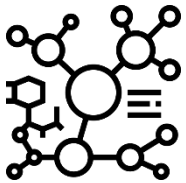
VERA

Virtual Extensive Read-Across

Un nuovo software per promuovere l'adozione di metodologie Read Across e Grouping

CONCERTREACH
CONCERTING EXPERIMENTAL DATA AND IN SILICO MODELS FOR REACH

VERA: un nuovo concetto di similarità

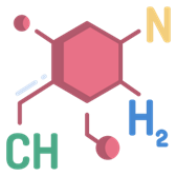


SIMILARITA' STRUTTURALE

VEGA

SIMILARITA' TOSSICOLOGICA

Allerte Strutturali

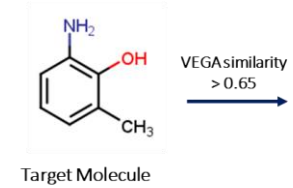


SIMILARITA' DI *GROUPING*

Gruppi Funzionali

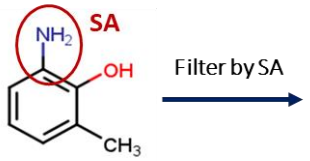
Come funziona?

1 ***Calcolo della similarità di VEGA*** → ***Simili con VEGA sim > 0.65***



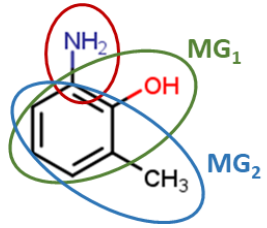
	Similarity	SMILES	Experimental value
0	0.938	COc1ccc(C)cc1N	1
1	0.915	COc1ccccc1N	1
2	0.914	COc1ccc(N)c(C)c1	1
3	0.910	COc1ccccc1[NH3+]	1
4	0.906	COc1ccc(N)cc1	0
...	...	...	...
483	0.651	CC(C)C(=O)Nc1ccc([N+](=O)[O-])c(C(F)(F)F)c1	1
484	0.650	COc1ccc2c3c(cccc13)OC([N+](=O)[O-])=C2	1
485	0.650	Clc1ccccc1	1
486	0.650	CC(C)(C)NCC(O)COc1cccc2c1CCCC2=O	1
487	0.650	COc1ccc(C(=O)C(Br)=CC(=O)O)cc1	1

2 ***Identificazione delle SAs nel target*** → ***Simili con SA***

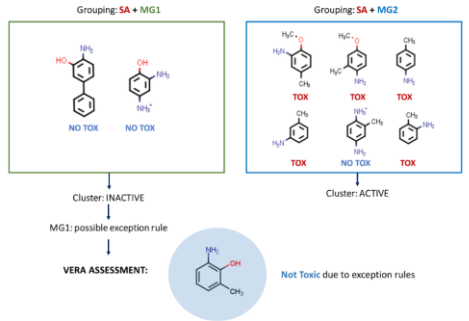


	SMILES	VEGA_Sim	Experimental value
	Cc1ccccc1N	0.875	1
	Cc1cccc(N)c1	0.890	1
	Cc1ccc(N)cc1	0.878	1
	Nc1ccc(-c2ccccc2)cc1O	0.837	0
	COc1ccc(C)cc1N	0.938	1
	COc1ccc(N)c(C)c1	0.914	1
	Cc1ccc(C)c(N)c1	0.884	1
	Cc1cc(-c2ccccc2C)ccc1N	0.742	1
	Cc1cc(C)c(N)cc1C	0.848	1
	CCn1c2ccccc2c2cc(N)ccc21	0.705	1

3 ***Identificazione dei MGs nel target*** → ***Calcolo della similarità di grouping***



4 ***Grouping*** → ***Clusters SA vs MGn***

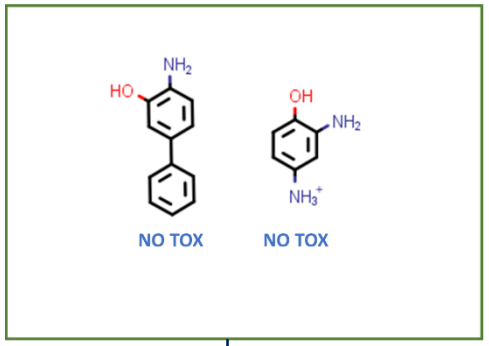


Endpoints

CARCINOGENICITY

Classification

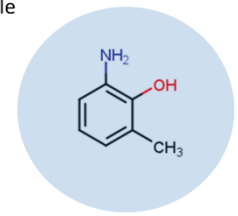
Grouping: SA + MG1



Cluster: INACTIVE

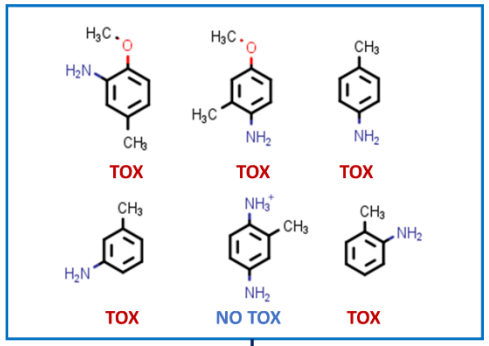
MG1: possible exception rule

VERA ASSESSMENT:



Not Toxic due to exception rules

Grouping: SA + MG2



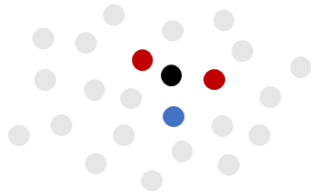
Cluster: ACTIVE

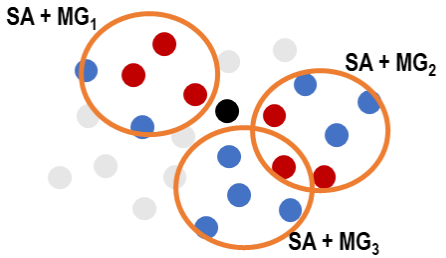
FISH ACUTE TOXICITY

Continuous

1. kNN model

If VEGA sim > 0.85

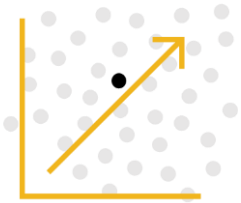




2. Grouping

If VEGA sim > 0.75

3. Local linear models



Pubblicazione

Open Access Article

Virtual Extensive Read-Across: A New Open-Access Software for Chemical Read-Across and Its Application to the Carcinogenicity Assessment of Botanicals

by Edoardo Luca Viganò [1], Erika Colombo [1], Giuseppa Raitano [1], Alberto Manganaro [2], Alessio Sommovigo [2], Jean Lou CM Dorne [3] and Emilio Benfenati [1,*]

[1] Department of Environmental Health Sciences, Istituto di Ricerche Farmacologiche Mario Negri IRCCS, 20156 Milano, Italy

[2] KODE Srl, 56122 Pisa, Italy

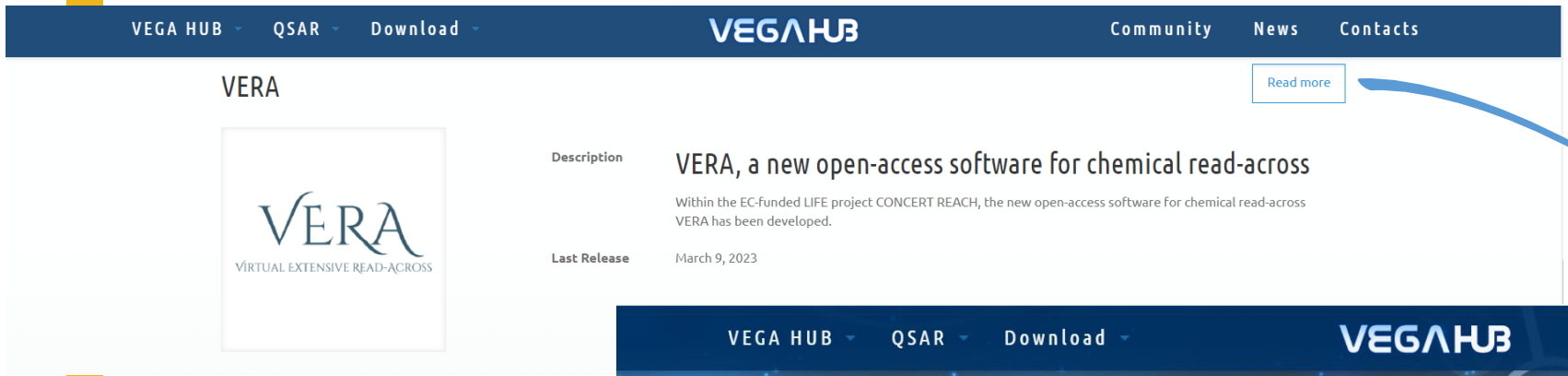
[3] Methodological and Scientific Support Unit, European Food Safety Authority, 43126 Parma, Italy

[*] Author to whom correspondence should be addressed.

Molecules **2022**, *27*(19), 6605; **https://doi.org/10.3390/molecules27196605**

Received: 22 August 2022 / Revised: 23 September 2022 / Accepted: 25 September 2022 / Published: 5 October 2022

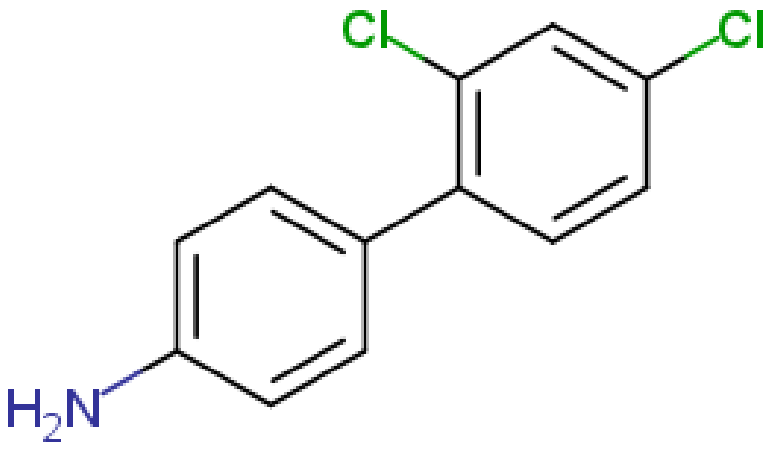
Open source!


VEGA HUB
QSAR
Download
VEGAHUB
Community
News
Contacts
VERA
Read more
VERA
VIRTUAL EXTENSIVE READ-ACROSS
Description
VERA, a new open-access software for chemical read-across
Within the EC-funded LIFE project CONCERT REACH, the new open-access software for chemical read-across VERA has been developed.
Last Release
March 9, 2023

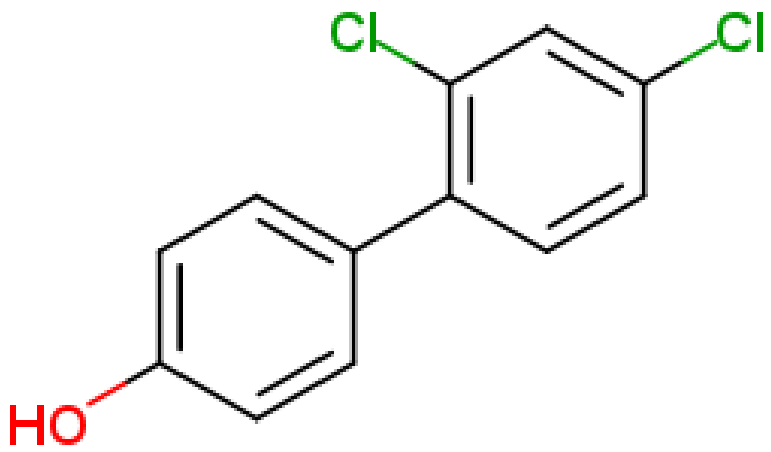

VEGA HUB
QSAR
Download
VEGAHUB
Community
News
Contacts
VERA
VERA Virtual-Extensive-Read-Across is a new open-access software for chemical read-across.
Within the EC-funded LIFE project CONCERT REACH, the new open-access software for chemical read-across VERA has been developed. Read-across applies the principle of similarity to identify the most similar substances to represent a given target substance in data-poor situations. However, differences between the target and the source substances exist. VERA (Virtual Extensive Read-Across) provides a means to assess the similarity between chemicals using structural alerts specific to the property, pre-defined molecular groups and structural similarity. The software finds the most similar compounds with a certain feature e.g. structural alerts and molecular groups and provides clusters of similar substances while comparing these similar substances within different clusters.
Introduction
Download
Screenshots

CASO STUDIO

CARCINOGENICITY



4-(2,4-dichlorophenyl)aniline



4-(2,4-Dichlorophenyl)Phenol

STEP futuri

① Implementazione di nuovi endpoints:

Skin Sensitization
Eye Irritation
Aromatase

② Aggiornamenti del software:

Nuovi dati sperimentali
Farmaci

Grazie per l'attenzione!

ISTITUTO DI RICERCHE FARMACOLOGICHE MARIO NEGRI · IRCCS

CONCERTREACH
CONCERTING EXPERIMENTAL DATA AND IN SILICO MODELS FOR REACH

erika.colombo@marionegri.it
edoardo.vigano@marionegri.it