ToxGPS® Read-Across

Relevant, Reliable, Consistent and Reproducible

ToxGPS® Read-Across is an easy-to-use and interactive workflow for read-across analysis. The workflow enables inclusion of various types of experimental or in silico information, including structural, physicochemical, biological and toxicological data. After lining up all available information, the user can select which evidence sources to combine to obtain a weight-of-evidence outcome with associated estimate of uncertainty. The workflow supports consistent, reproducible and transparent decision making by read-across.

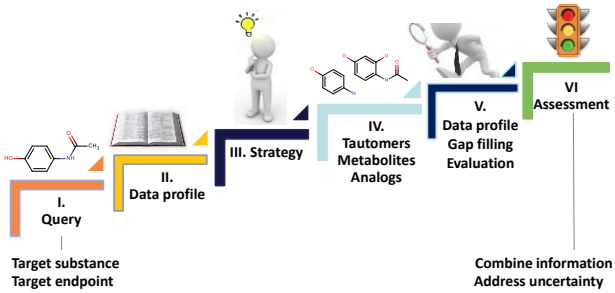
ToxGPS Read-Across

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 selected evidence
- Presentation and display of final assessment results in convenient table view

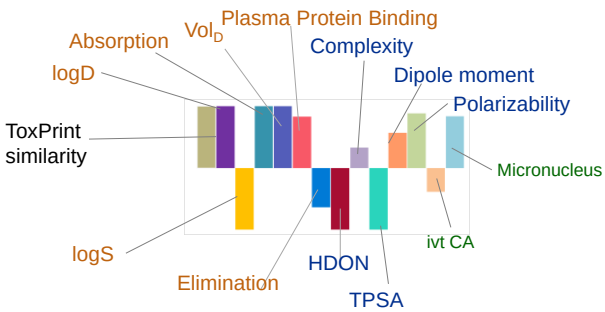
Workflow Strategy

- Data for target compound determine steps to be taken in the Read-Across workflow



Analog Retrieval

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



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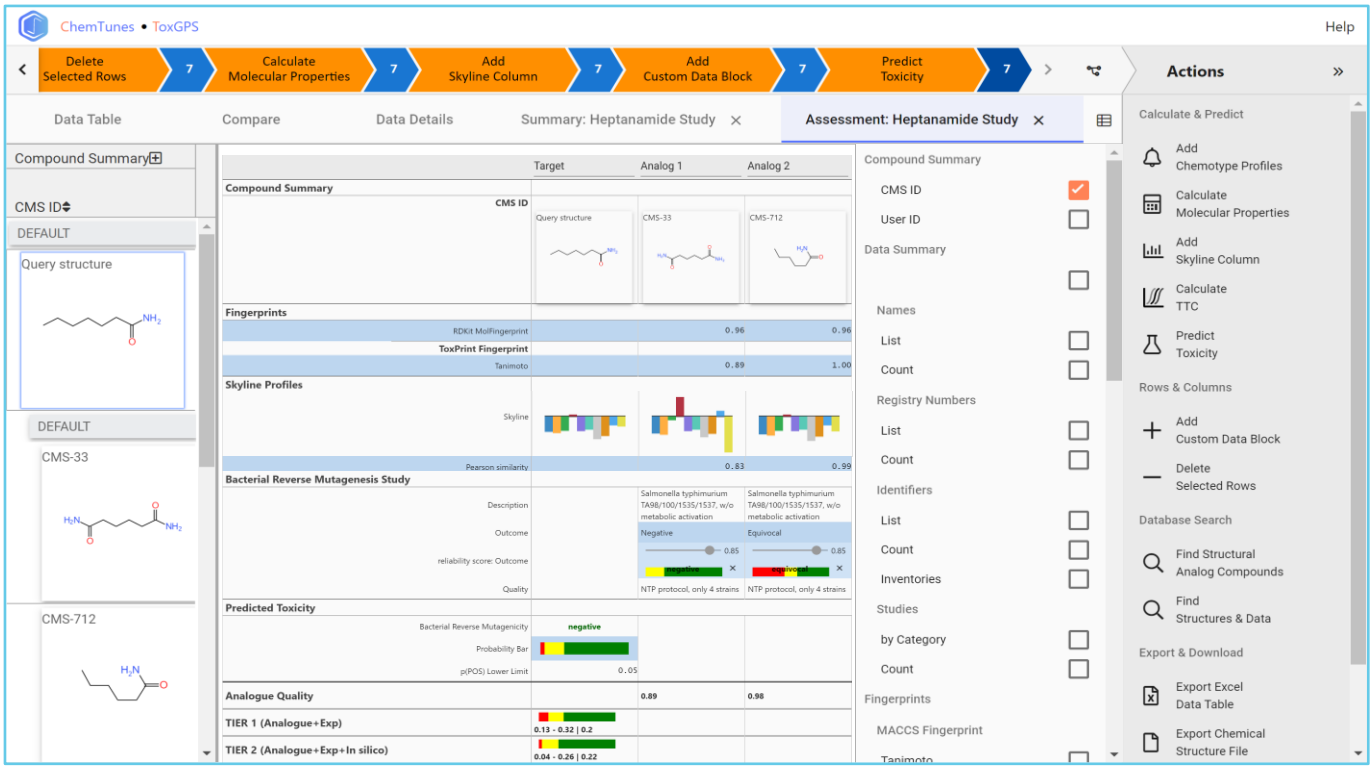
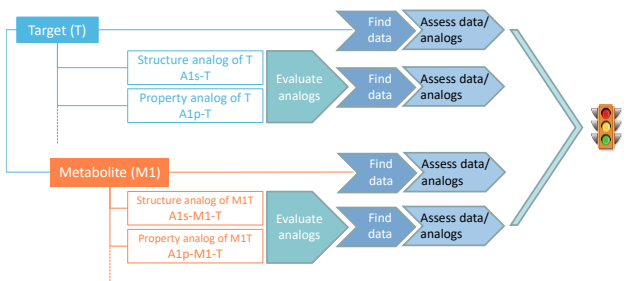
ToxGPS® Read-Across provides an interactive workflow that tracks the actions and steps performed by a scientist during a read-across analysis. Workflows can be stored and shared among scientists at any stage for review and discussion. This allows for a systematic and transparent generation of a read-across outcome for assessing chemical safety, including such analyses in a regulatory context.



Read-Across Tree

- Inclusion of chemical species, e.g., metabolites, to consider 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)
  - Minimum 10 GB disk space, 8 GB RAM

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