ToxPHACTS

VERSION 2.0 RELEASE NOTE

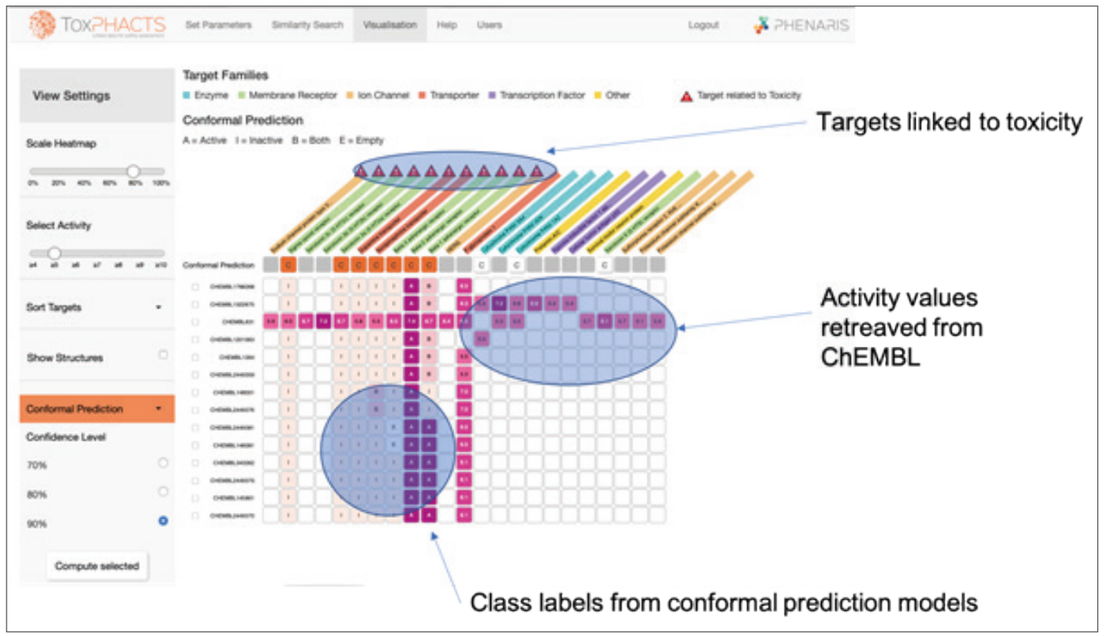
ToxPHACTS version 2.0 has been released. Besides improvements in target-toxicity associations and chemical structure representation, it offers conformal prediction models for a set of off-targets. Please check the quick guide below and contact office@phenaris.com for a Demo.

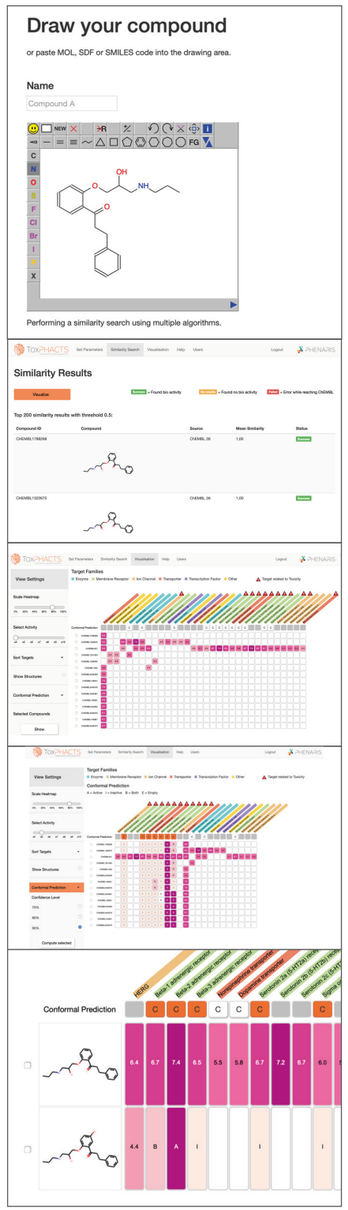
NEW FEATURES & ENHANCEMENTS

Target-toxicity associations
Constantly increased list of proteins associated with adverse drug events

New standardized representation of chemical structures
The standardized structure representation using RDKit (Version 2020.03.2) allows fast and simple comparison of structures in order to identify off-target SAR in your hit list

Conformal prediction models
This major enhancement allows a fast assessment of all compounds similar to your query structure using robust conformal prediction models





QUICK GUIDE

Draw your Compound — STEP 1
Simple and fast drawing of your query structure using the tool from Peter Ertl and Bruno Bienfait.

Similarity Results — STEP 2
Retrieve similar compounds and their bioactivity data from ChEMBL using a consensus of 5 different similarity algorithms.

Data Visualization — STEP 3
Intuitive presentation of all data retrieved as heat map, highlighting target-toxicity annotations.

Predictions — STEP 4
Predict compound-target activity classes (active – inactive – both – empty) using conformal prediction models.

Comparison — STEP 5
Standardised chemical structure representation using RDKit (Version 2020.03.2) allows fast and simple comparison of structures in order to identify off-target SAR in your hit list.