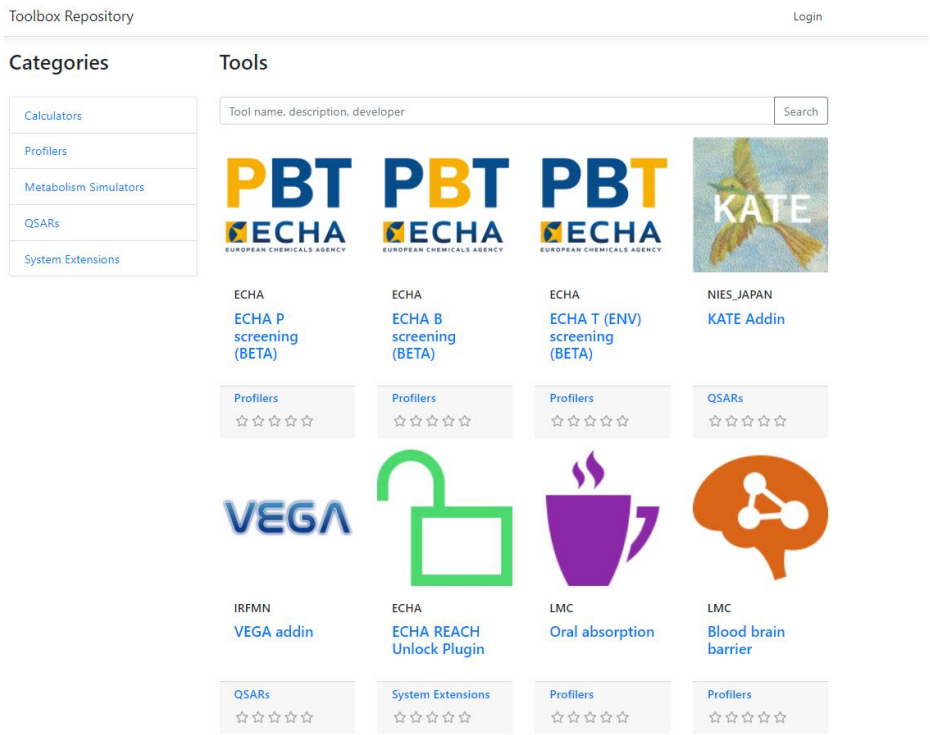
THE OECD QSAR TOOLBOX:
MORE THAN QSAR PREDICTIONS

Patience Browne
OECD Environment Directorate
30 November, 2021

BETTER POLICIES FOR BETTER LIVES

Governance

- ECHA and OECD co-own and co-develop the Toolbox
  - Work executed by LMC
- Activities under the OECD umbrella, core developments contracted by ECHA
  - Coordination group: OECD, ECHA, IT developer
  - Toolbox management group: Coordination group + experts from industry, authorities , NGOs
- Other partners also invest in the development
  - e.g. EPA contracted the link with their tool ONCOLOGIC and Japan developed a plug-in for their QSAR tool KATE
- Now third parties can make their own extensions (e.g. profilers, QSAR models) available through the TB repository.



QSAR TOOLBOX

Global Use by Regulators

Environment and Climate Change Canada

Health Canada

NIH NIEHS

United States Environmental Protection Agency

Agência Nacional de Vigilância Sanitária

ECHA European Chemicals Agency

anses French agency for food, environmental and occupational health & safety — Investigate, evaluate, protect

BfR Bundesinstitut für Risikobewertung

Istituto Superiore di Sanità

Ministry of Environment and Food of Denmark Environmental Protection Agency

Cefas

経済産業省 Ministry of Economy, Trade and Industry

環境省 Ministry of the Environment

Australian Government Department of Health National Industrial Chemicals Notification and Assessment Scheme

QSAR TOOLBOX

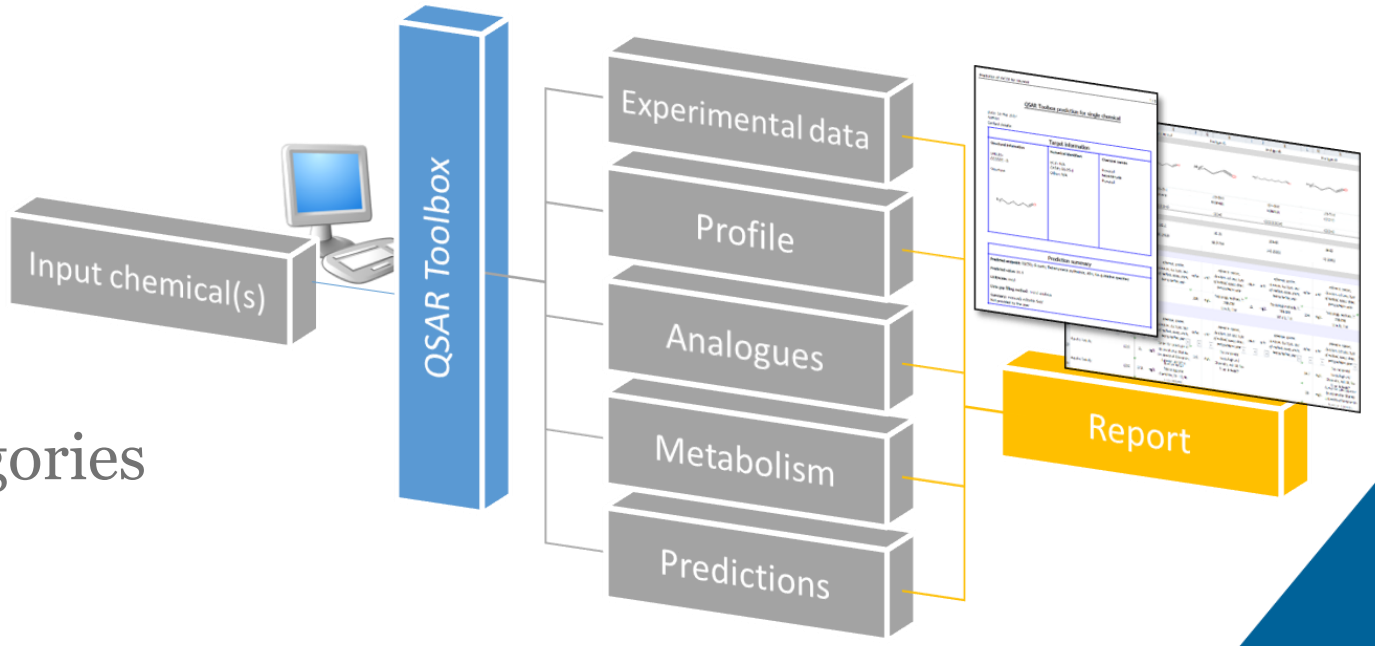
More than QSAR predictions

QSAR TOOLBOX

The QSAR Toolbox is a free software application that supports (eco)toxicologists in performing reproducible and transparent chemical hazard assessment using **non-animal methods**.

Key functionalities:

- retrieve experimental data
- profiling properties of chemical
- simulate metabolism
- identify analogues and build categories
- predict properties



Experimental data

QSAR TOOLBOX

No need to perform new experimental studies if the information is already (publicly) available.

Toolbox searches **experimental data** on chemicals from 59 databases, including 100 000 chemicals and over 3 million data points.

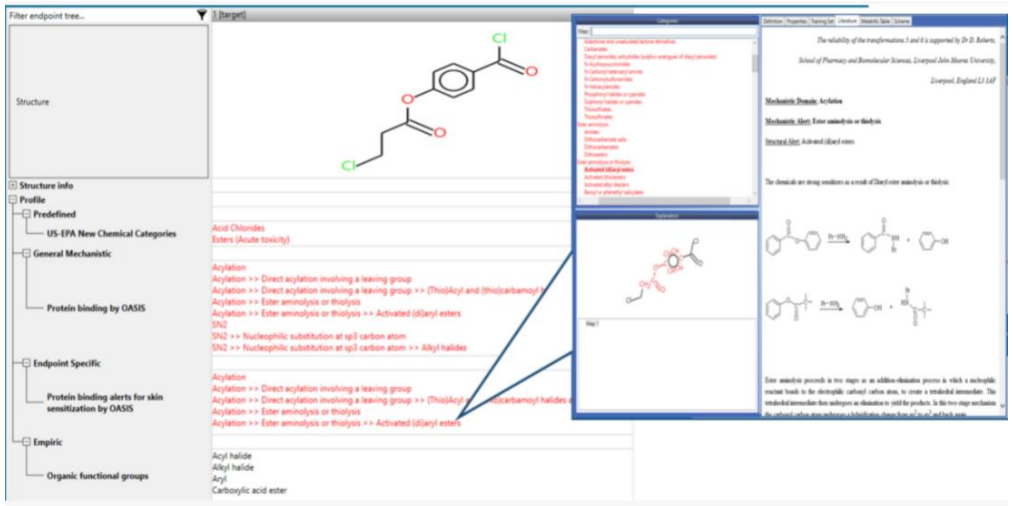
Experimental data from analogues can also be used for read-across predictions.

Profiling

QSAR TOOLBOX

Structural profilers support the identification of structurally similar substances.

Mechanistic profilers provide an understanding of the mode of action, which is key to predict the activity of substances or to form mechanistically sound categories.



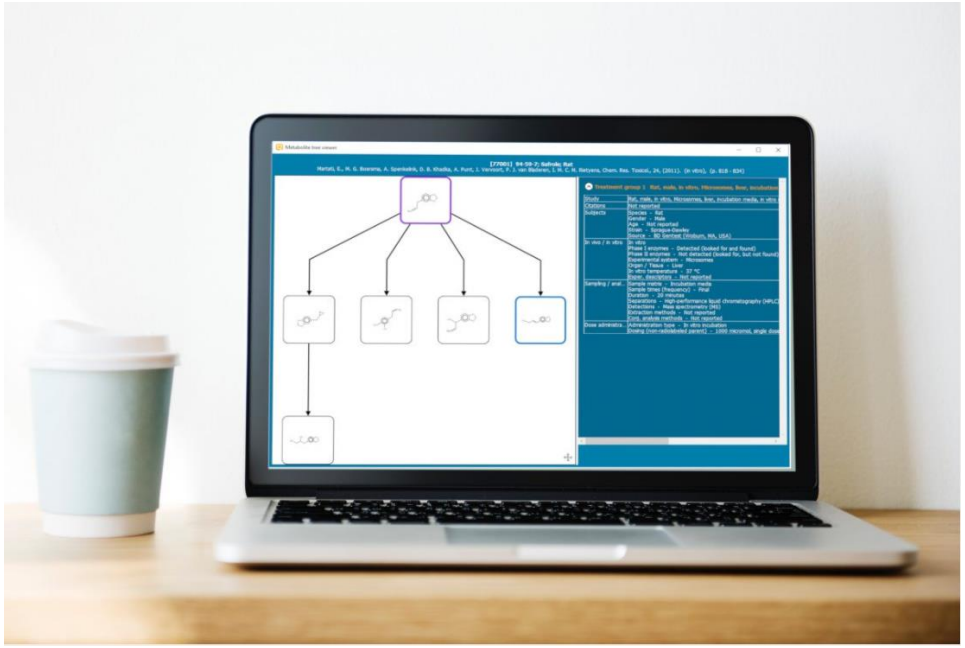
The results of the profilers in the Toolbox, include descriptions and references to scientific papers to explain the outcome.

Metabolism

QSAR TOOLBOX

Metabolism influences the activity of substances in many cases. It is important to take it into account when making predictions of forming categories.

Results from 5 experimental metabolic databases and 11 metabolic simulators can be taken into account when assessing a single substance or categories.

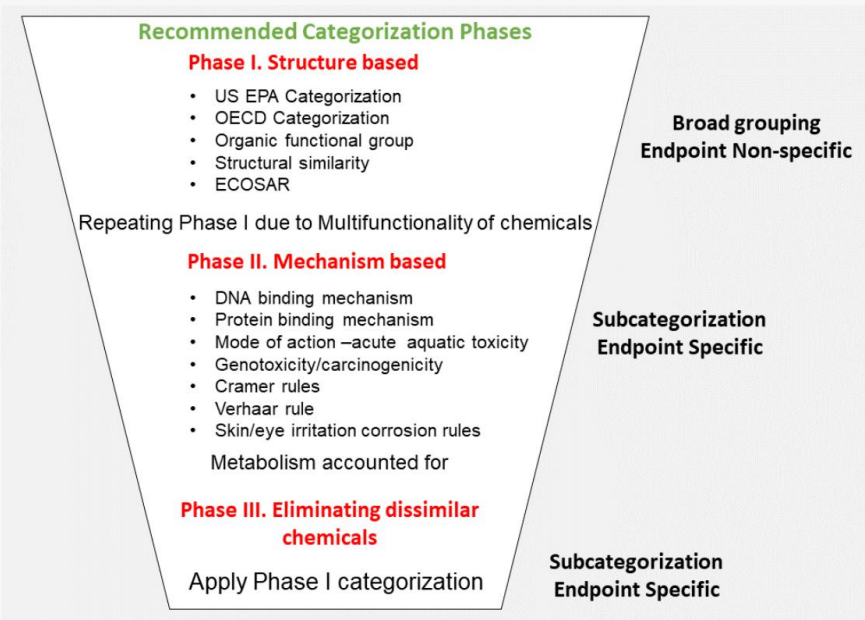


Analogues and categories

QSAR TOOLBOX

Data from analogues can be used to predict the property of a target substance using read-across or trend-analysis.

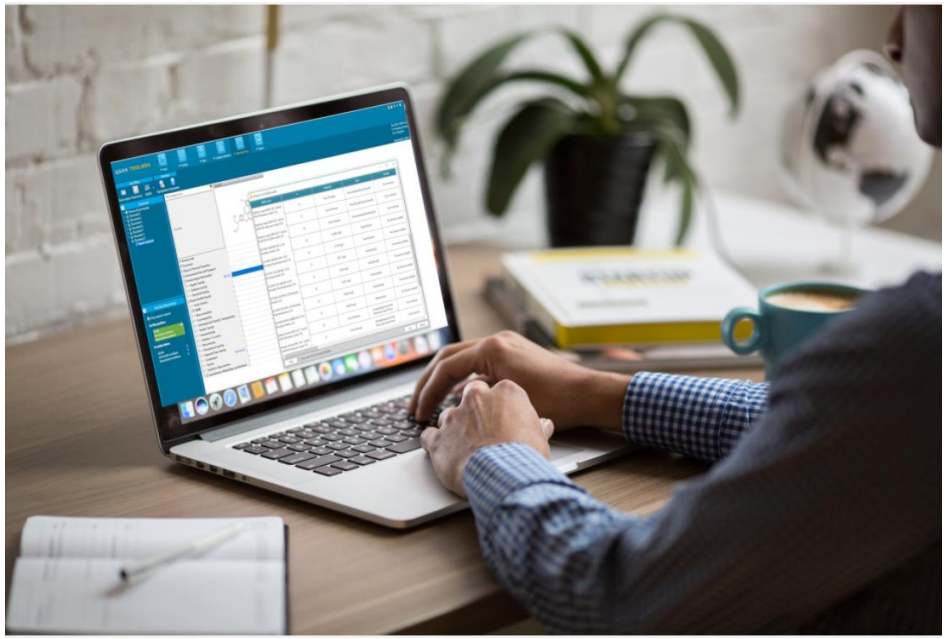
Toolbox can take into account structural, mechanistic and metabolic aspects to find toxicologically relevant analogues with data on the property of interest.



Predict properties

QSAR TOOLBOX

Toolbox can also predict properties by using existing QSAR models, which do not require the (manual) identification of analogues.



Examples of external QSARs included in the Toolbox are:

- EPISuite models by US EPA
- Danish QSAR Database predictions

Conclusions

QSAR TOOLBOX

- The QSAR Toolbox offers many possibilities to assess chemical properties with non-animal methods.
- In addition to QSAR models, existing data, metabolic and mechanistic information can be used to fill data gaps.
- The Toolbox development is a group effort! The project is managed by ECHA and OECD and implemented by LMC, but also 3rd parties contribute to its success, with e.g.:
  - The donation of data, profilers and models.
  - Feedback and suggestions, especially by the QSAR Toolbox management group.
  - The financing of tutorials and other developments.