CONCERTREACH
CONCERTING EXPERIMENTAL DATA AND IN SILICO MODELS FOR REACH

VERA: VIRTUAL EXTENSIVE READ-ACROSS

A new tool for automated read-across

CASE STUDY:

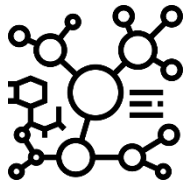
using the new VERA tool, for automated read-across assessment of carcinogenicity

ISTITUTO DI RICERCHE FARMACOLOGICHE MARIO NEGRI · IRCCS

knoell

VERA: the new concept of similarity

VERA
VIRTUAL EXTENSIVE READ-ACROSS



STRUCTURAL SIMILARITY

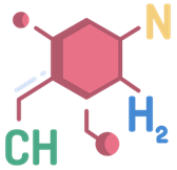
VEGA

Endpoint Specific

SAs

TOXICOLOGICAL SIMILARITY

Based on literature searching and implemented as SMARTS



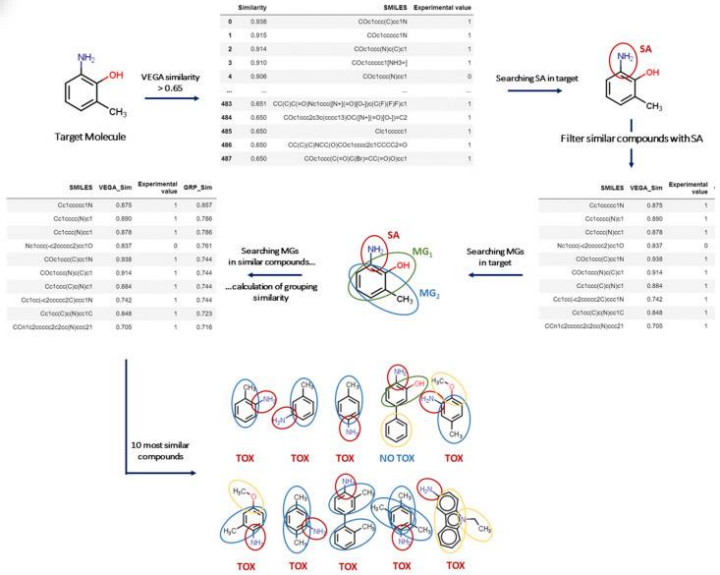
GROUPING SIMILARITY

MGs

From RdKit and other manually implemented as SMARTS

General Workflow of VERA

VERA
VIRTUAL EXTENSIVE READ-ACROSS



1. **Calculation of VEGA sim.** → *and filtering VEGA sim > 0.65*
2. **Searching SA *in the target*** → *and filtering by SA*
3. **Searching MGs *in the target*** → *calculation of grouping similarity* → *Considering MG in common and not with the target*
4. **Reasoning** → *Clusters SA vs MG_n*

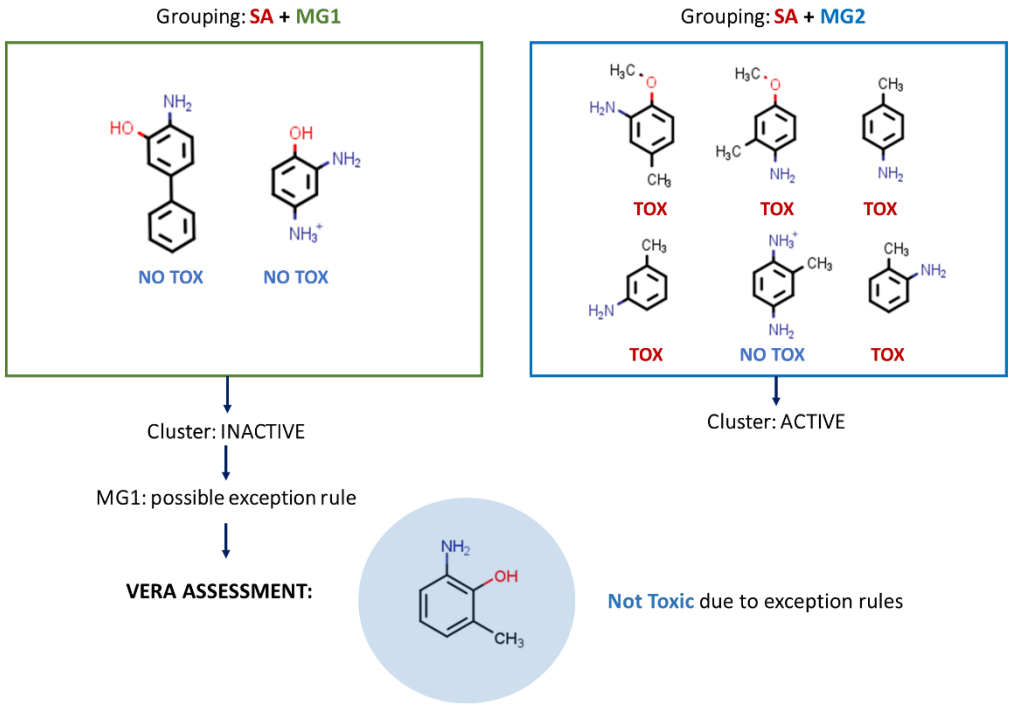
$$GSI = \frac{\frac{1+nMGs \in common}{ntargetMGs}}{2} - \frac{\frac{nMGsNOT \in common}{nsimilarMGs}}{8}$$

Endpoints

VERA
VIRTUAL EXTENSIVE READ-ACROSS

CARCINOGENICITY

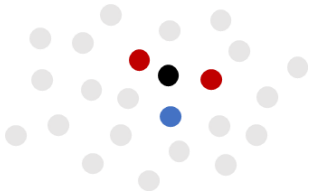
Classification

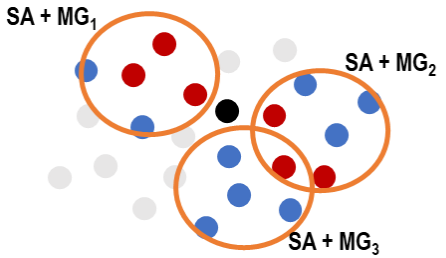


FISH ACUTE TOXICITY

Continuous

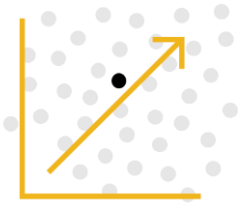
1. kNN model
   If VEGA sim > 0.85





2. Grouping
   If VEGA sim > 0.75

3. Local linear models



Pubblication

VERA
VIRTUAL EXTENSIVE READ-ACROSS

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,*]

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Availability

VERA
VIRTUAL EXTENSIVE READ-ACROSS

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VERA

Read more

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

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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

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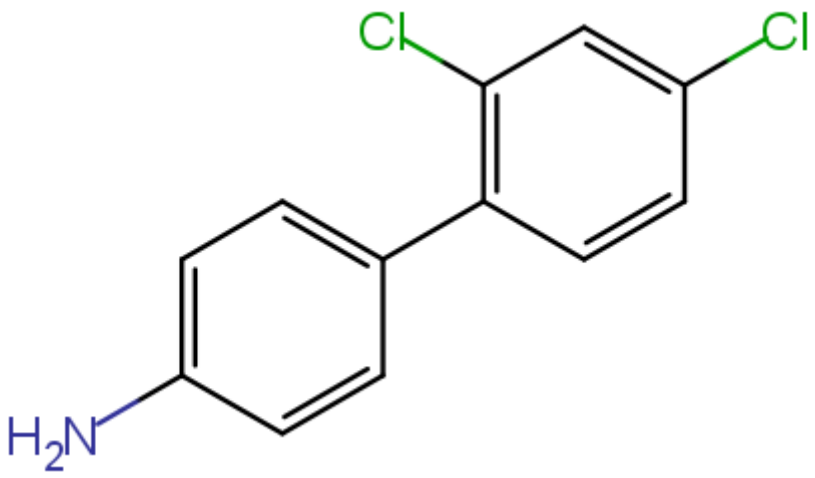
Screenshots

VEGAHUB

CASE STUDY

CARCINOGENICITY

VERA
VIRTUAL EXTENSIVE READ-ACROSS



4-(2,4-dichlorophenyl)aniline

- Pharmaceutical precursor
- Pesticide precursor
- Starting material for synthesizing dyes
- Potentially building block for polymers