ToxGPS Read-Across

Relevant, Reliable, Consistent and Reproducible

ToxGPS Read-Across is an easy-to-use and transparent workflow to perform read-across studies and experiments. The workflow considers various types of information, such as chemical and physicochemical, biological and toxicological data, either experimental or predicted, and is capable of lining up and combining their evidences and uncertainties to support the decision for a consistent and reproducible read-across outcome.

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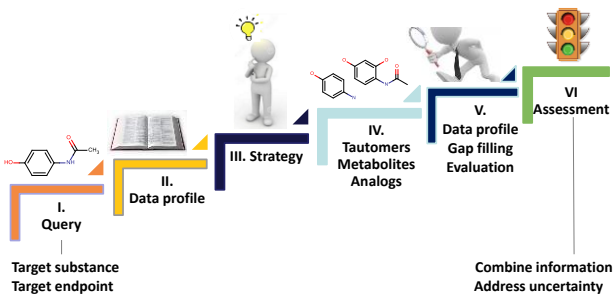
Key Features

- Rigorous cheminformatics workflows applied to Read-Across
- Evidence-based assessment of experimental target and source compound data provided in ChemTunes Safety Evaluation Database
- Assessment including study quality, species and human relevance and data variation
- Chemical speciation of target compound, metabolites and tautomers, by knowledge-based approaches
- Retrieval and quality assessment of analogs from ChemTunes Databases based on structural, physicochemical and biological similarity
- Final and overall assessment by combination of all evidences for outcome and uncertainty
- Presentation and display of final assessment in convenient table view

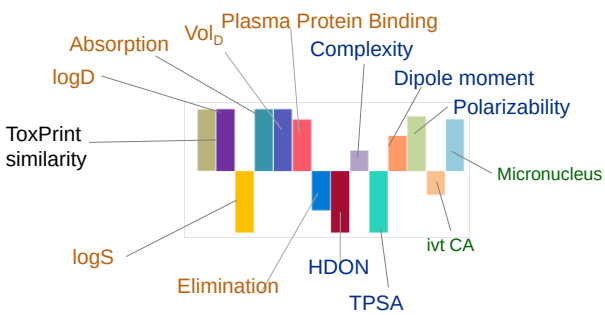
Workflow Strategy

- Various steps depending on availability of target data



Analog Retrieval

- Various criteria for similarity
  - Structure similarity
  - Physicochemical properties
  - Biological assay activity
- Visualization of similarity through chemical structures and skyline plots



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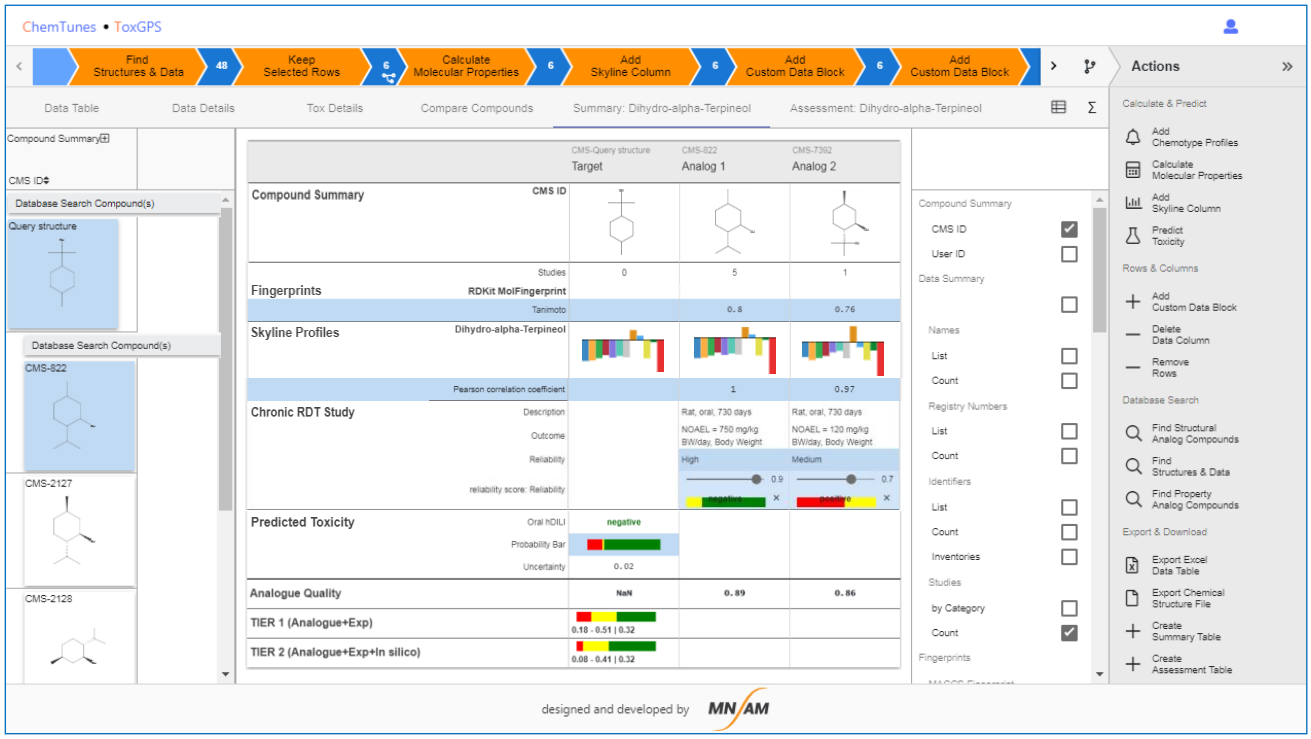
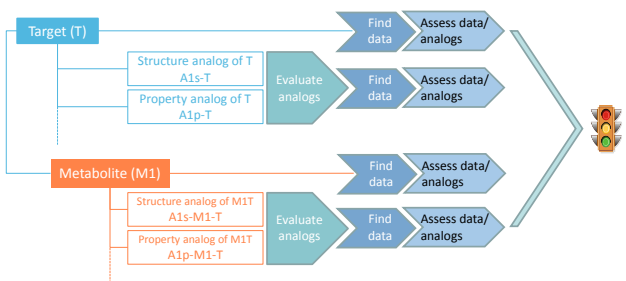
ToxGPS Read-Across provides an interactive workflow that tracks the actions and steps performed by a scientist during the read-across study. Thus, workflows can be stored and even shared among scientists at any stage for review and discussion. This allows for a fully reliable, consistent and transparent generation of a read-across outcome, also in a regulatory context.



Read-Across Tree

- Inclusion of chemical species, *e.g.*, metabolites, to take into account metabolic activation



Technical Requirements

- Frontend
  - Standard web browser (Chrome or Firefox recommended)
  - Interface to existing workflows on request
- Backend
  - Linux (Ubuntu 14/16 LTS, RedHat 6/7)
  - Microsoft® Windows® 7, Server 2008/2012
  - ORACLE v.11.2 database server
  - Minimum 10 GB disk space, 8 GB RAM

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