In silico Toxicity Prediction

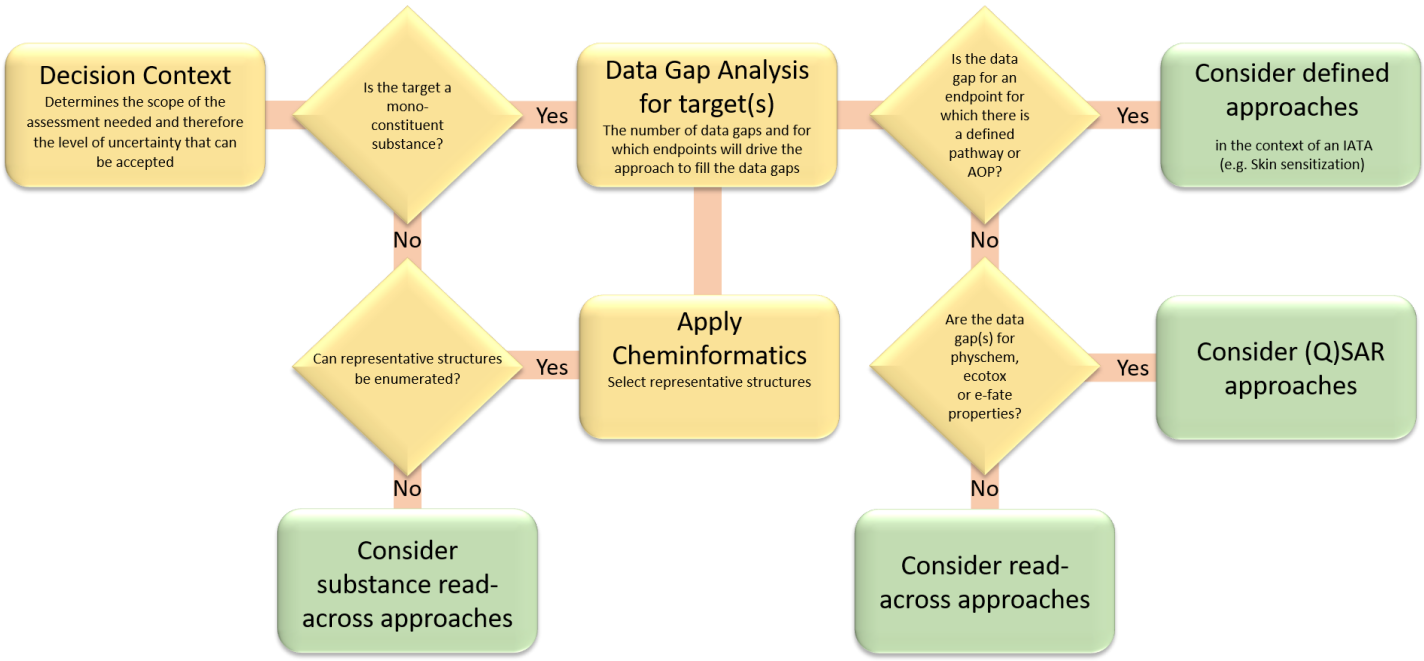
Regulators are encouraging the use of computational toxicology as a mean of reducing your *in vivo* and *in vitro* testing based on existing knowledge. The key issue is to retain the credibility of your chemical risk assessment to the regulator.

ToxNavigation provides a cost effective *in silico* toxicology service using (Q)SAR and read-across to estimate the toxicity of your substances.

Before you order, **a free feasibility study** is conducted prior to acceptance of your project to ensure there is experimental data available to support a reliable prediction.

If your substance is a UVCB, ToxNavigation has experience in selecting representative structures for *in silico* predictions by applying cheminformatics.

The approach is defined by applying the workflow outlined below:



QSAR Approach

1. **Predictions**
   Statistical models, Rules based model, Profilers
2. **Reliability check**
   Expert assessment of the reliability of each model
3. **Combine results**
   Expert assessment, combining all predictions into a final call

Toxicology

- Acute toxicity
- Skin / Eye irritation
- Skin sensitization
- Mutagenicity/Genotoxicity
- Carcinogenicity§
- Developmental toxicity§
- Endocrine System Disruption§

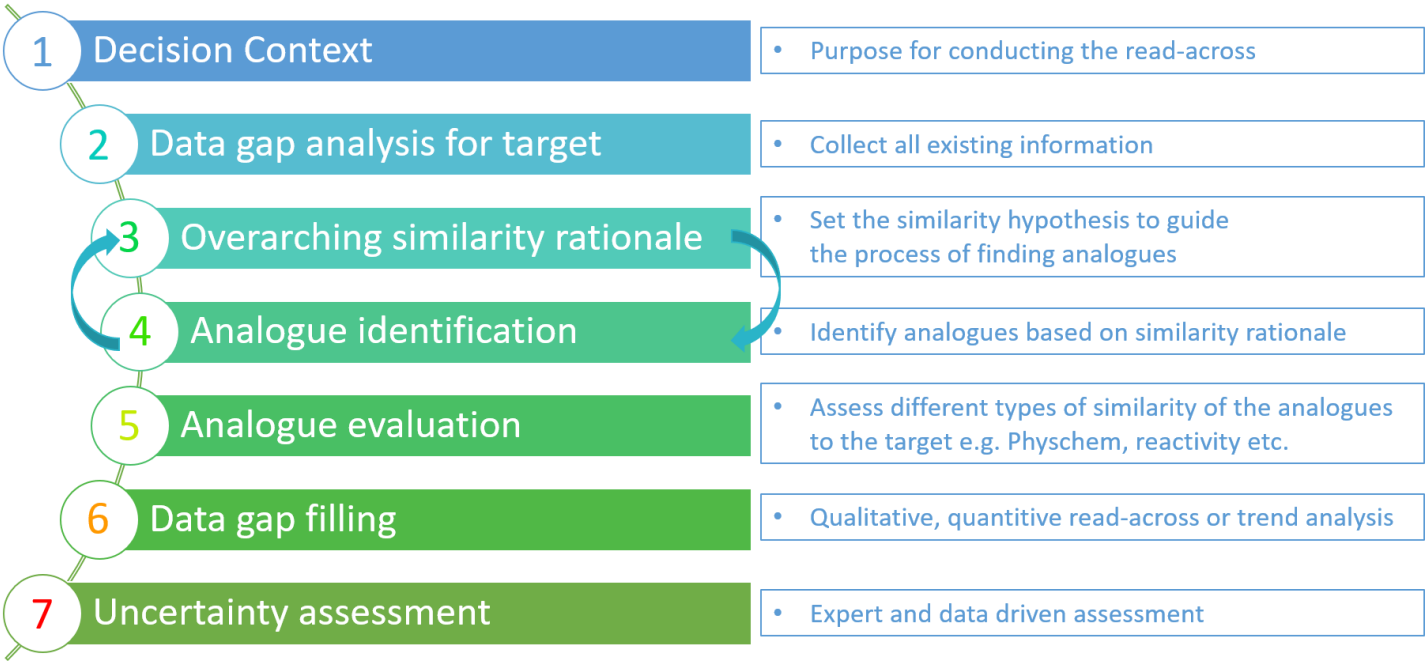
Phys-chem

- Water solubility
- $logK_{ow}$ or logP
- Dissociation constant (pK_a)

The **standard report** is structured as the QSAR Prediction Reporting Format described by ECHA.
A bespoke report is also available upon request.

§ Main applications: *in silico* toxicology hazard profile to give information on possible hazard of the chemical useful to prioritize and design the tests *in vitro*

Read-across Approach



A video explaining the above workflow in more detail can be viewed: https://www.toxnavigation.com/read-across

Two levels of service are provided: **Standard and Extensive analogue evaluation**

The **Standard analogue evaluation** includes the analysis of the similarity between your target and the analogues carried out in four steps:

- Step 1: Physicochemical similarity analysis
- Step 2: Structural similarity analysis
- Step 3: Toxicokinetic similarity analysis
- Step 4: Mechanistic similarity analysis

The standard report includes the read-across result, a prediction report for the target substance, the list of analogues, their evaluation and their experimental values used in assigning the final read-across prediction. The report is structured in line with the Read-Across Assessment Framework (RAAF). A bespoke report is also available upon request.

The scope and the content of the **Extensive analogue evaluation** will vary case-by-case. For example a review of a read-across initially rejected by a regulator to strengthen the initial justification including a metabolic, a toxicokinetic or a toxicodynamic similarity analysis.

In all evaluations it is imperative the read-across must be both scientifically justified and fully documented to meet the expectations of regulators.

The scientists at ToxNavigation have more than 25 years of experience in *in silico* modelling to predict the effects of chemicals on humans and in the environment and can generate **reliable safety data *in silico*** by combining results from **(Q)SAR** models, **chemical categories**, **grouping** and **read-across**

CONTACT US

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