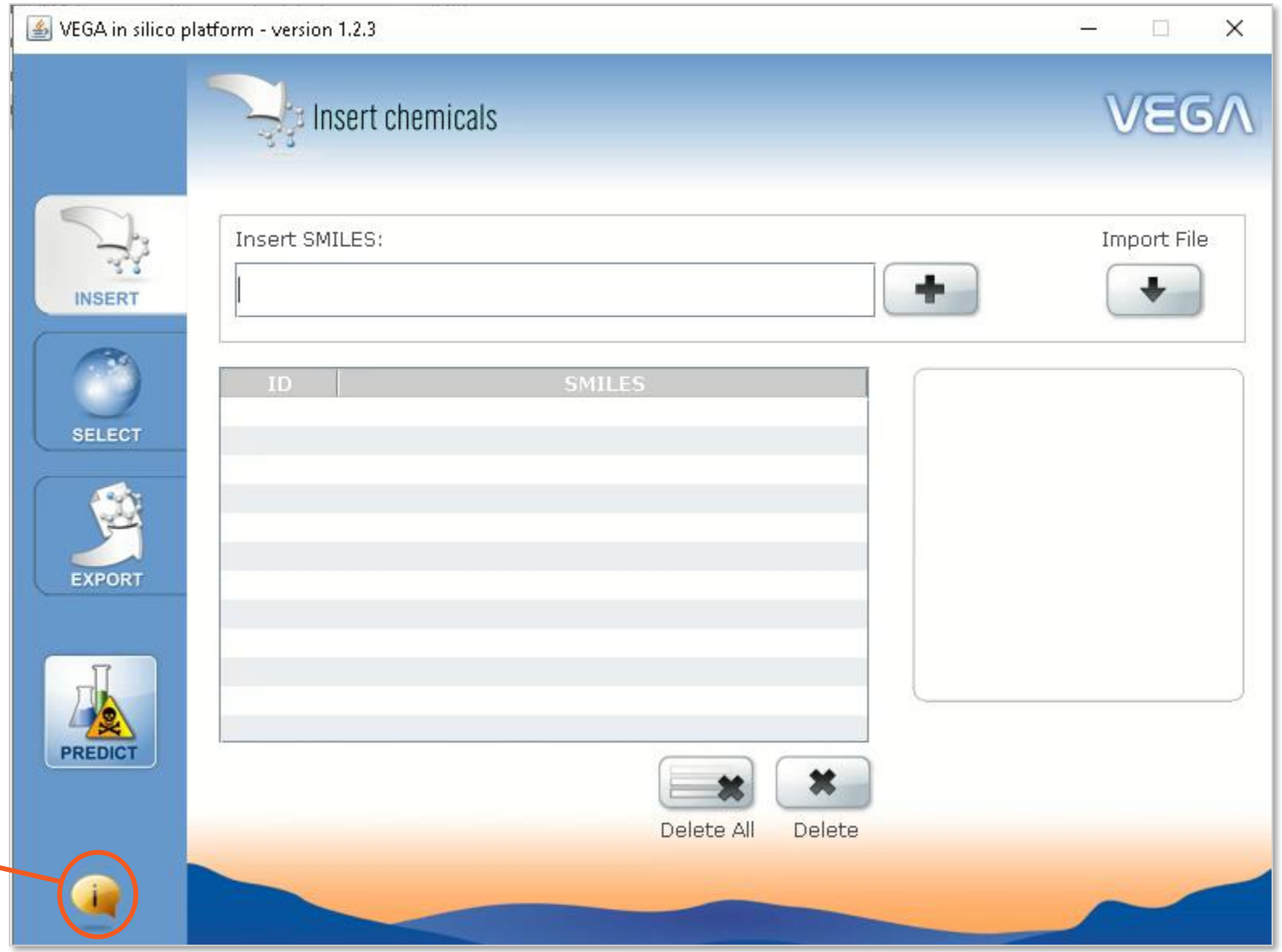
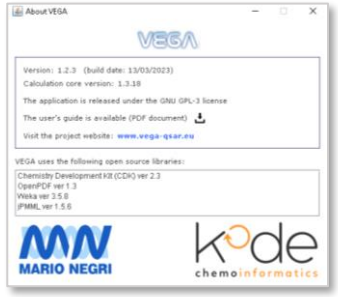
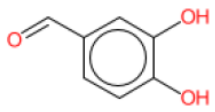
VEGA: running predictions





VEGA: result analysis



Prediction:

Prediction is NON-Mutagenic with a consensus score of 0.675, on 4 models.

Compound: Molecule 0
Compound SMILES: O=Cc1ccc(O)c(O)c1
Used models: 4
Predicted Consensus Mutagen activity: NON-Mutagenic
Mutagenic Score: 0.05
Non-Mutagenic Score: 0.675
Model Caesar assessment: NON-Mutagenic (GOOD reliability)
Model ISS assessment: Mutagenic (LOW reliability)
Model SarPy assessment: Possible NON-Mutagenic (GOOD reliability)
Model KNN assessment: NON-Mutagenic (GOOD reliability)
Remarks:
none

VEGA Mutagenicity (Ames test) model (CAESAR) 2.1.14 page 2

1. Prediction Summary

VEGA Mutagenicity (Ames test) model (SarPy-IRFMN) 1.0.8 page 10

1. Prediction Summary

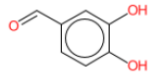
VEGA Mutagenicity (Ames test) model (KNN-Read-Across) 1.0.1 page 14

1. Prediction Summary

VEGA Mutagenicity (Ames test) model (ISS) 1.0.3 page 5

1. Prediction Summary

Prediction for compound Molecule 0 -



Prediction: Reliability:

Prediction is Mutagenic, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- similar molecules found in the training set have experimental values that disagree with the predicted value
- some atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 infrequent_fragments found)
The following alerts have been found: SA11 Simple aldehyde

Compound: Molecule 0
Compound SMILES: O=Cc1ccc(O)c(O)c1
Experimental value: -
Predicted Mutagen activity: Mutagenic
Structural Alerts: SA11 Simple aldehyde
Reliability: The predicted compound is outside the Applicability Domain of the model
Remarks:
none

- **Stars** for ...ility from 1 to 3 (high)
...mary of the ...ation

The reliability of the prediction **is based on** an automated check of the molecule **compliance with the applicability domain of the model**.

VEGA: result analysis

Applicability Domain Index (ADI) ranges **from 0 (not in AD) to 1 (in AD)**
The ADI is calculated based on other indices, **each one taking into account a particular issue** of the applicability domain (AD)

3.2 Applicability Domain:
Measured Applicability Domain Scores

Global AD Index AD index = 0.965 Explanation: The predicted compound is into the Applicability Domain of the model.
Similar molecules with known experimental value Similarity index = 0.932 Explanation: Strongly similar compounds with known experimental value in the training set have been ..
Accuracy of prediction for similar molecules Accuracy index = 1 Explanation: Accuracy of prediction for similar molecules found in the training set is good..
Concordance for similar molecules Concordance index = 1 Explanation: Similar molecules found in the training set have experimental values that agree with the predicted value..
Atom Centered Fragments similarity check ACF index = 1 Explanation: all atom centered fragment of the compound have been found in the compounds of the training set..

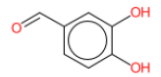
Symbols explanation:

- The feature has a good assessment, model is reliable regarding this aspect.
- The feature has a non optimal assessment, this aspect should be reviewed by an expert.
- The feature has a bad assessment, model is not reliable regarding this aspect.

VEGA — Mutagenicity (Ames test) model (KNN-Read-Across) 1.0.1 — page 14

1. Prediction Summary

Prediction for compound Molecule 0 -



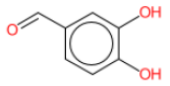
Prediction: Reliability:

Prediction is NON-Mutagenic, the result appears reliable. Anyhow, you should check it through the evaluation of the information given in the following sections.

Compound: Molecule 0
Compound SMILES: O=Cc1ccc(O)c(O)c1
Experimental value: -
Predicted Mutagen activity: NON-Mutagenic
Molecules used for prediction: 4
Reliability: The predicted compound is into the Applicability Domain of the model
Remarks:
none

Number of considered similar molecules and number and type of indexes are **model dependent**

VEGA: example of the automated AD/reliability evaluation



Prediction: Reliability:

Prediction is NON-Mutagenic, the result appears reliable. Anyhow, you should check it through the evaluation of the information given in the following sections.

Compound: Molecule 0
Compound SMILES: O=Cc1ccc(O)c(O)c1
Experimental value: -
Predicted Mutagen activity: NON-Mutagenic
Molecules used for prediction: 4
Reliability: The predicted compound is into the Applicability Domain of the model
Remarks:
none

Global AD Index
AD index = 0.965
Explanation: The predicted compound is into the Applicability Domain of the model.

Similar molecules with known experimental value
Similarity index = 0.932
Explanation: Strongly similar compounds with known experimental value in the training set have been ..

Accuracy of prediction for similar molecules
Accuracy index = 1
Explanation: Accuracy of prediction for similar molecules found in the training set is good..

Concordance for similar molecules
Concordance index = 1
Explanation: Similar molecules found in the training set have experimental values that agree with the predicted value..

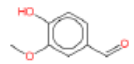
Atom Centered Fragments similarity check
ACF index = 1
Explanation: all atom centered fragment of the compound have been found in the compounds of the training set..

All the SCs are TN

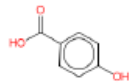
All EXPs=prediction

VEGA — Mutagenicity (Ames test) model (KNN-Read-Across) 1.0.1 — page 15

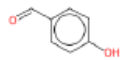
3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



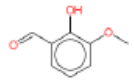
Compound #1
CAS: 121-33-5
Dataset id:873 (Training Set)
SMILES: O=Cc1ccc(O)c(OC)c1
Similarity: 0.938
Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic



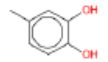
Compound #2
CAS: 99-96-7
Dataset id:5596 (Training Set)
SMILES: O=C(O)c1ccc(O)cc1
Similarity: 0.938
Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic



Compound #3
CAS: 123-08-0
Dataset id:932 (Training Set)
SMILES: O=Cc1ccc(O)cc1
Similarity: 0.927
Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic



Compound #4
CAS: 148-53-8
Dataset id:1548 (Training Set)
SMILES: O=Cc1cccc(OC)c1(O)
Similarity: 0.926
Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic



Compound #5
CAS: 452-86-8
Dataset id:3123 (Training Set)
SMILES: Oc1ccc(cc1(O))C
Similarity: 0.909
Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic

Compound #6
CAS: 90-02-8
Dataset id:5134 (Training Set)
SMILES: O=Cc1ccccc1(O)
Similarity: 0.909
Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic

VEGA: result analysis

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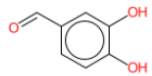
3.2 Applicability Domain:
Measured Applicability Domain Scores

✖	Global AD Index AD index = 0 Explanation: The predicted compound is outside the Applicability Domain of the model.
✔	Similar molecules with known experimental value Similarity index = 0.861 Explanation: Strongly similar compounds with known experimental value in the training set have been ..
✔	Accuracy of prediction for similar molecules Accuracy index = 1 Explanation: Accuracy of prediction for similar molecules found in the training set is good..
✖	Concordance for similar molecules Concordance index = 0 Explanation: similar molecules found in the training set have experimental values that disagree with the predicted value..
⚠	Atom Centered Fragments similarity check ACF index = 0.85 Explanation: some atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 infrequent_fragments found)..

VEGA — Mutagenicity (Ames test) model (ISS) 1.0.3 — page 5

1. Prediction Summary

Prediction for compound Molecule 0 -



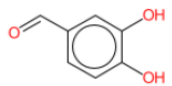
Prediction: Reliability:

Prediction is Mutagenic, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- similar molecules found in the training set have experimental values that disagree with the predicted value
- some atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 infrequent_fragments found)

The following alerts have been found: SA11 Simple aldehyde

Compound: Molecule 0
Compound SMILES: O=Cc1ccc(O)c(O)c1
Experimental value: -
Predicted Mutagen activity: Mutagenic
Structural Alerts: SA11 Simple aldehyde
Reliability: The predicted compound is outside the Applicability Domain of the model
Remarks:
none

VEGA: example of the automated AD/reliability evaluation



Prediction: Reliability:

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Structural Alerts: SA11 Simple aldehyde
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All the SCs are TN

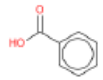
All EXPs≠prediction

VEGA — Mutagenicity (Ames test) model (ISS) 1.0.3 — page 6

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

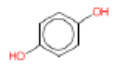
Compound #1

CAS: 120-80-9
Dataset id:817 (Training Set)
SMILES: Oc1ccccc1(O)
Similarity: 0.866
Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic



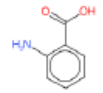
Compound #2

CAS: 65-85-0
Dataset id:798 (Training Set)
SMILES: O=C(O)c1ccccc1
Similarity: 0.856
Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic



Compound #3

CAS: 123-31-9
Dataset id:673 (Training Set)
SMILES: Oc1ccc(O)cc1
Similarity: 0.852
Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic

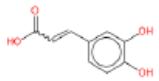


Compound #4

CAS: 118-92-3
Dataset id:96 (Training Set)
SMILES: O=C(O)c1ccccc1(N)
Similarity: 0.849
Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic

Compound #5

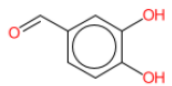
CAS: 108-46-3
Dataset id:298 (Training Set)
SMILES: Oc1cccc(O)c1
Similarity: 0.849
Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic



Compound #6

CAS: 331-39-5
Dataset id:813 (Training Set)
SMILES: O=C(O)C=Cc1ccc(O)c(O)c1
Similarity: 0.835
Experimental value : NON-Mutagenic
Predicted value : NON-Mutagenic

VEGA: example of the automated AD/reliability evaluation



Prediction: Reliability:

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Structural Alerts: SA11 Simple aldehyde
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Remarks:
none

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⚠	Atom Centered Fragments similarity check ACF index = 0.85 Explanation: some atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 infrequent_fragments found)..

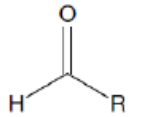
- Lower similarity
- Other SAs not present in the target

VEGA — Mutagenicity (Ames test) model (ISS) 1.0.3 — page 8

4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on fragments/structural alerts :.

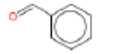
Fragment found: SA11 Simple aldehyde



R= aliphatic or aromatic carbon
α,β unsaturated aldehydes are excluded

Aliphatic and aromatic aldehydes. The alfa,beta-unsaturated aldehydes are excluded

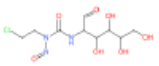
Following, the most similar compounds from the model's dataset having the same fragment.



CAS: 100-52-7
Dataset id:661 (Training Set)
SMILES: O=Cc1ccccc1
Similarity: 0.815

Experimental value : NON-Mutagenic
Predicted value : Mutagenic

Alerts (found also in the target): SA11 Simple aldehyde



CAS: 54749-90-5
Dataset id:826 (Training Set)
SMILES: O=NN(C(=O)NC(C=O)C(O)C(O)C(O)CO)CCCl
Similarity: 0.48

Experimental value : Mutagenic
Predicted value : Mutagenic

Alerts (found also in the target): SA11 Simple aldehyde

Alerts (not found also in the target): SA8 Aliphatic halogens; SA21 Alkyl and aryl N-nitroso groups

CAS: 107-20-0
Dataset id:820 (Training Set)
SMILES: O=CCCl
Similarity: 0.469

Experimental value : Mutagenic
Predicted value : Mutagenic

Alerts (found also in the target): SA11 Simple aldehyde

Alerts (not found also in the target): SA8 Aliphatic halogens

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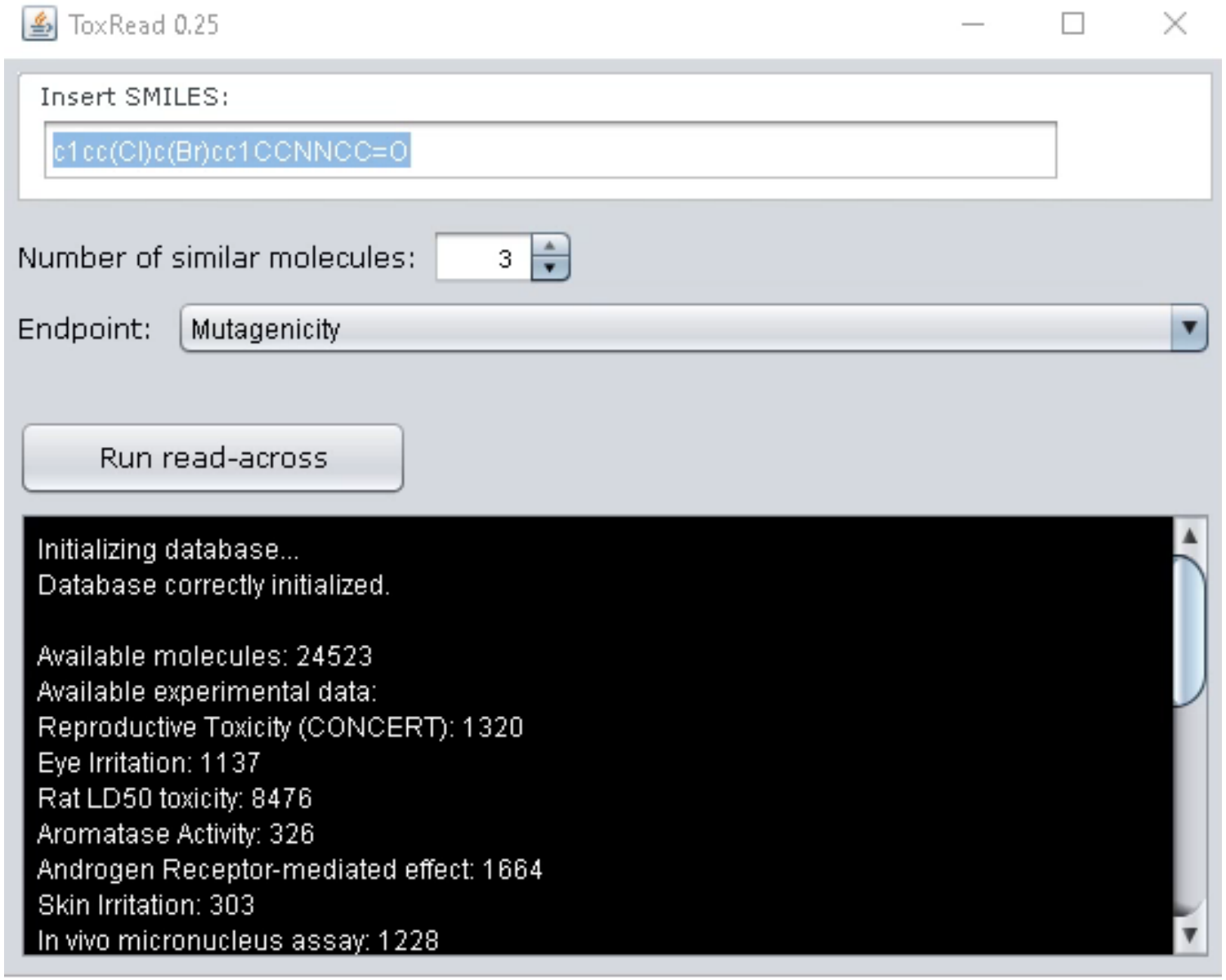
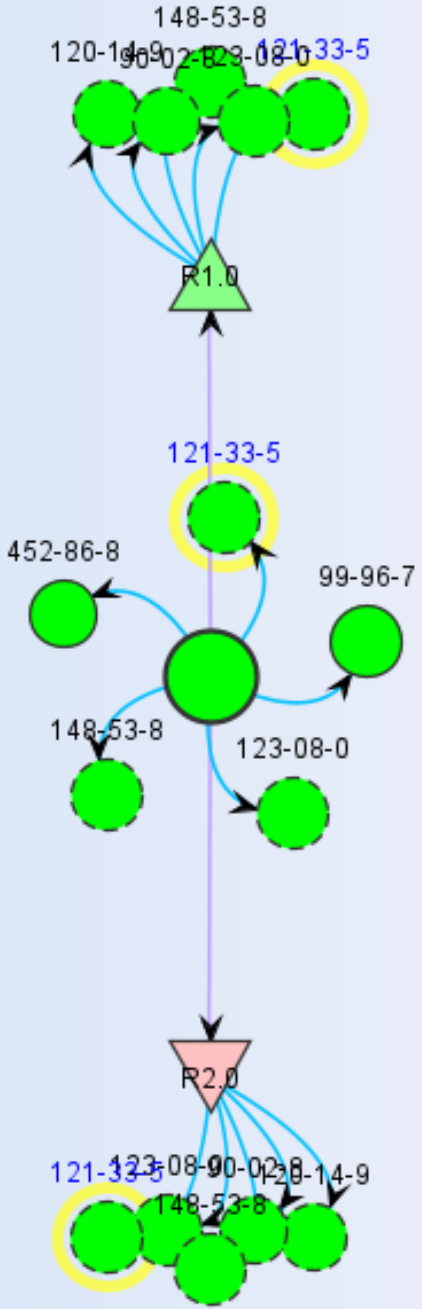
TOXREAD: running read-across

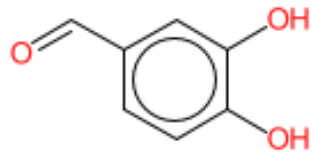


Dataset = 6060 substances and their public data

4 different rulesets:

- ISS (46, 100% **P**)
- SARpy (205, 55% **P**)
- CSR4 (238, 41% **P**)
- IRFMN (282, 57% **P**)





Molecular Weight: 138.14
LogP (experimental): 1.09

Label	Rule Set
R2.0	Aliphatic and aromatic aldehydes. The alfa,beta-unsaturat...
R1.0	IRFMN alert n. 106 for NON-Mutagenicity, defined by the S...

target compound

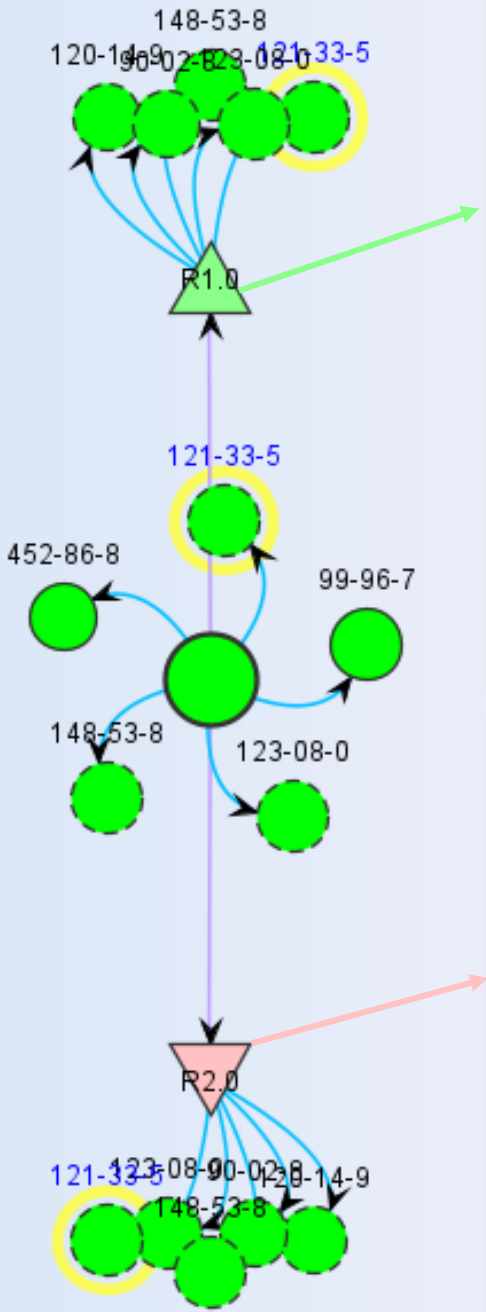
intensity of red related to the value of mutagenicity

intensity of green related to the value of non-mutagenicity

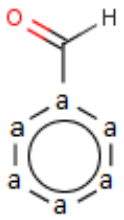
non-toxicity or toxicity rule, size related to the Fisher Test P-Value of the rule

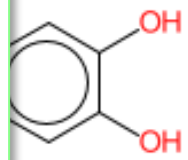
circle size related to the similarity with the target compound

repeated compound



Details of rule MNM106



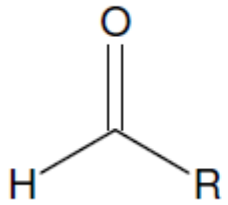


Details of rule MNM106

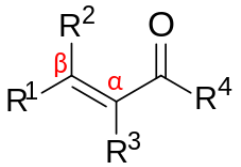
Name: MNM106
Description: IRFMN alert n. 106 for NON-Mutagenicity
Experimental accuracy: 0.71
Fisher test p-value: 0.00319

Label Rule Set

Details of rule SA11 Simple aldehyde



R= aliphatic or aromatic carbon
α,β unsaturated aldehydes are excluded

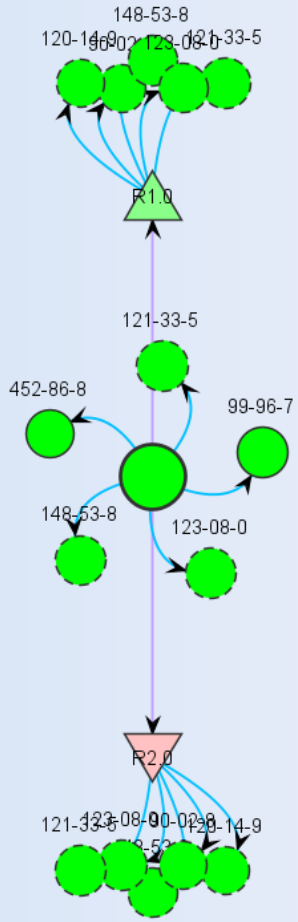


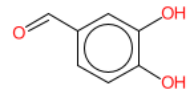
Details of rule SA11 Simple aldehyde

Name: SA11 Simple aldehyde
Description: Aliphatic and aromatic aldehydes. The alfa,beta-unsatu
Experimental accuracy: 0.43
Experimental accuracy (only on biocide compounds): 1
Fisher test p-value: 0.02957

,beta-unsaturat...
defined by the S...

Read-Across chart - Endpoint: Mutagenicity





Target molecule prediction

```
Overall assessment: NON-MUTAGENIC

Read-Across assessment: Non-Mutagenic
Read-Across Mutagenic score = 0
Read-Across Non-Mutagenic score = 1

QSAR consensus assessment: NON-Mutagenic (Consensus score: 0.675)
Predicted Consensus Mutagen activity = NON-Mutagenic
Mutagenic Score = 0.05
Non-Mutagenic Score = 0.675
Model Caesar assessment = NON-Mutagenic (GOOD reliability)
Model ISS assessment = Mutagenic (LOW reliability)
Model SarPy assessment = Possible NON-Mutagenic (GOOD reliability)
Model KNN assessment = NON-Mutagenic (GOOD reliability)
```

a-unsaturated aldehydes are excluded

hed by the SMARTS: [C;D2;H1](=O)a1aaaaa1

ITA 15:42 29/05/2023

CONCERTREACH
CONCERTING EXPERIMENTAL DATA AND IN SILICO MODELS FOR REACH

LIFE17 GIE/IT/000461

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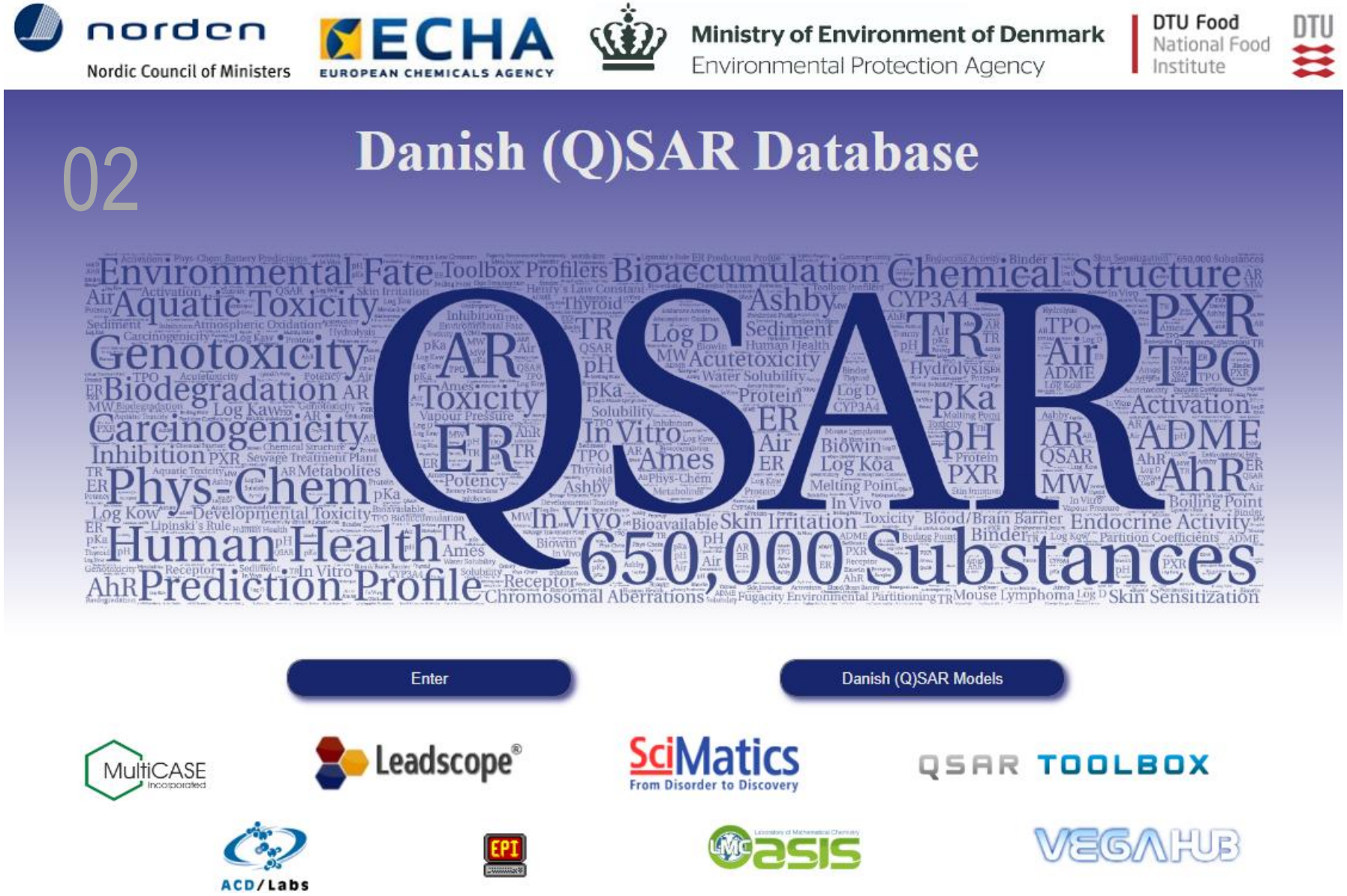
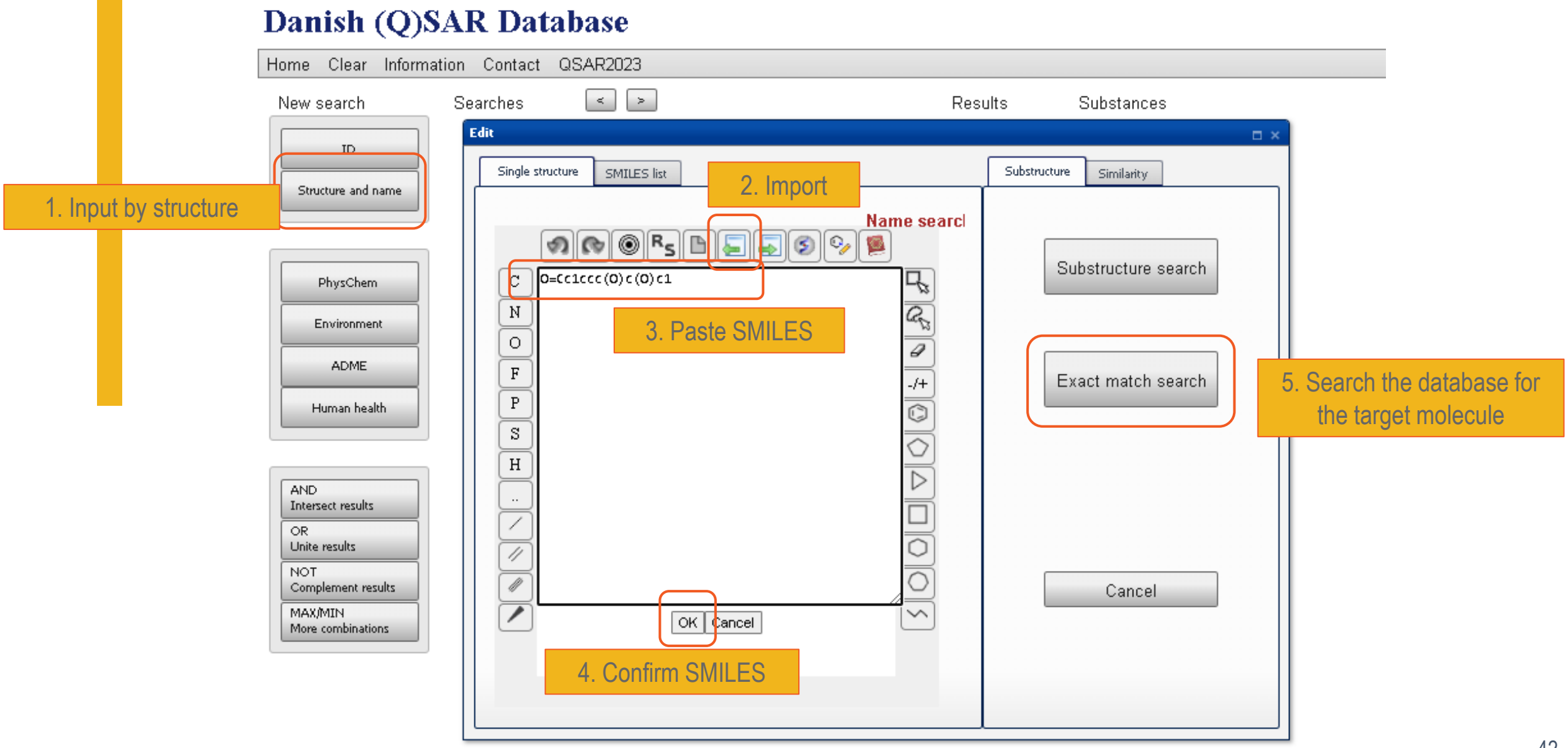
Danish (Q)SAR Database: introduction



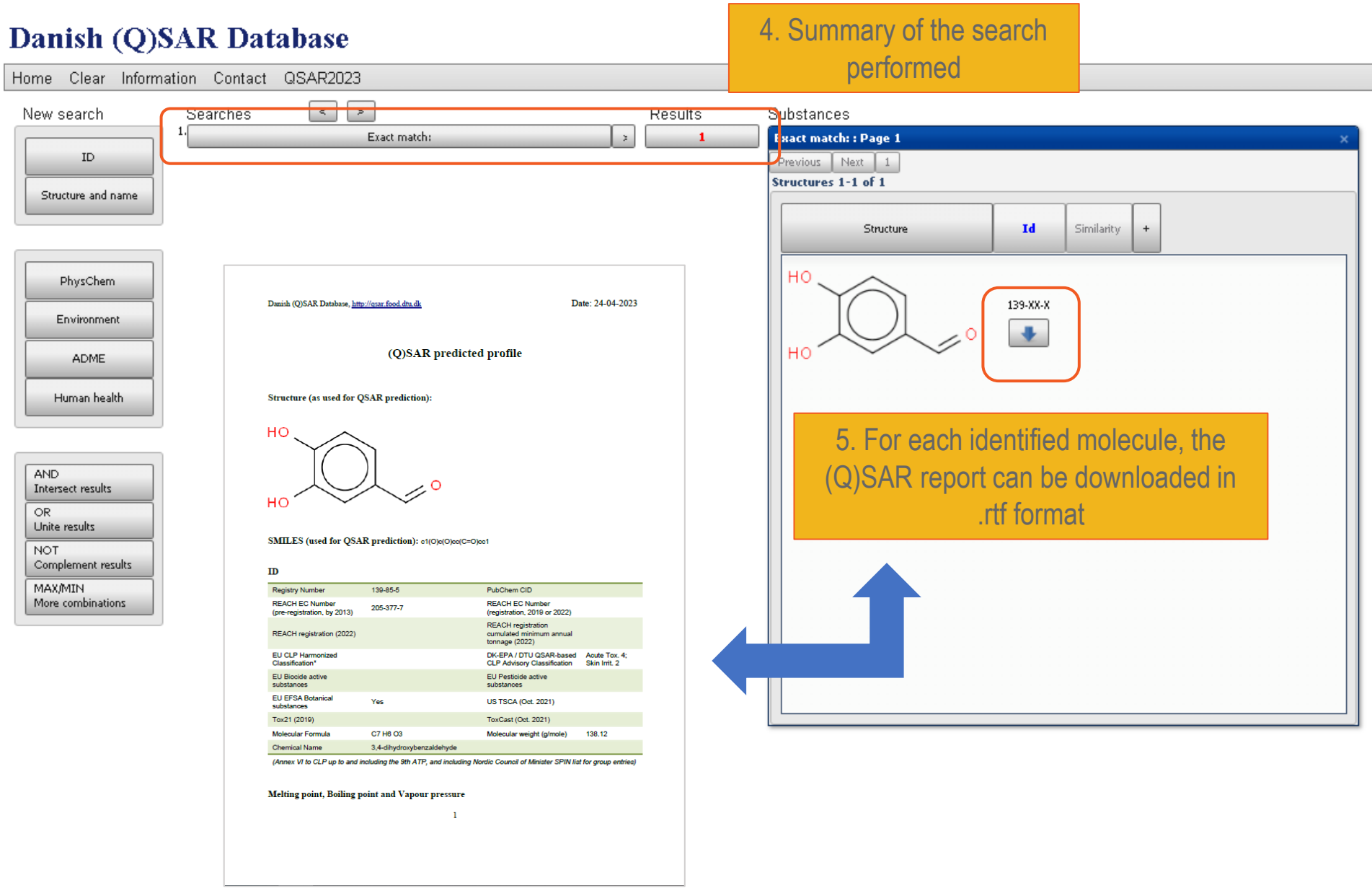
Danish (Q)SAR Database **can be searched** for molecules, based on available **experimental data, (Q)SAR predictions, structural alerts**, etc., for the endpoint of interest

- The results of the QSAR predictions
- Identification of similar molecules
- Stepwise approach

Danish (Q)SAR Database: gathering (Q)SAR results



Danish (Q)SAR Database: gathering (Q)SAR results



Danish (Q)SAR Database: results for in vitro gene mutation in bacteria

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***In vitro* Genotoxicity - Bacterial Reverse Mutation Test (Ames test)**

	Exp	Battery	CASE Ultra	Leadscope	SciQSAR
Ames test in S. typhimurium (*in vitro*)		NEG_IN	NEG_IN	NEG_IN	NEG_OUT
*Direct Acting Mutagens (without S9)	N/A	INC_OUT	NEG_OUT	INC_OUT	INC_OUT
*Base-Pair Ames Mutagens	N/A	NEG_OUT	NEG_OUT	NEG_IN	INC_OUT
*Frameshift Ames Mutagens	N/A	INC_OUT	POS_OUT	POS_IN	NEG_IN
*Potent Ames Mutagens, Reversions ≥ 10 Times Controls	N/A	POS_IN	POS_IN	POS_IN	POS_IN

DTU-developed models

* The four models (Direct Acting mutagens (without S9), Base-Pair Ames Mutagens, Frameshift Ames Mutagens, Potent Ames Mutagens) should not be used to determine if substances are Ames mutagens, but can be used for indication of mechanism or potency for cases where the main Ames model (Ames test in S. typhimurium (*in vitro*)) is POS_IN.

The target molecule was evaluated as **compliant with AD** except for SciQSAR model.
The other four models should not be considered.

Within LIFE CONCERT REACH, results from the four VEGA models and the Consensus model have been integrated

	VEGA	Mut. / Non-mut. scores	Used models
Mutagenicity consensus	NEG	0.05 / 0.68	4

Mutagenicity (Ames) consensus model version 1.0.2 contained in VEGA version 1.1.4 with calculation core version 1.2.4

Prediction: POS = Mutagenic, NEG = Non-mutagenic.

VEGA			
ISS	CAESAR	SarPy	KNN
POS_Low	NEG_Good	POSS.NEG_Good	NEG_Good

Four individual models in mutagenicity consensus model version 1.0.2 contained in VEGA version 1.1.4 with calculation core version 1.2.4

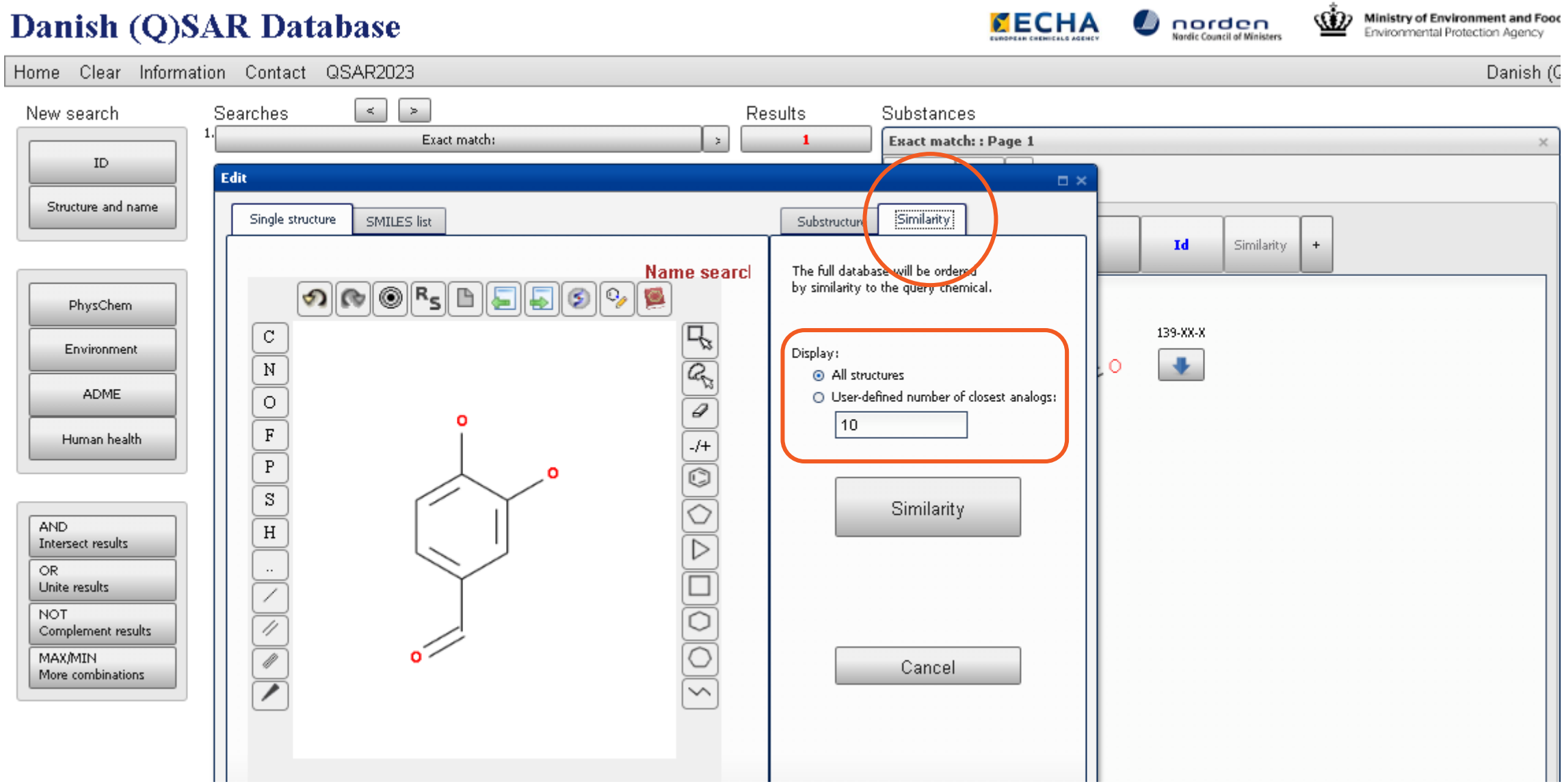
Structural alerts identified by two endpoint-specific profilers present in the OECD QSAR Toolbox

DNA alerts for AMES by OASIS, alerts in:	
- parent only	No alert found
In vitro mutagenicity (Ames test) alerts by ISS, alerts in:	
- parent only	Simple aldehyde

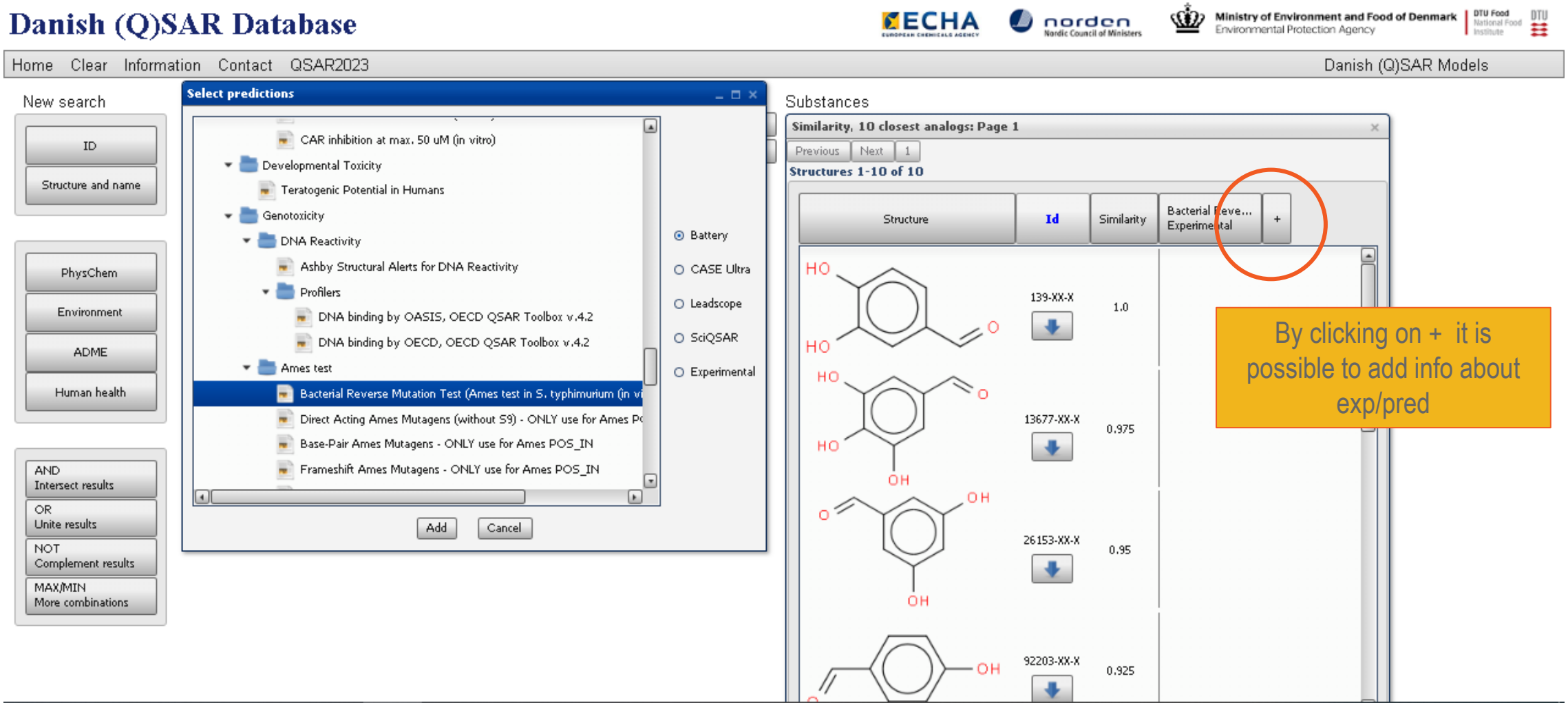
OECD QSAR Toolbox v.4.2 profilers

Profiler predictions are supporting information to be used together with the relevant QSAR predictions

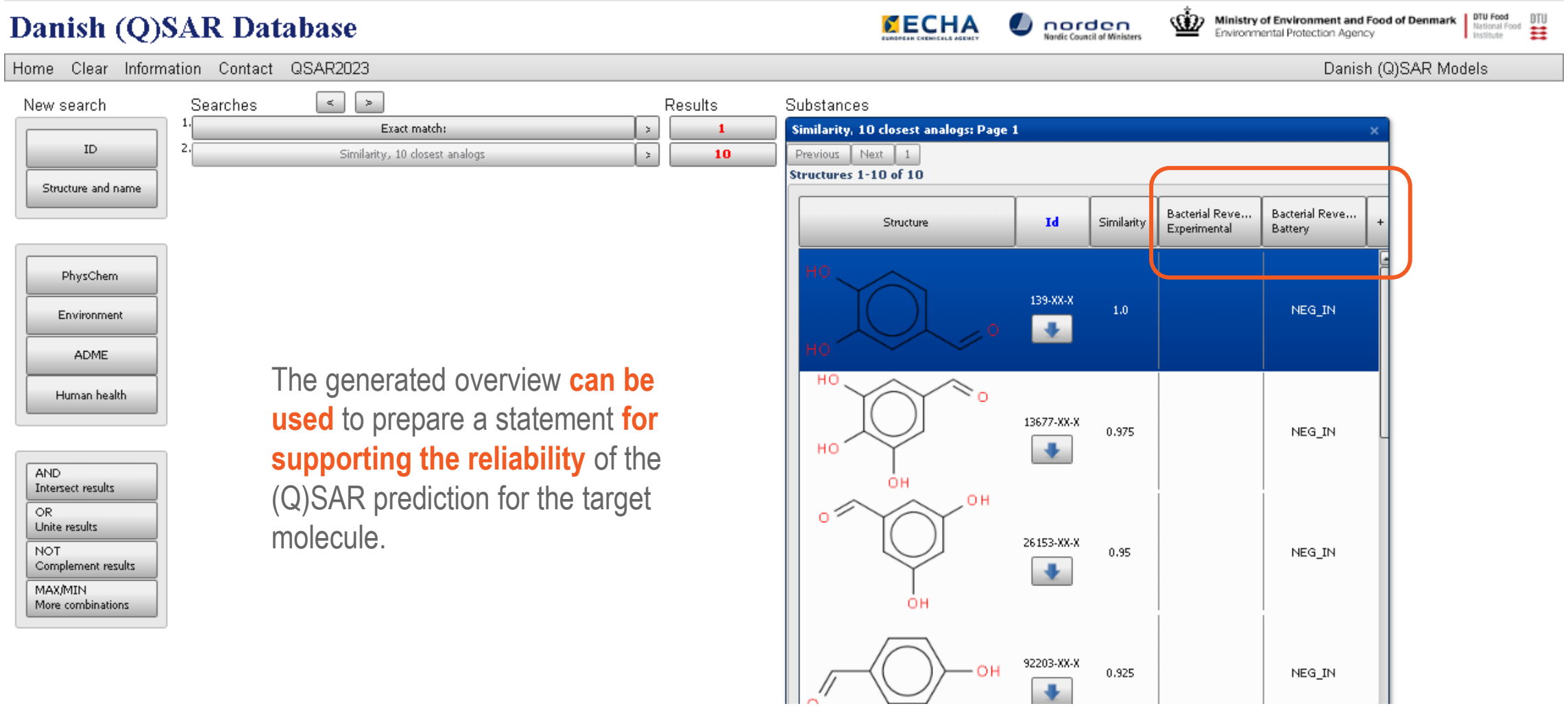
Danish (Q)SAR Database: identification of similar molecules



Danish (Q)SAR Database: identification of similar molecules



Danish (Q)SAR Database: identification of similar molecules

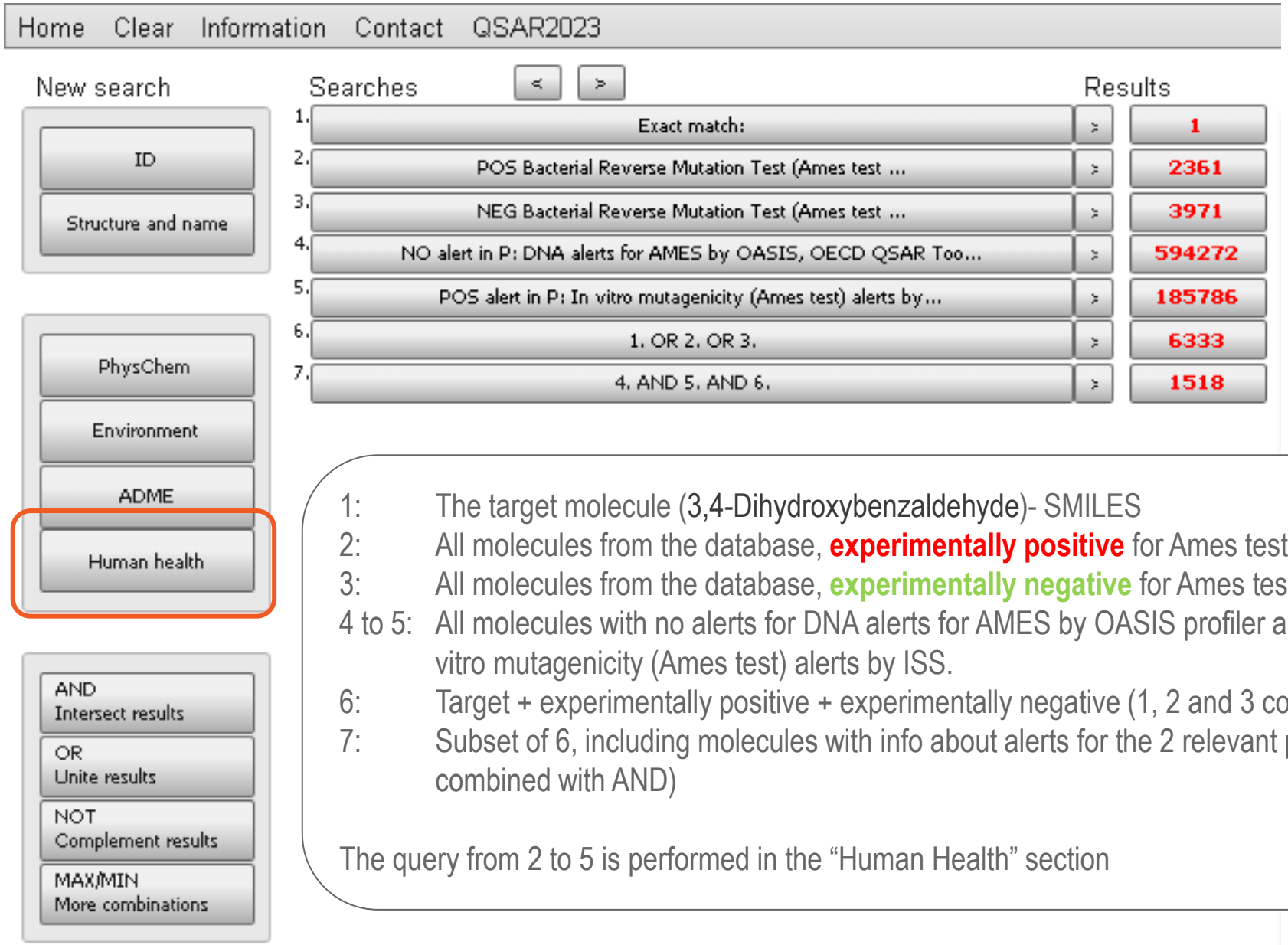


The generated overview **can be used** to prepare a statement **for supporting the reliability** of the (Q)SAR prediction for the target molecule.

Danish (Q)SAR Database: identification of similar molecules

- **Stepwise approach**
- Danish (Q)SAR Database **can be searched** for molecules, based on available **experimental data, (Q)SAR predictions, structural alerts**, etc., for the endpoint of interest
- For each query, a **list of molecules is retrieved**
- The lists **can be merged**, using logical operators such as **AND** or **OR**

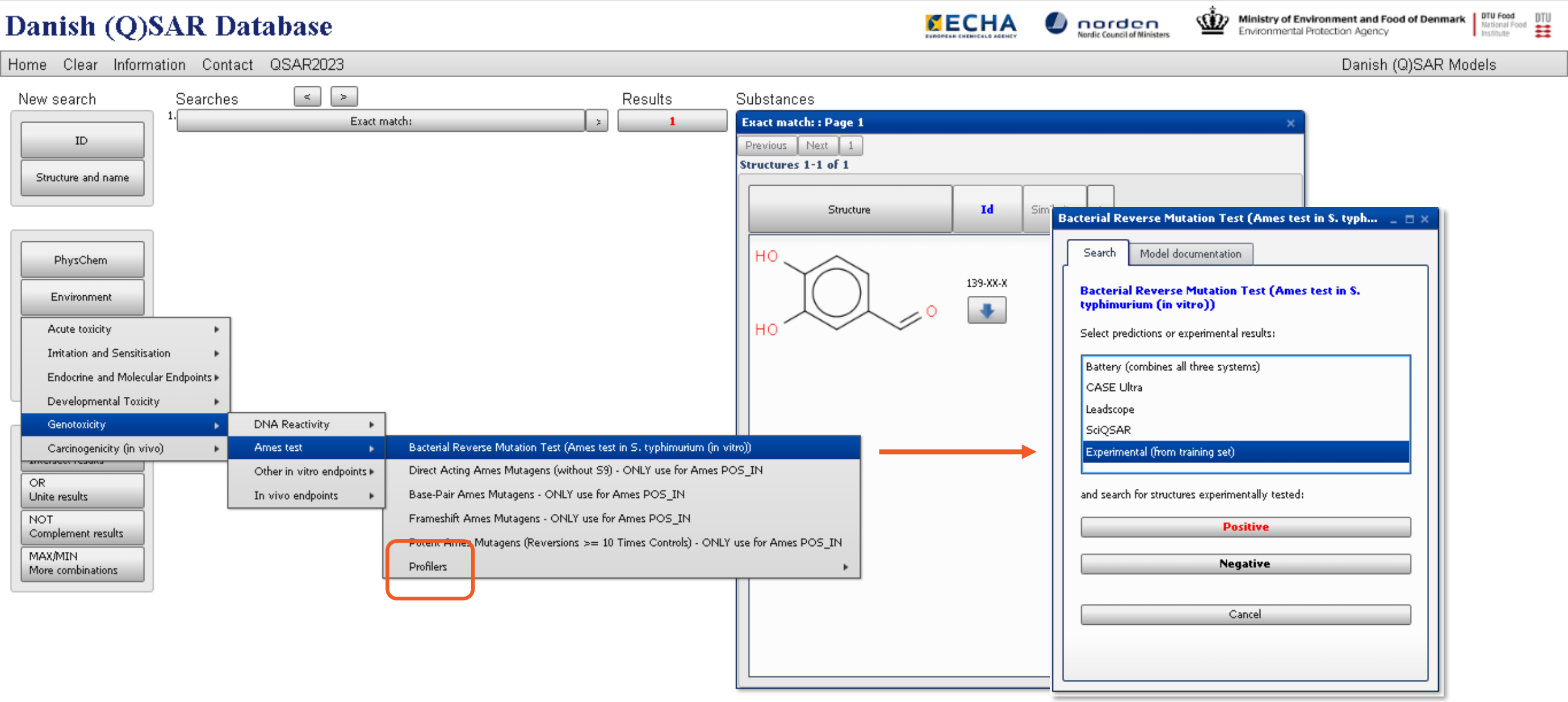
Danish (Q)SAR Database: identification of similar molecules



1: The target molecule (3,4-Dihydroxybenzaldehyde)- SMILES
2: All molecules from the database, **experimentally positive** for Ames test
3: All molecules from the database, **experimentally negative** for Ames test
4 to 5: All molecules with no alerts for DNA alerts for AMES by OASIS profiler and at least one alert for In vitro mutagenicity (Ames test) alerts by ISS.
6: Target + experimentally positive + experimentally negative (1, 2 and 3 combined with OR)
7: Subset of 6, including molecules with info about alerts for the 2 relevant profilers (6, 4 and 5 combined with AND)

The query from 2 to 5 is performed in the “Human Health” section

Danish (Q)SAR Database: identification of similar molecules



Danish (Q)SAR Database: identification of similar molecules

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Danish (Q)SAR Database

ECHA EUROPEAN CHEMICALS AGENCY · norden Nordic Council of Ministers · Ministry of Environment and Food of Denmark Environmental Protection Agency · DTU Food National Food Institute · DTU

Home | Clear | Information | Contact | QSAR2023 | Danish (Q)SAR Models

New search

- ID
- Structure and name
- PhysChem
- Environment
- ADME
- Human health
- AND Intersect results
- OR Unite results
- NOT Complement results
- MAX/MIN More combinations

Searches < >

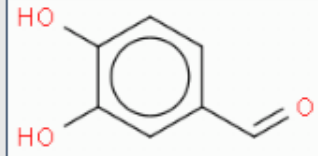
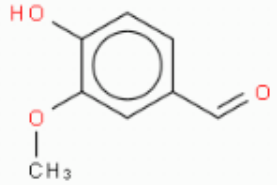
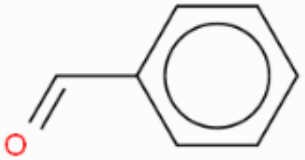
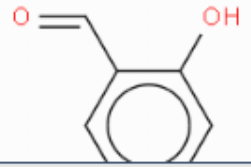
	Searches	Results
1.	Exact match:	1
2.	POS Bacterial Reverse Mutation Test (Ames test ...	2361
3.	NEG Bacterial Reverse Mutation Test (Ames test ...	3971
4.	NO alert in P: DNA alerts for AMES by OASIS, OECD QSAR Too...	594272
5.	POS alert in P: In vitro mutagenicity (Ames test) alerts by...	185786
6.	1. OR 2. OR 3.	6333
7.	4. AND 5. AND 6.	1518

Substances

4. AND 5. AND 6.: Page 1

Previous | Next | 1 | 2 | 3 | 152

Structures 1-10 of 1518

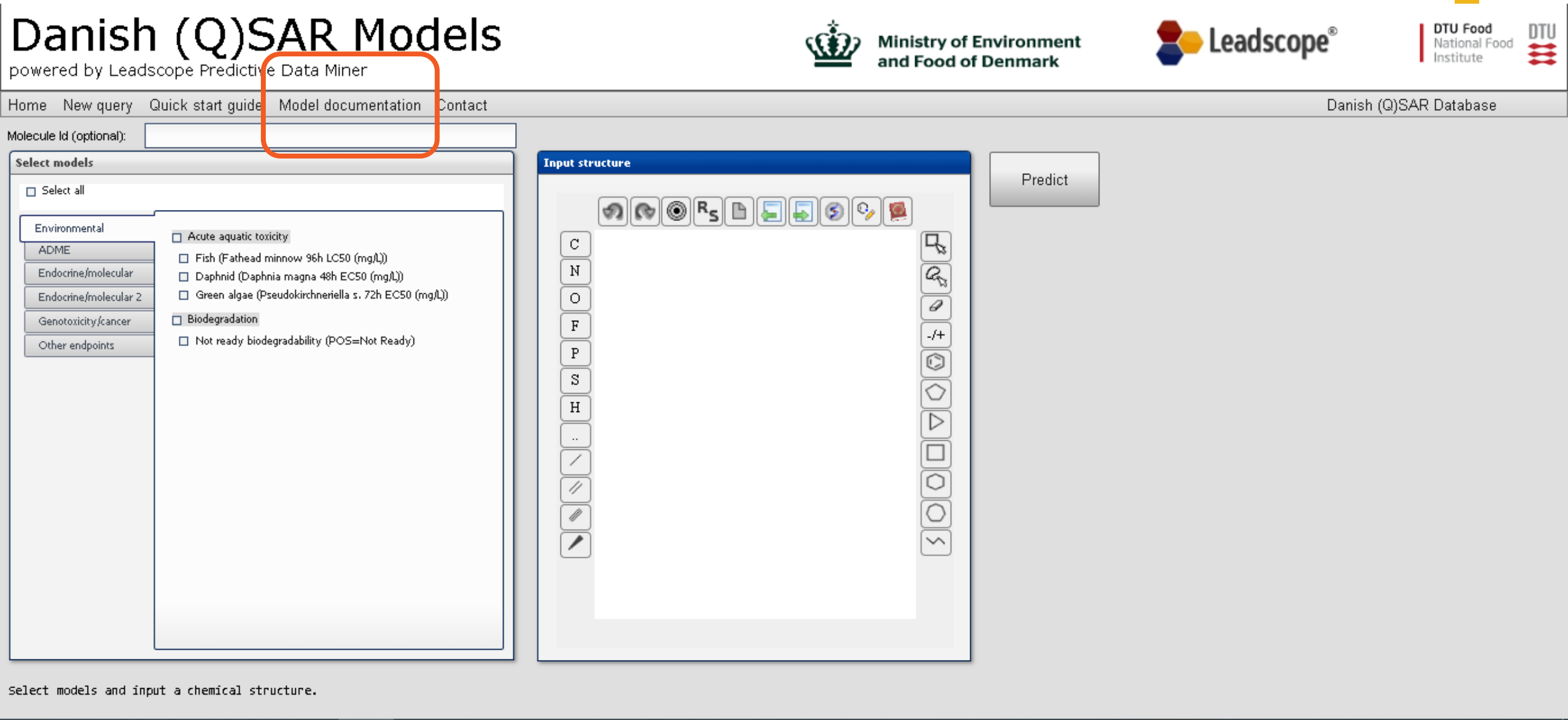
Structure	Id	Similarity	Bacterial Reve... Experimental	+
	XXX-XX-X	1.0		
	XXX-XX-X	0.886	NEG	
	XXX-XX-X	0.846	NEG	
	XX-XX-X	0.829	NEG	

Danish (Q)SAR Database: running predictions

Genotoxicity/Cancer
Ames test

Leadscope model

Danish (Q)SAR Database: running predictions



in vitro) NEW			(2*5-fold cross-validation)
Pregnane X Receptor (PXR) Activation (Human in vitro)	2176	Leadscope	Sens=89.1, Spec=98.6, BA=93.9 (2*5-fold cross-validation)
Pregnane X Receptor (PXR) Activation (Rat in vitro)	2330	Leadscope	Sens=86.5, Spec=97.4, BA=92.0 (2*5-fold cross-validation)
CYP3A4 Induction (Human in vitro)	2271	Leadscope	Sens=86.7, Spec=98.2, BA=92.5 (2*5-fold cross-validation)
Constitutive Androstane Receptor (CAR) activation at max. 20 µM	924	Leadscope	Sens=72.2, Spec=93.5, BA=82.8 (2*5-fold cross-validation)
Constitutive Androstane Receptor (CAR) activation at max. 50 µM	1903	Leadscope	Sens=78.4, Spec=91.4, BA=84.9 (2*5-fold cross-validation)
Constitutive Androstane Receptor (CAR) inhibition at max. 20 µM	1408	Leadscope	Sens=58.4, Spec=97.1, BA=77.8 (2*5-fold cross-validation)
Constitutive Androstane Receptor (CAR) inhibition at max. 50 µM	1870	Leadscope	Sens=72.4, Spec=91.6, BA=82.0 (2*5-fold cross-validation)
Bacterial reverse mutation test (Ames test in S. typhimurium in vitro)	4102	Leadscope	Sens=84.3, Spec=85.7, Conc=84.9
Chromosome aberrations in CHL cells (*in vitro*)	688	Leadscope	Sens=74.6, Spec=75.2, Conc=74.9
Mutations in thymidine kinase locus in mouse lymphoma cells (*in vitro*)	555	Leadscope	Sens=85.1, Spec=83.8, Conc=84.4
Mutations in HGPRT locus in CHO cells (*in vitro*)	239	Leadscope	Sens=81.7, Spec=78.4, Conc=80.5
Unscheduled DNA synthesis (UDS) in rat hepatocytes (*in vitro*)	415	Leadscope	Sens=74.1, Spec=70.1, Conc=72.4
Syrian hamster embryo (SHE) cell transformation (*in vitro*)	363	Leadscope	Sens=71.6, Spec=76.5, Conc=74.5
Sex-linked recessive lethal (SLRL) test in Drosophila m. (*in vivo*)	367	Leadscope	Sens=79.1, Spec=80.3, Conc=79.6

4. Defining the algorithm

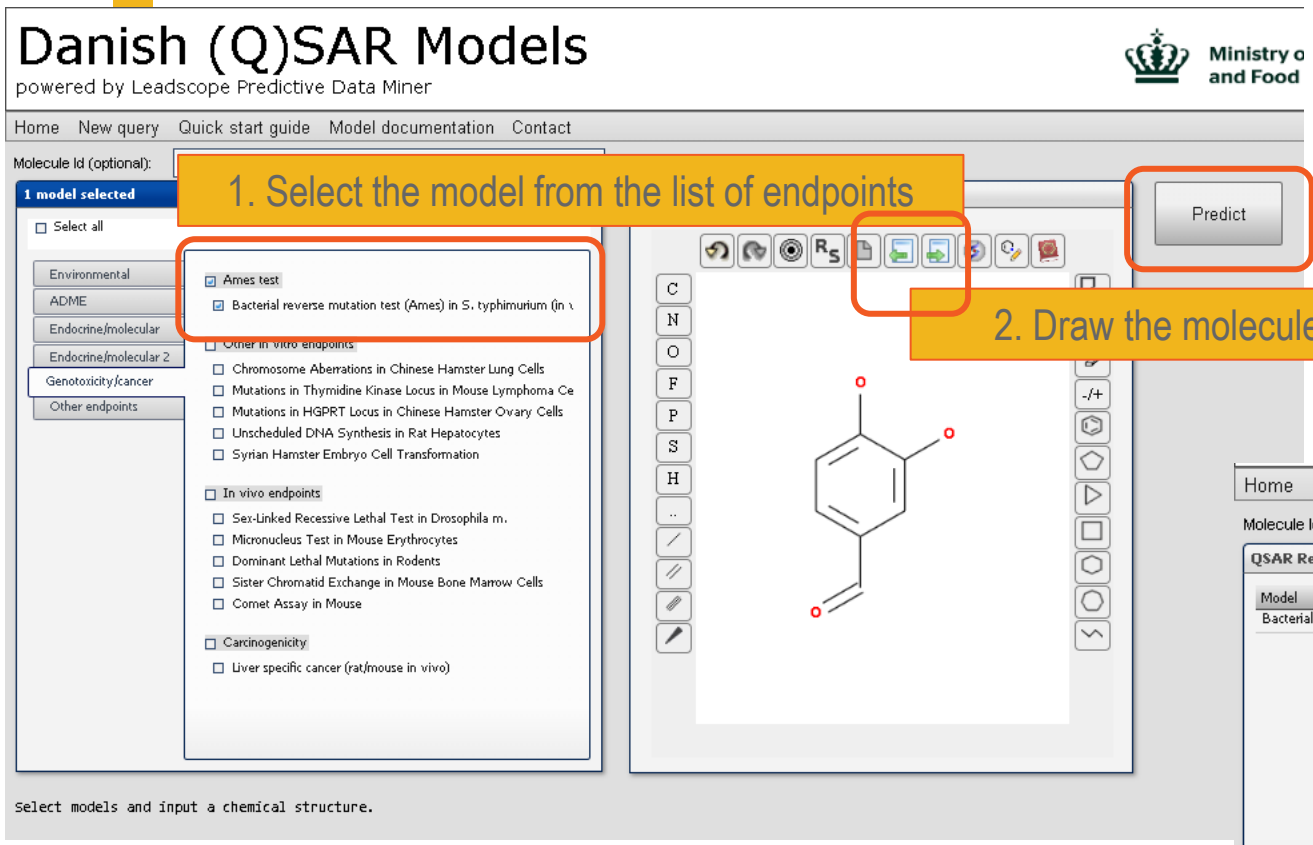
4.1 Type of model

A categorical (Q)SAR model based on structural features and numeric molecular descriptors.

4.2 Explicit algorithm

This is a categorical (Q)SAR model made by use of partial logistic regression (PLR). The model is a composite model consisting of 2 submodels, using all the negatives (1803 chemicals) in each of these and different sub-sets of the positives (see 4.5). The specific implementation is proprietary within the Leadscope software.

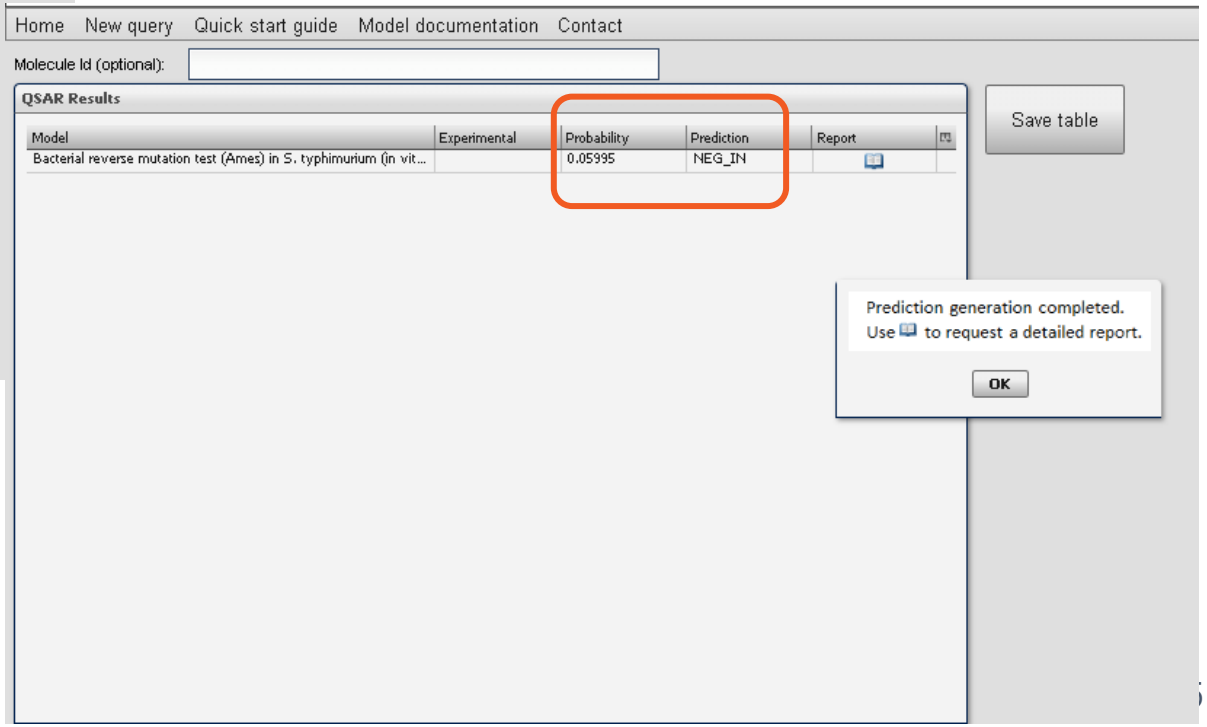
Danish (Q)SAR Database: running QSAR model



1. Select the model from the list of endpoints

2. Draw the molecule/paste the SMILES

3. Click predict



The target chemical is predicted as Positive or Negative with respect to the Ames endpoint based on the **probability** associated with the **prediction** generated **by** a partial logistic regression **(PLR) model**. In this case, the model returns a probability of **0.05995**, leading to a negative prediction.

Danish (Q)SAR Database: running QSAR model

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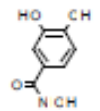
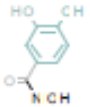
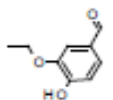
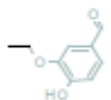
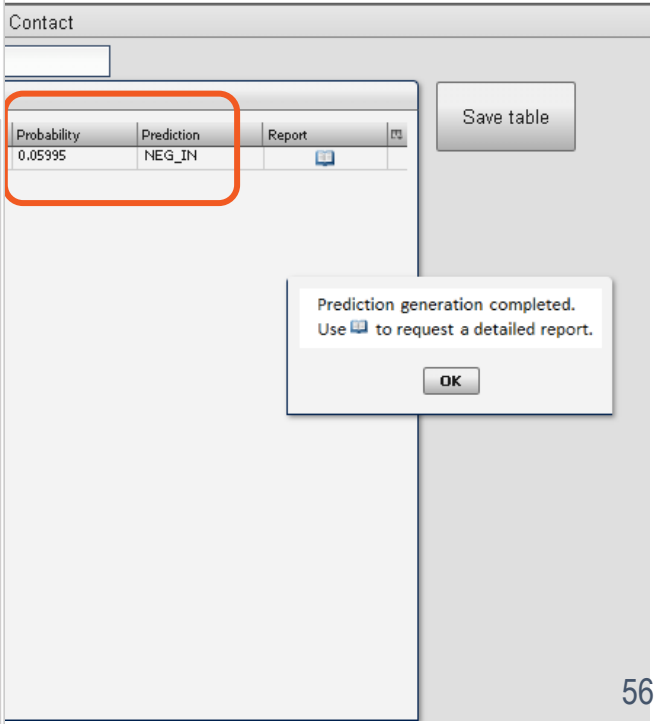
Model Features:
Danish_QSAR_DB_Bacterial_Reverse_Mutation_Test_Ames_mutagenicity_(S.typhimurium)_QSARmodels.food.dtu.dk v1

Model Features: DKDB_Ames_Mutagenicity_Multiple_Model-1 v1

Model Features: DKDB_Ames_Mutagenicity_Multiple_Model-2 v1

Analog Structures from Model Training Set

Structure	Similarity	Experimental Value - Danish_QSAR_DB_Bacterial_Reverse_Mutation_Test_Ames_mutagenicity_(S.typhimurium)_QSARmodels.food.dtu.dk	Danish_QSAR_DB_Bacterial_Reverse_Mutation_Test_Ames_mutagenicity_(S.typhimurium)_QSARmodels.food.dtu.dk - Highlights	Danish_QSAR_DB_Bacterial_Reverse_Mutation_Test_Ames_mutagenicity_(S.typhimurium)_QSARmodels.food.dtu.dk - Call	Danish_QSAR_DB_Bacterial_Reverse_Mutation_Test_Ames_mutagenicity_(S.typhimurium)_QSARmodels.food.dtu.dk - Prob.
 DKDB_2018_2561	0.7	Positive	 DKDB_2018_2561	Negative	0.287
	0.62	Negative		Negative	0.0271



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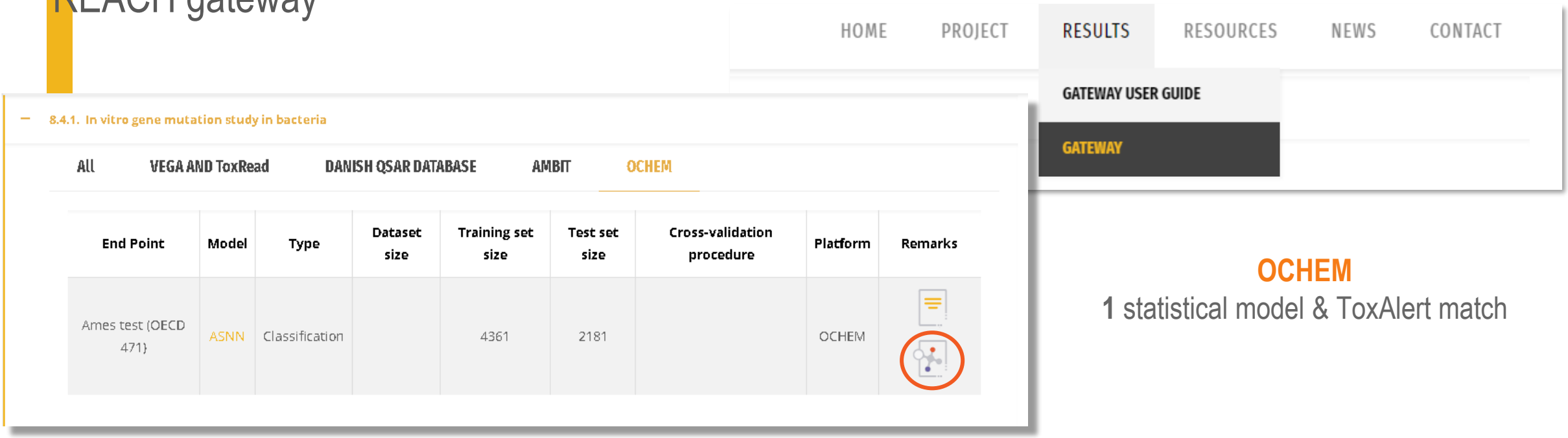
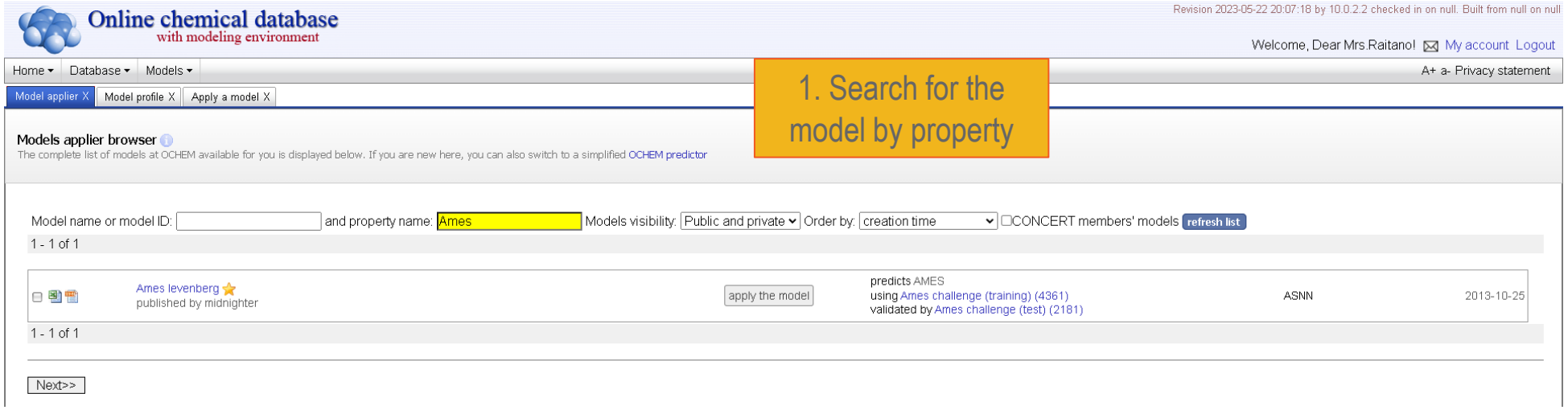
Checking the availability of the tools for in vitro gene mutation in bacteria in the CONCERT REACH gateway



OCHEM

1 statistical model & ToxAlert match



OCHEM: running model & ToxAlerts

CONCERTREACH
CONCERTING EXPERIMENTAL DATA AND IN SILICO MODELS FOR REACH

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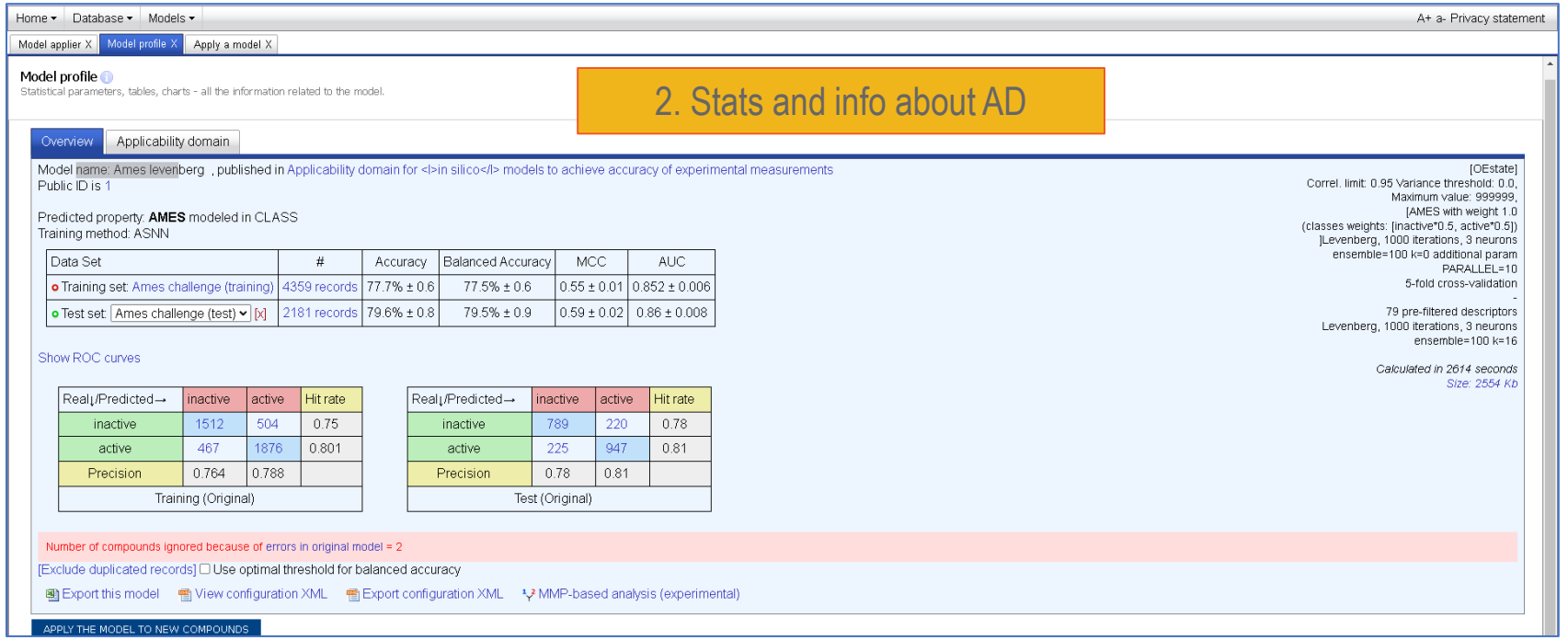
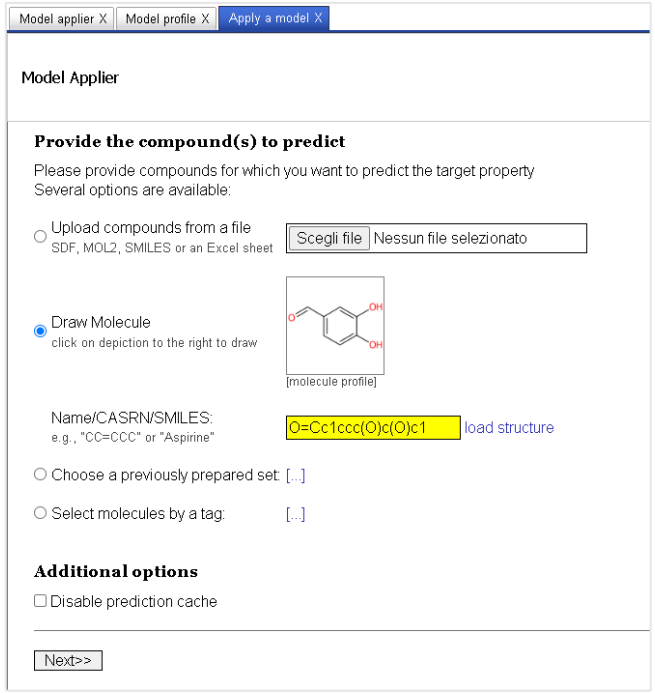


3. Paste the SMILES



OCHEM: running model & ToxAlerts

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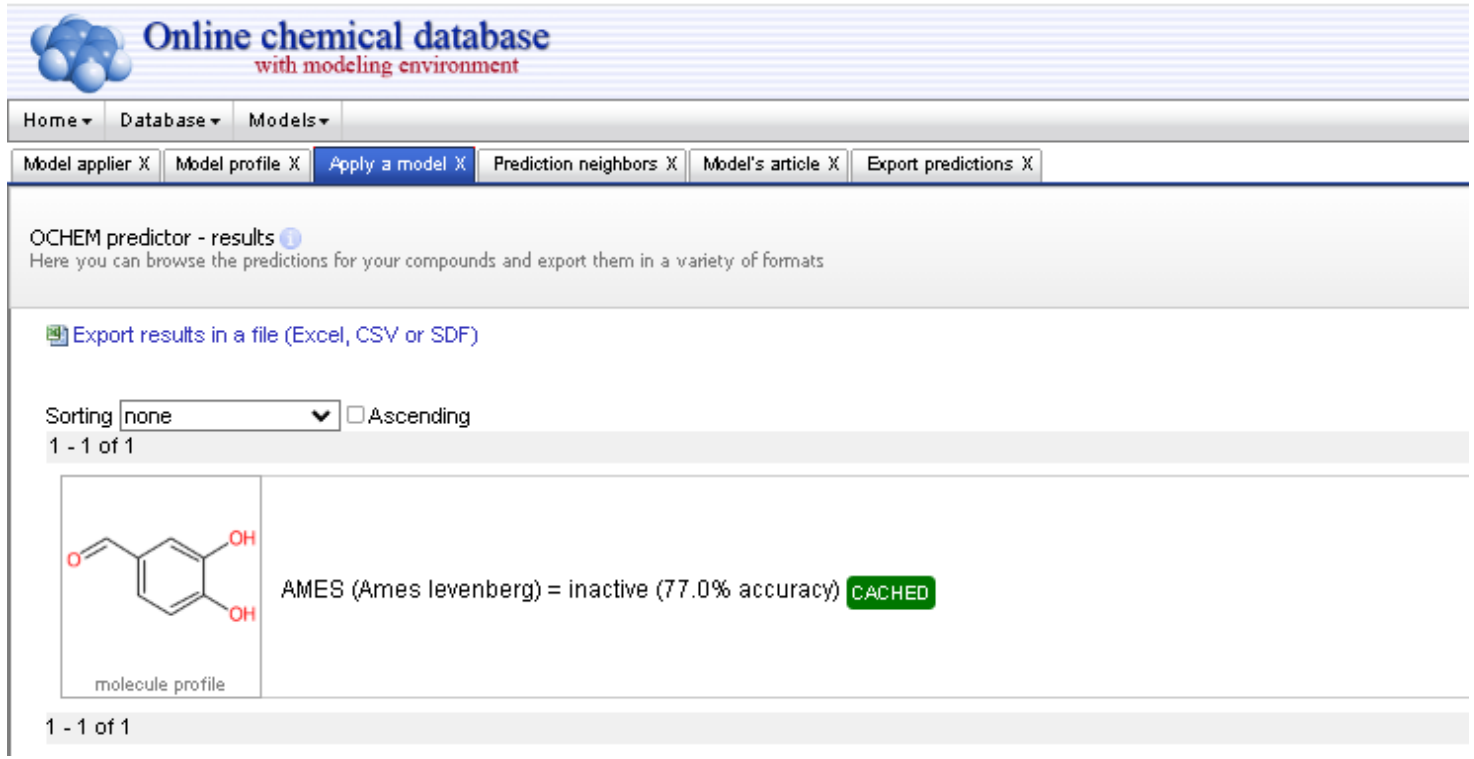


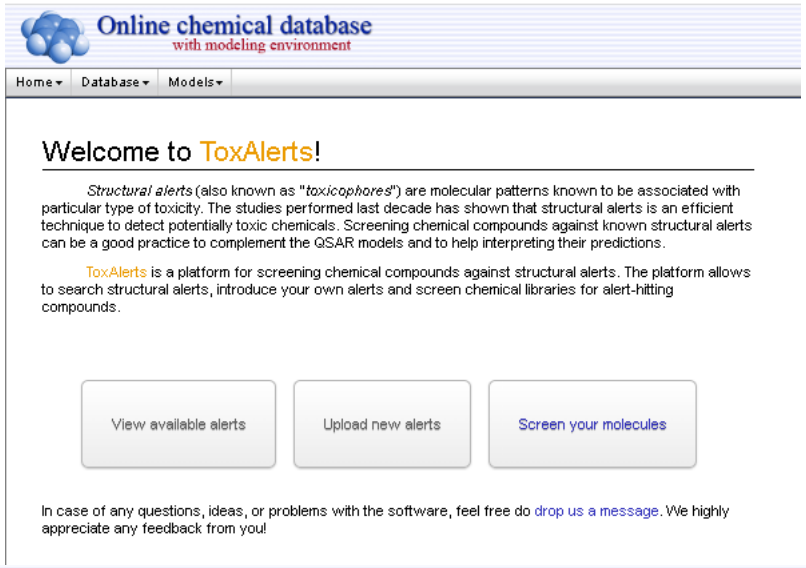
4.Online result

5. Export result: excel, CSV or SDF

SMILES	CASRN	EXTERNAL	N	NAME	ARTICLEID	PUBMEDID	PAGE	TABLE	ERROR	AMES {predicted by ochem.eu/model/1}	Numeric prediction for AMES {predicted by ochem.eu/model/1}	PROB-STD{AMES by Ames levenberg}	ASNN-STDEV{AMES by Ames levenberg}	CLASS-LAG{AMES by Ames levenberg}	ASNN-CORREL{AMES by Ames levenberg}	Estimated accuracy{AMES predicted by Ames levenberg}	APPLICABILITY_DOMAIN	
OC1=CC=C(C=O)C=C1O					-	-	-	-		inactive	0.2437	0.18	0.09	0.49	0.26	0.77	TRUE	-

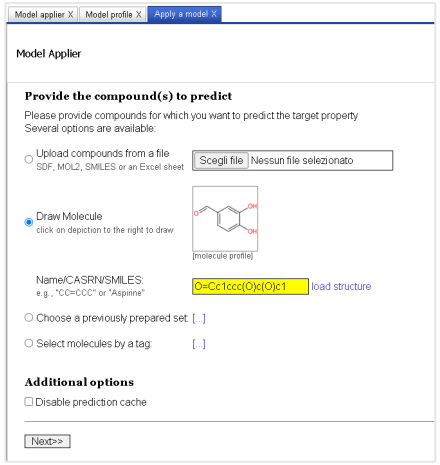
OCHEM: running model & **ToxAlerts**

117 ToxAlerts for Genotoxic carcinogenicity, mutagenicity



Online chemical database
with modeling environment

Paste the SMILES



Home | Database | Models | A+ a- Privacy statement

Model templates X | Screen compounds against alerts X

ToxAlerts: Screening results
The compounds that matched any alerts grouped by endpoints, publications and by alerts themselves

X

ENDPOINTS

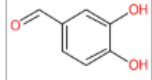
Skin sensitization	1 compounds
Genotoxic carcinogenicity, mutagenicity	1 compounds
Reactive, unstable, toxic	1 compounds
Acute Aquatic Toxicity	1 compounds
Potential electrophilic agents	1 compounds
Idiosyncratic toxicity (RM formation)	1 compounds
Custom filters	1 compounds
Extended Functional Groups (EFG)	1 compounds
Promiscuity	1 compounds
PAINS compounds	1 compounds
Biodegradable compounds	1 compounds
Nonbiodegradable compounds	1 compounds
Non-genotoxic carcinogenicity	1 compounds
UNIFAC	1 compounds
Glaxo Wellcome	1 compounds
Dundee	1 compounds
LINT	1 compounds
Inpharmatica	1 compounds
MLSMR	1 compounds
SureChEMBL	1 compounds
SMARTCyp	1 compounds

PUBLICATIONS

1994 Barratt	1 compounds
2004 Gerner	1 compounds
1994 Payne	1 compounds
2008 Benigni	1 compounds
2008 Enoch	1 compounds
2011 ChemDiv	1 compounds
1990 Hermens	1 compounds
1992 Verhaar,H.J.M.	1 compounds
2011 Enoch	1 compounds
2005 Kalgutkar	1 compounds
2011 Life_Chemicals	1 compounds
2011 Enamine	1 compounds
2011 "Ontario"_filters	1 compounds
2011 Maybridge	1 compounds
2012 Tetko, I.V.	1 compounds
2005 CheckMol	1 compounds
2015 Salmina, ES	1 compounds
2006 Pearce, BC	1 compounds
2010 Baell, JB	1 compounds
2003 Environment	1 compounds
2013 Benigni, R	1 compounds
1991 Hansen	1 compounds
2003 Wittig	1 compounds
1999 Hann	1 compounds
2008 Brenk	1 compounds
2019 Blake JF	1 compounds
2017 Inpharmatica	1 compounds

View records for the filtered compounds | Tag the 1 filtered molecules | Export the screening results

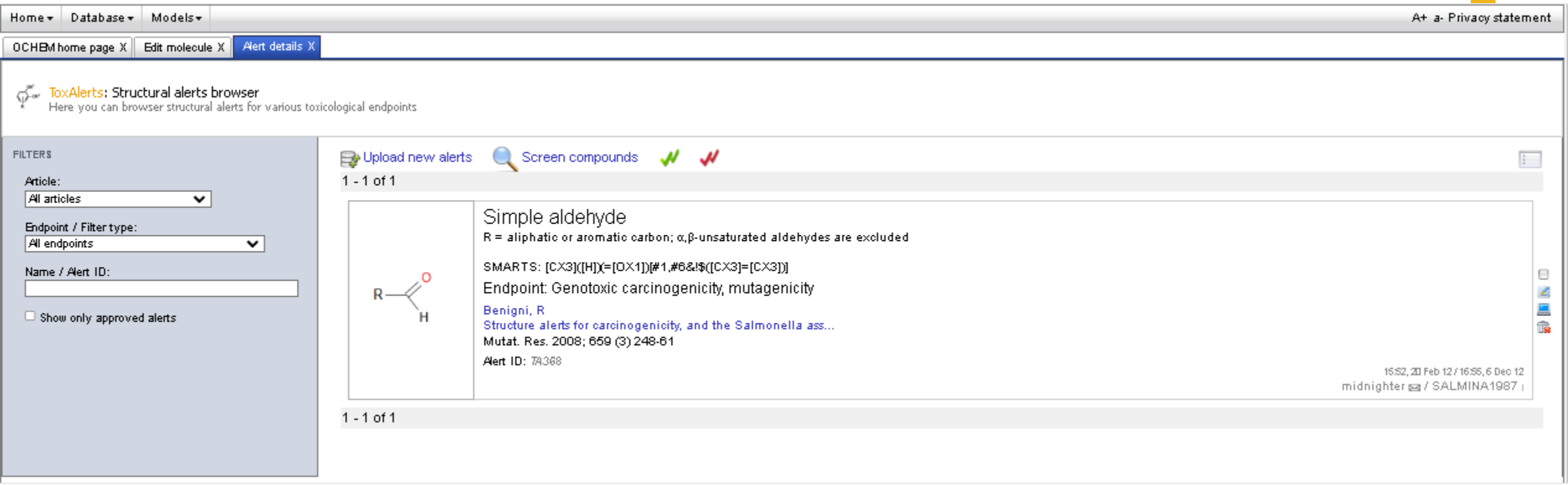
1 - 1 of 1



molecule profile

Catechols and O-alkyl precursors (for Skin sensitization in 3894 Barratt)
Aldehydes (for Skin sensitization in 3894 Barratt)
Aldehydes (for Skin sensitization in 3904 Gerner)
Catechols, resorcinols, hydroquinones (for Skin sensitization in 3904 Gerner)
Aldehydes and precursors (for Skin sensitization in 3894 Payne)
Catechols (for Skin sensitization in 3894 Payne)
Di- or polyhydroxy aromatic compounds and their precursors (for Skin sensitization in 3894 Payne)
1,2-Dihydroxy aromatic compounds (for Skin sensitization in 3894 Payne)
Simple aldehyde (for Genotoxic carcinogenicity, mutagenicity in 3908 Benigni)
Aromatic aldehydes (for Skin sensitization in 3908 Enoch)
Ortho-disubstituted benzenes (for Skin sensitization in 3908 Enoch)
Aldehydes (for Reactive, unstable, toxic in 3911 ChemDiv)
Ortho-substituted phenols, primary and secondary amines (for Skin sensitization in 3908 Enoch)
Aldehydes (for Acute Aquatic Toxicity in 3890 Hermens)
Aldehydes (for Acute Aquatic Toxicity in 3892 Verhaar,H.J.M.)
Hydroquinones (for Potential electrophilic agents in 3911 Enoch)
Mono-aldehydes (for Potential electrophilic agents in 3911 Enoch)
Ortho- or parahydroquinones (for Idiosyncratic toxicity (RM formation) in 3905 Kalgutkar)
Aldehydes (for Reactive, unstable, toxic in 3911 Life_Chemicals)
Hydroquinone (for Reactive, unstable, toxic in 3911 Life_Chemicals)
Aldehydes (for Reactive, unstable, toxic in 3911 Enamine)
C, N, O, P and S atoms in unusual valence states (for Reactive, unstable, toxic in 3911 Enamine)
Aldehydes (for Reactive, unstable, toxic in 3911 "Ontario"_filters)
Catechols (for Reactive, unstable, toxic in 3911 "Ontario"_filters)
Aldehydes (including aminoformyl moieties) (for Reactive, unstable, toxic in 3911 Maybridge)
Simple anilines and phenols (for Reactive, unstable, toxic in 3911 Maybridge)
Atoms supported in ALOGPS program (for Custom filters in 3912 Tetko, I.V.)
Organic chemistry atoms (for Custom filters in 3912 Tetko, I.V.)
Carbonyl compouns: aldehydes or ketones (for Extended Functional Groups (EFG) in 3905 CheckMol)
Aldehydes (for Extended Functional Groups (EFG) in 3905 CheckMol)
Hydroxy compounds: alcohols or phenols (for Extended Functional Groups (EFG) in 3905 CheckMol)
Phenols (for Extended Functional Groups (EFG) in 3905 CheckMol)
Diphenols (for Extended Functional Groups (EFG) in 3915 Salmina, ES)
Aromatic compounds (for Extended Functional Groups (EFG) in 3905 CheckMol)
Arenes (for Extended Functional Groups (EFG) in 3915 Salmina, ES)
Nonmetals (for Extended Functional Groups (EFG) in 3915 Salmina, ES)
Chalcogens (oxygen group) (for Extended Functional Groups (EFG) in 3915 Salmina, ES)
Tetragens (carbon group) (for Extended Functional Groups (EFG) in 3915 Salmina, ES)
aldehyde (for Promiscuity in 3906 Pearce, BC)
Catechol_A (for PAINS compounds in 3910 Baell, JB)
1,2 – Diphenols (for Extended Functional Groups (EFG) in 3905 CheckMol)
Alcohols (for Biodegradable compounds in 3903 Environment)
Aldehyde (for Biodegradable compounds in 3903 Environment)
MoreThanTwoHydroxyOnAromaticRing (for Nonbiodegradable compounds in 3903 Environment)
Molecules with at least one carbon (for Custom filters in 3912 Tetko, I.V.)
Simple aldehyde (for Non-genotoxic carcinogenicity in 3913 Benigni, R)
3 - Aromatic carbon (for UNIFAC in 3891 Hansen)
8 - Aromatic carbon-alcohol (for UNIFAC in 3891 Hansen)
10 - Aldehyde (for UNIFAC in 3891 Hansen)
10 - ACH (3 - Aromatic carbon) (for UNIFAC in 3903 Wittig)
11 - AC (3 - Aromatic carbon) (for UNIFAC in 3903 Wittig)
18 - ACOH (8 - Aromatic carbon-alcohol) (for UNIFAC in 3903 Wittig)
21 - CHO (10 - Aldehyde) (for UNIFAC in 3903 Wittig)
A33 - phenol (for Glaxo Wellcome in 3899 Hann)

OCHEM: running model & **ToxAlerts**



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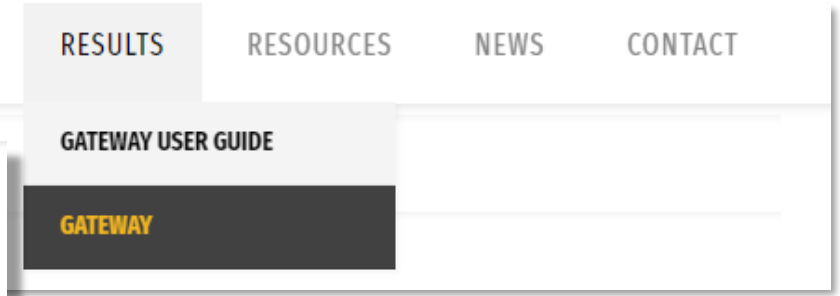
Checking the availability of the tools for in vitro gene mutation in bacteria in the CONCERT REACH gateway



8.4.1. In vitro gene mutation study in bacteria

All | VEGA AND ToxRead | DANISH QSAR DATABASE | AMBIT | OCHEM

End Point	Model	Type	Dataset size	Training set size	Test set size	Cross-validation procedure	Platform	Remarks
Ames test (OECD 471)	ASNN	Classification		4361	2181		OCHEM	

OCHEM

1 statistical model & ToxAlert match

All | VEGA AND ToxRead | DANISH QSAR DATABASE | AMBIT | OCHEM

End Point	Model	Type	Dataset size	Training set size	Test set size	Cross-validation procedure	Platform	Remarks
TOX 7.6.1. Genetic toxicity in vitro	Dataset		50366				AMBIT	

AMBIT

1 dataset

Using AMBIT database and results analysis

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LRI AMBIT2 Read Across tool - new version!

Chemical substance database with read across workflow : IUCLID6 support; featuring OpenFoodToxData and VEGA integration

Simple search

Enter chemical name, identifiers, SMILES, InChI

formaldehyde Search

Advanced: Structure search | Search substances by identifiers | Search substances by endpoint data | Free text search

Legal notice:

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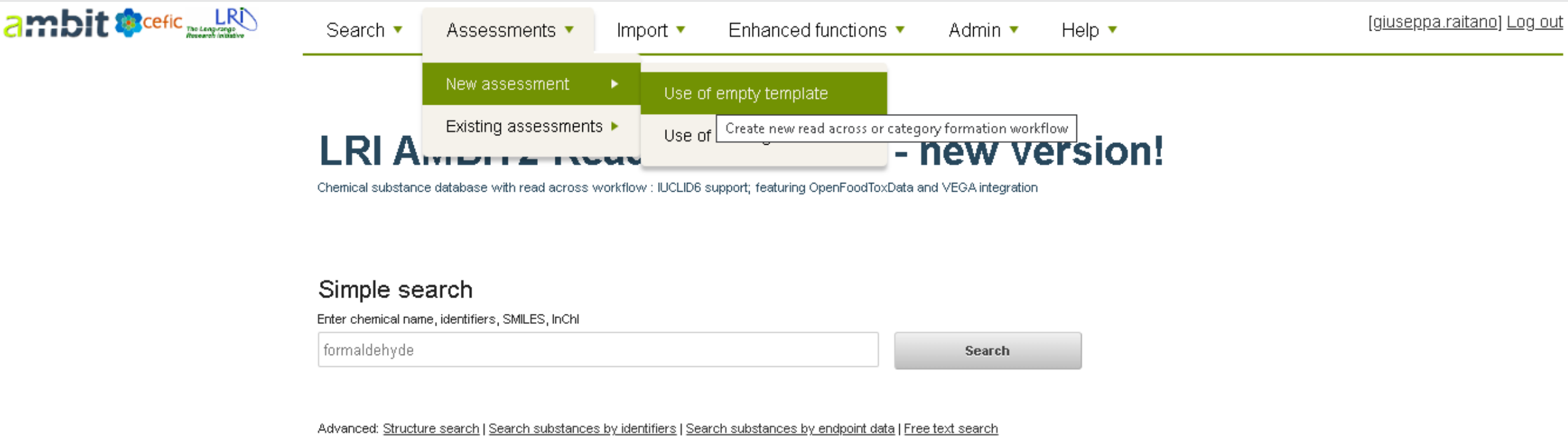

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Home 〉 All assessments 〉

1. Assessment identifier

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

Assessment title* :	3,4-Dihydroxybenzaldehyde
Owner* :	Nelly
Purpose* :	QSAR2023 course
Version :	?.?
Version start date :	
Version last modified on :	
Status :	
Assessment code* :	read across1
Assessment Doclink(s)* :	local
Assessment ID :	
Users with write access :	Save
Users with read access :	Save

Start

Automatic generation of the ID assessment

Five steps assessment

category formation. REACH guidance

The assessment workflow is organized in five main tabs:

1. Assessment identifier
2. Collect structures
3. Endpoint data used
4. Assessment details
5. Report

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Home 〉 All assessments 〉

2. Collect structures, for the **target** as well as for the **analogues** and **category members**

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

Collect structures | List collected

Search for the target: CAS N, SMILES, drawing etc..

Search

Exact structure | Similarity | Substructure | URL

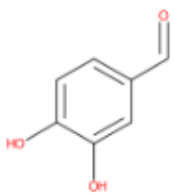
target

Enable fragment search

O=Cc1ccc(O)c(O)c1

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

Filter...

	Diagram	CasRN	EC number	Names	Rationale
T S SM		139-85-5	205-377-7	3,4-Dihydroxybenzaldehyde | 3,4-dihydroxybenzaldehyde	Reason for selection_

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Home 〉 All assessments 〉

2. Collect structures, for the target as well as for the analogues and category members

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

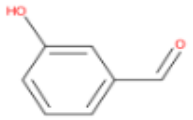
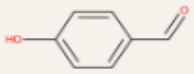
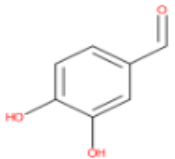
Collect structures | List collected

Search

Exact structure | Similarity | Substructure | URL

Only hits with substance data 0.8 O=Cc1ccc(O)c(O)c1

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

	Diagram	CasRN	EC number	Names	Similarity	Rationale
T S CM		100-83-4	202-892-9	| 3-hydroxybenzaldehyde | Benzaldehyde, 3-hydroxy-	0.91	
T S CM		123-08-0	204-599-1	4-Hydroxybenzaldehyde | 4-hydroxybenzaldehyde	0.85	
T S CM		139-85-5	205-377-7	3,4-Dihydroxybenzaldehyde | 3,4-dihydroxybenzaldehyde	1	

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3. Endpoint data used

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

Search substance(s) | Selection of endpoints

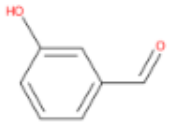
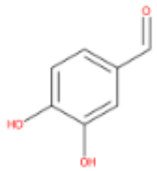
Expand all | Collapse all

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

Filter...

B. Select the endpoint of interest

A. Expand all the info about the chemicals and then select

	Diagram	CasRN	EC numbe		Rational	
- 1 -		100-83-4	202-892-9	hydroxybenzaldehyde | Benzaldehyde, 3-hydroxy-		
- 2 -		123-08-0	204-599-1	4-Hydroxybenzaldehyde | 4-hydroxybenzaldehyde		S
- 3 -		139-85-5	205-377-7	3,4-Dihydroxybenzaldehyde | 3,4-dihydroxybenzaldehyde		T

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3. Endpoint data used

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

Search substance(s) | Selection of endpoints

☑ Show all endpoints

Filter...

▸ P-Chem — select all unselect all [91169]

▸ Env Fate — select all unselect all [55690]

▸ Eco Tox — select all unselect all [115597]

▾ Tox — select all unselect all [228703]

Showing 18 endpoint(s) (1 to 18)

☐	7.2.1. Acute toxicity - oral	[26076]
☐	7.2.2. Acute toxicity - inhalation	[9213]
☐	7.2.3. Acute toxicity - dermal	[11852]
☐	7.3.1. Skin irritation / Corrosion	[21694]
☐	7.3.2. Eye irritation	[18430]
☐	7.4.1. Skin sensitisation	[16404]
☐	7.5.1. Repeated dose toxicity - oral	[20212]
☐	7.5.2. Repeated dose toxicity - inhalation	[6657]
☐	7.5.3. Repeated dose toxicity - dermal	[2139]
☑	7.6.1. Genetic toxicity in vitro	[50366]
☐	7.6.2. Genetic toxicity in vivo	[10232]
☐	7.7. Carcinogenicity	[6288]

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4. Assessment details

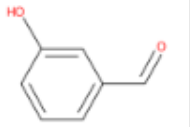
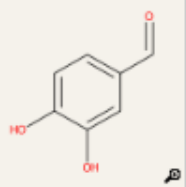
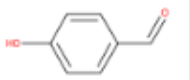
Assessment identifier | Collect structures | Endpoint data used | Assessment details | Report

Initial matrix | Working matrix | Final matrix

1) Initial matrix: all the available info is listed
2) Working matrix: it is possible to add or eliminate data
3) Final matrix

Identifiers | TOX

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

Substance Name	I5UUID	Data source	Tag	Diagram	Constitu	7.6.1
3-hydroxybenzaldehyde	ECHA-8a...	-	S		Benzaldeh hydroxy-	Structural Alert for S. typhimurium mutagenicity = Y Potential S. typhimurium TA100 mutagen based on QSAR = NO Mutagenicity (Ames test) model (CAESAR) - prediction = NON-Mutagenic No alerts for S. typhimurium mutagenicity = NO Unlikely to be a S. typhimurium TA100 mutagen based on QSAR = NO
3,4-DIHYDROXYBENZALDEHYDE	FOOD-64...	OpenFoodToxData	T		3,4-Dihydroxy	Structural Alert for S. typhimurium mutagenicity = YES Potential S. typhimurium TA100 mutagen based on QSAR = NO Mutagenicity (Ames test) model (CAESAR) - prediction = NON-Mutagenic No alerts for S. typhimurium mutagenicity = NO Unlikely to be a S. typhimurium TA100 mutagen based on QSAR = NO Negative (EFSA opinion) Negative (EFSA opinion) Negative (EFSA opinion) Negative (EFSA opinion) Negative (EFSA opinion)
4-HYDROXYBENZALDEHYDE	FOOD-a4...	OpenFoodToxData	S		4-Hydroxybe	Structural Alert for S. typhimurium mutagenicity = YES Potential S. typhimurium TA100 mutagen based on QSAR = NO Mutagenicity (Ames test) model (CAESAR) - prediction = NON-Mutagenic No alerts for S. typhimurium mutagenicity = NO

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5. Report

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Create Word file

Ambit Assessment Report

3,4-Dihydroxybenzaldehyde

Author: Nelly
Date: 03.06.2023
Assessment code: ecd6a503-83e3-40c8-a1f2-8bca2eee1036
Purpose: QSAR2023 course

1. Assessment Identifiers

Assessment title:	3,4-Dihydroxybenzaldehyde
Owner:	Nelly
Purpose:	QSAR2023 course
Version:	1
Status:	draft
Version start date:	03.06.2023
Version last modified on:	03.06.2023
Published:	draft
Assessment code:	read across1
Assessment DocLink:	local

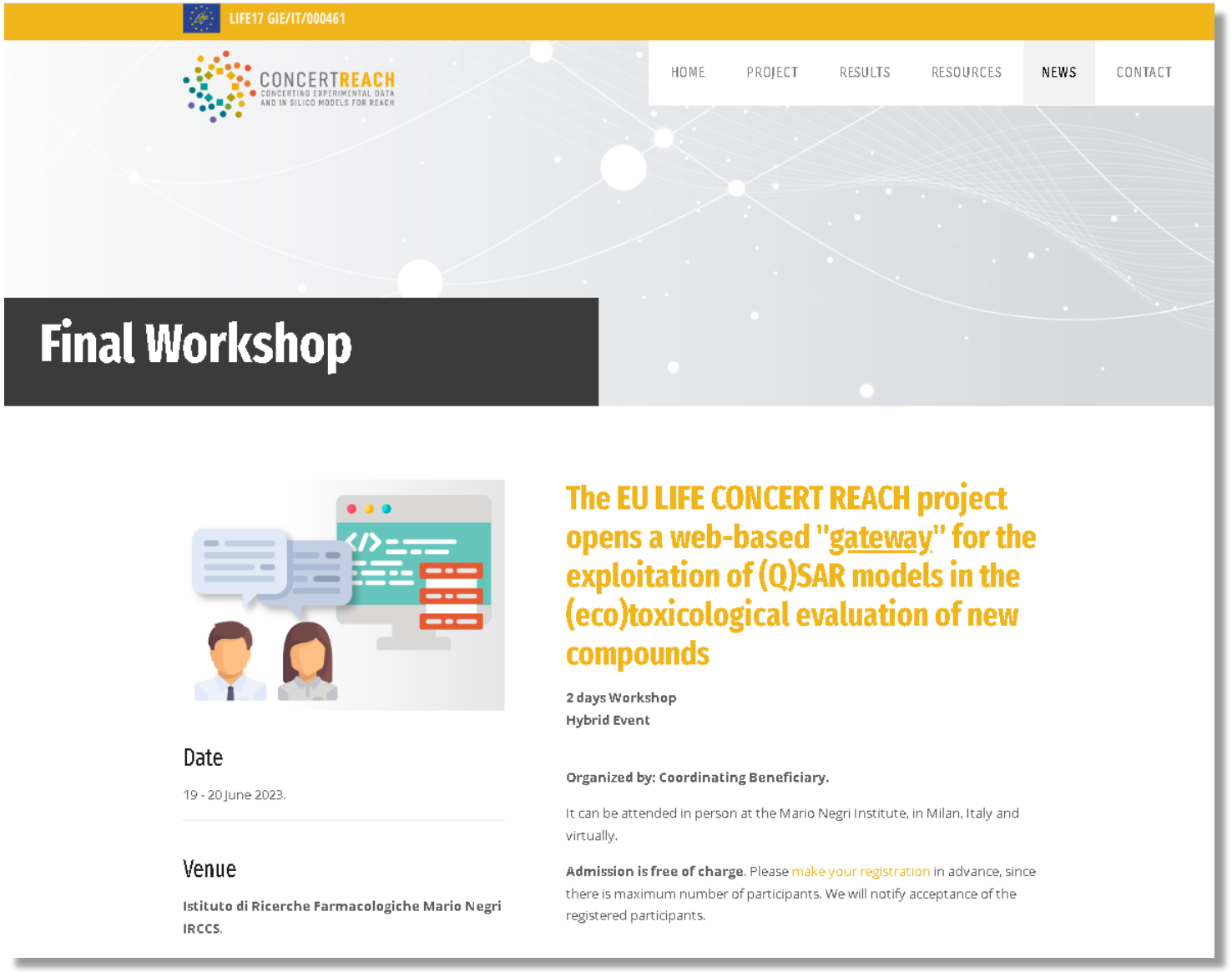
2-day workshop

Monday 19/06, full day

Workshop presentations

Tuesday 20/06, morning

Training sessions



https://www.life-concertreach.eu/final-workshop-19-and-20-june-2023/

THANKS

Does anyone have any questions?
https://www.life-concertreach.eu/

Acknowledgment:
My colleagues,
All the partners of the project,
Rodolfo Gonella Diaza from Knoell

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ISTITUTO DI RICERCHE FARMACOLOGICHE MARIO NEGRI · IRCCS
giuseppa.raitano@marionegri.it

Target molecule

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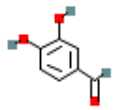
SEARCH FOR

3,4-Dihydroxybenzaldehyde

Treating this as a text search.

BEST MATCH



3,4-Dihydroxybenzaldehyde; Protocatechualdehyde; 139-85-5; PROTOCATECHUIC ALDEHYDE; Rancinamycin IV; Benzaldehyde, 3,4-Dihydroxy-; 4-Formyl-1,2-Dihydroxybenzene; 3,4-Dihydroxybenzenecarbonal; ...

Compound CID: 8768

MF: $C_7H_6O_3$ **MW:** 138.12g/mol

IUPAC Name: 3,4-dihydroxybenzaldehyde

Isomeric SMILES: C1=CC(=C(C=C1C=O)O)O

InChIKey: IBGBGRVKPALMCQ-UHFFFAOYSA-N

InChI: InChI=1S/C7H6O3/c8-4-5-1-2-6(9)7(10)3-5/h1-4,9-10H

Create Date: 2005-03-26

Summary Similar Structures Search Related Records

01

Welcome to the VEGA HUB

Offering a family of tools to evaluate chemical hazard: VEGA, ToxRead, SWAN, VERA, ToxWeight, ToxDelta, and JANUS.

VEGA is the QSAR software with tens of models for individual properties.

Do you need assistance for a property prediction ?

CONTACT US

Our philosophy

The In silico methods can be very useful, if correctly applied

We want to enhance

We want to enhance the capability of the in silico methods to assess the properties of chemical substances.

We sustain

We sustain the correct use of in silico methods

We provide

We provide computer tools to support the human experts

We support

We support the evaluation of chemicals safety

https://www.vegahub.eu/download/

01

VEGA QSAR

Try out VEGA QSAR and its features

All the VEGA models are also available in a unique stand-alone application.

With the VEGA application you can easily execute all the models on your local machine without sending any information to our server. VEGA is the ideal application for batch processing large dataset. VEGA can be installed and used on any operative system supporting JAVA technology (for any doubt please visit JAVA website).

Free download VEGA QSAR Application

Visit the link to download the application.

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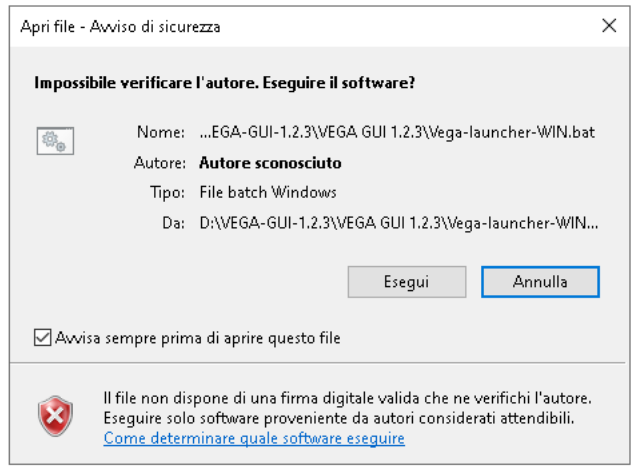
Ultima modifica
Tipo
Dimensione
jdk-11.0.6
24/05/2023 09:18
Cartella di file
README
24/05/2023 09:17
Documento di testo
2 KB
Vega-GUI-1.2.3
24/05/2023 09:18
Executable Jar File
254,025 KB
Vega-launcher-LINUX.sh
24/05/2023 09:18
File SH
1 KB
Vega-launcher-WIN
24/05/2023 09:18
File batch Windows
1 KB


Apri file - Avviso di sicurezza
Impossibile verificare l'autore. Eseguire il software?
Nome: ...EGA-GUI-1.2.3\VEGA GUI 1.2.3\Vega-launcher-WIN.bat
Autore: Autore sconosciuto
Tipo: File batch Windows
Da: D:\VEGA-GUI-1.2.3\VEGA GUI 1.2.3\Vega-launcher-WIN...
Esegui
Annulla
Avvisa sempre prima di aprire questo file
Il file non dispone di una firma digitale valida che ne verifichi l'autore. Eseguire solo software proveniente da autori considerati attendibili.
Come determinare quale software eseguire

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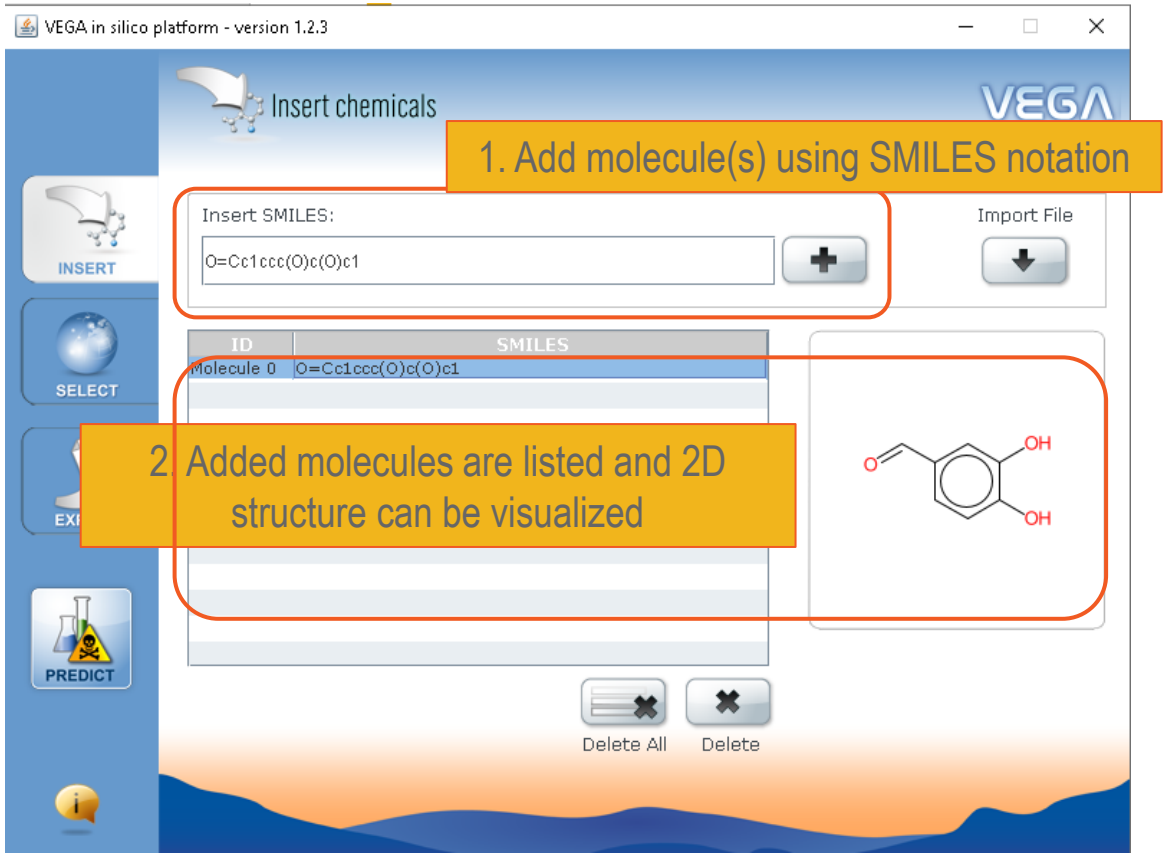
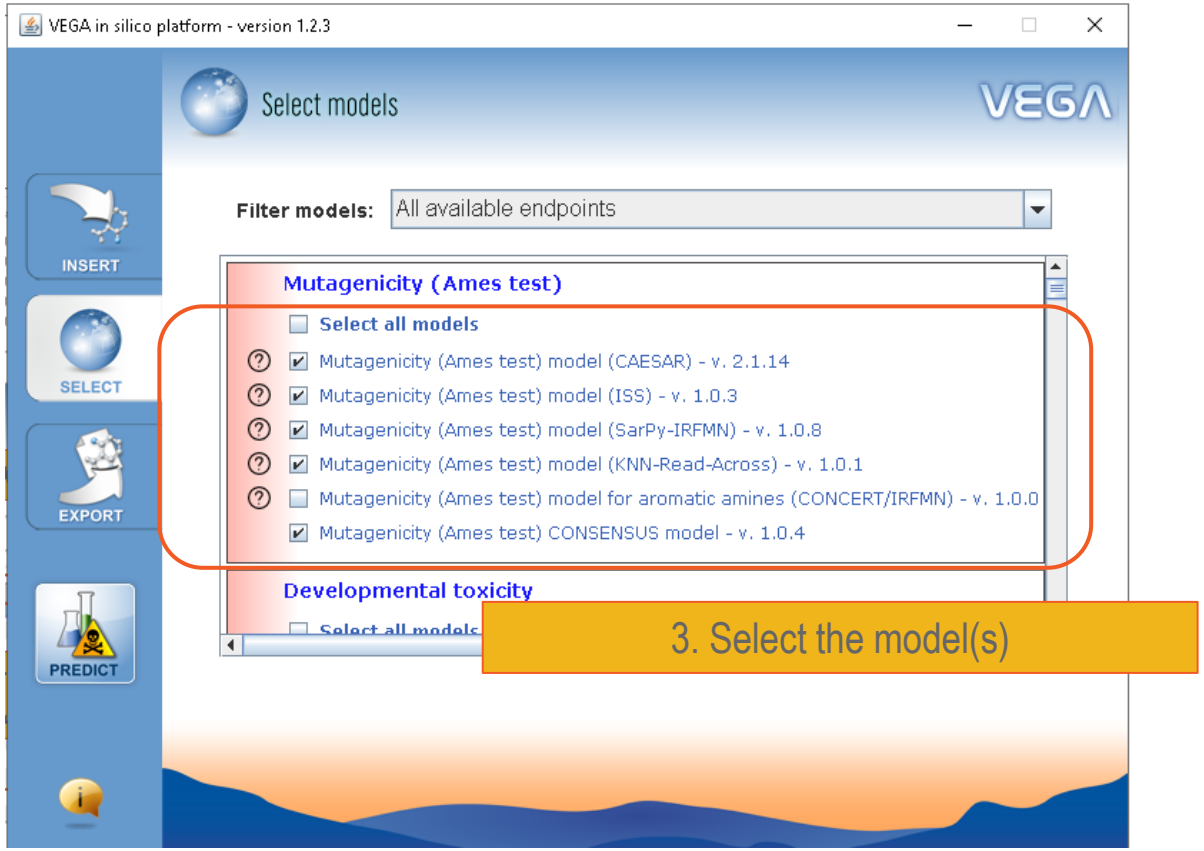
VEGA: running predictions





VEGA: running predictions

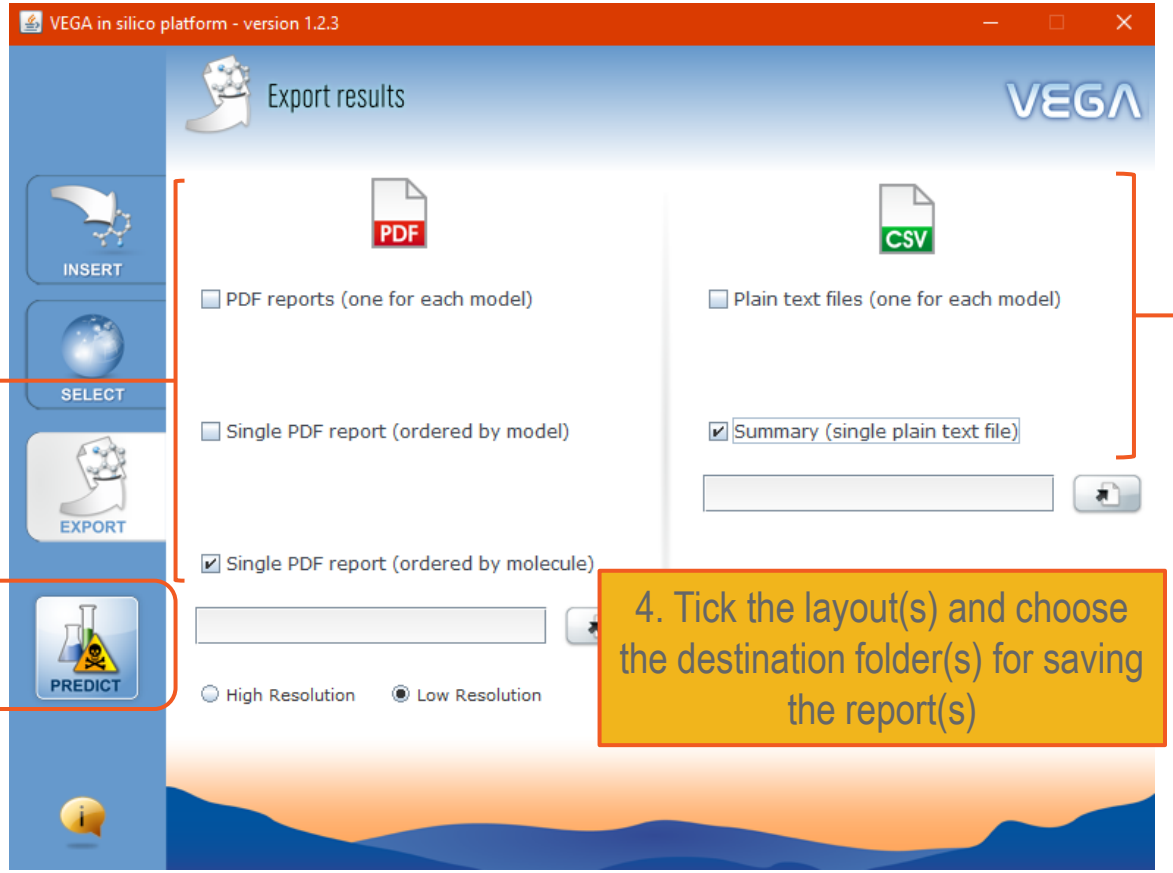
CONCERTREACH
CONCERTING EXPERIMENTAL DATA AND IN SILICO MODELS FOR REACH

LIFE17 GIE/IT/000461

Full PDF reports:

- prediction(s) results
- applicability domain
- experimental data of the target (if any)
- most similar substances
- other supporting info (if any)

5. Click on «Predict»

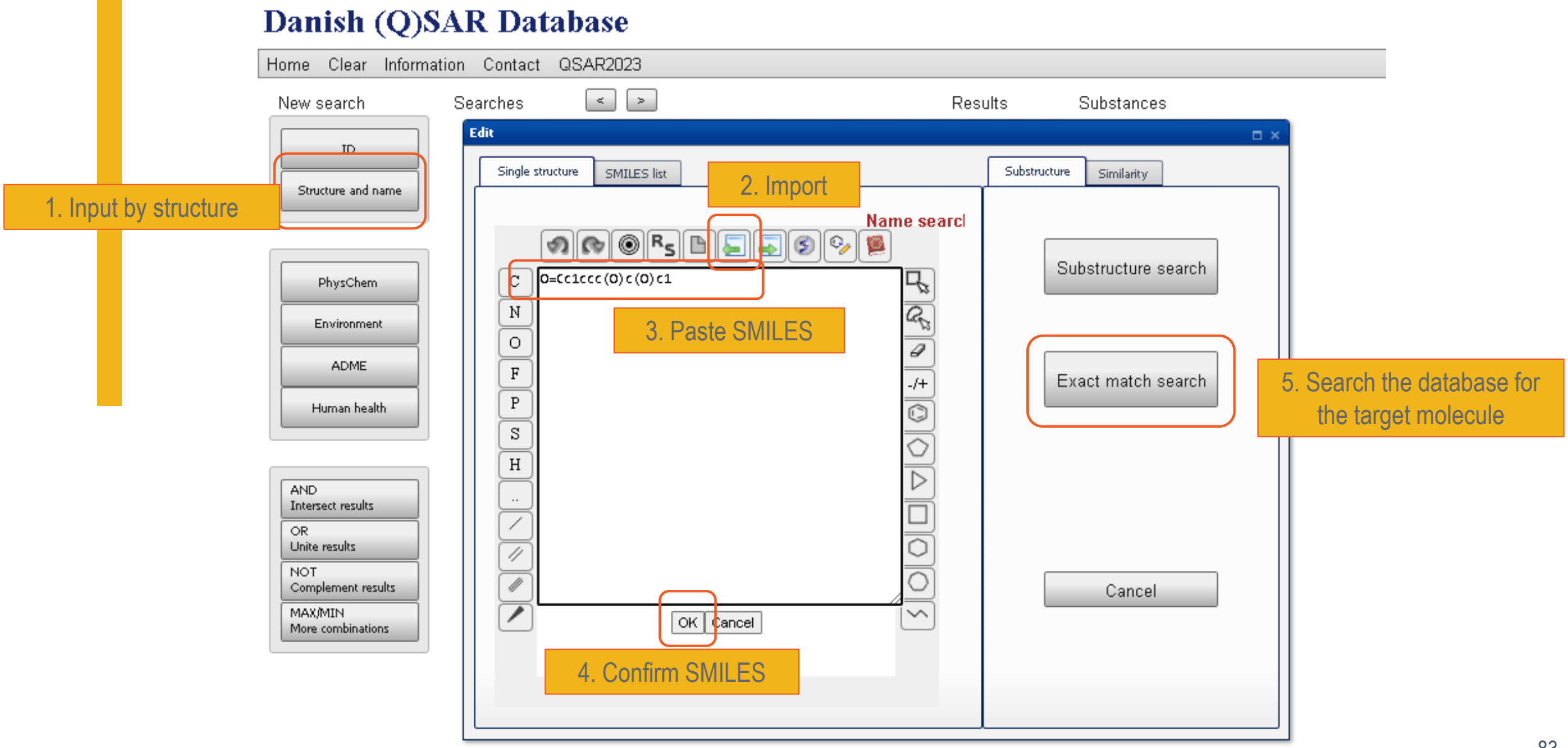


4. Tick the layout(s) and choose the destination folder(s) for saving the report(s)

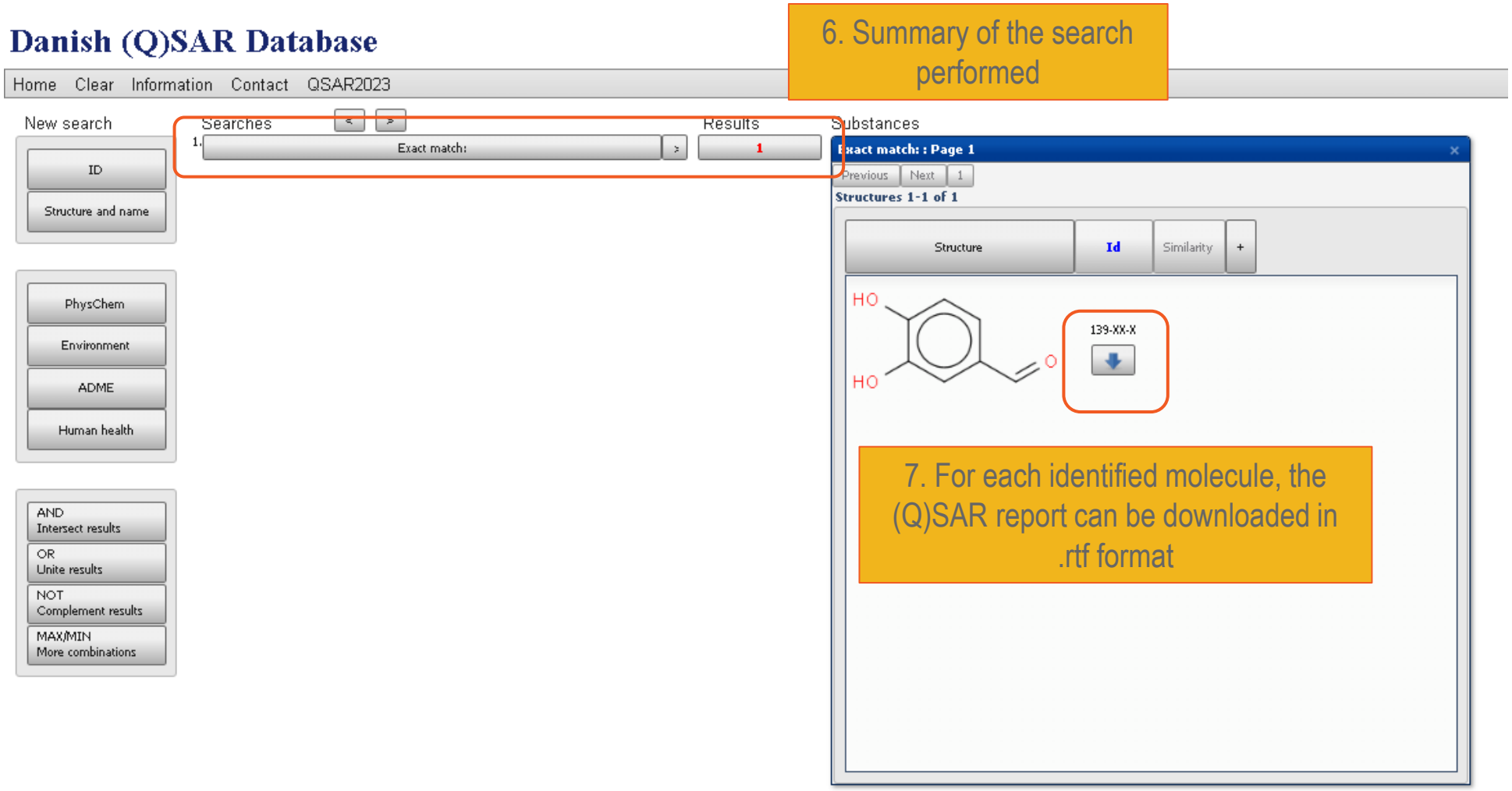
Simplified text reports

(useful for excel import)

Danish (Q)SAR Database: gathering (Q)SAR results



Danish (Q)SAR Database: gathering (Q)SAR results



The GATEWAY

Why it will be useful both for regulators and the industry

Feedback from regulators & end-users (via workshops):

- Regulators recommend multiple systems.
  - Within the 4 platforms are available **several in silico models**

- Difficulties: access, quality/choice, use, interpretation, integration
  - Access. Which models? Commercial/public. **We cover both**
  - Quality. Any tool possible, providing doc. **We focus on 4 well-known systems**
  - Use. CONCERT **improves the use and explanation**
  - Integration. CONCERT **improves integration**

The GATEWAY

Why it will be useful both for regulators and the industry

- Website active for 5 years after the end of the project
- Selection of the endpoints for other regulations then REACH (cosmetics…)
- Continuous updating by adding new tools and platforms

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in silico tool	Prediction	reliability
Mutagenicity (Ames test) CONSENSUS model-assessment	**NON-Mutagenic (Consensus score: 0.675)**	0.675
Mutagenicity (Ames test) model (CAESAR)	**NON-Mutagenic (GOOD reliability)**	0.96
Mutagenicity (Ames test) model (ISS)	Mutagenic (LOW reliability)	0
Mutagenicity (Ames test) model (SarPy-IRFMN)	**Possible NON-Mutagenic (GOOD reliability)**	0.96
Mutagenicity (Ames test) model (KNN-Read-Across)	**NON-Mutagenic (GOOD reliability)**	0.965
Toxread	**NON-Mutagenic**	
Battery	**NEG_IN**	
CASE Ultra	**NEG_IN**	
Leadscope	**NEG_IN**	aggiungere probability
SciQSAR	NEG_OUT	
OCHEM	**INACTIVE**	0.77
OCHEM ToxAlerts	Simple Aldehyde	
AMBIT	negative	