



# THE OECD QSAR TOOLBOX: CURRENT STATUS & FUTURE DEVELOPMENTS

Patience Browne  
OECD Environment Directorate  
30 November, 2021



# What is the OECD QSAR Toolbox?

The Toolbox (TB) is a free software application that supports (eco)toxicologists in performing reproducible and transparent chemical hazard assessment.

More than “just” a QSAR tool!

# QSAR TOOLBOX

Key functionalities:

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



## Supports alternatives to animal testing

---

- **Inform testing strategies** - By forming categories and identifying data gaps, intelligent testing strategies can be designed to optimise costs and number of animals required.
- **Predict properties** - TB predictions can replace information requirements for regulatory purposes (industry) or be used as input for authorities work e.g. prioritisation, substance evaluation
- **Sustainable development and green chemistry** - The toxicity of substances can be predicted even before they are produced.



- 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.

The screenshot shows the 'Toolbox Repository' website. At the top right is a 'Login' link. On the left is a 'Categories' sidebar with links for 'Calculators', 'Profilers', 'Metabolism Simulators', 'QSARs', and 'System Extensions'. The main area is titled 'Tools' and features a search bar with the placeholder text 'Tool name, description, developer'. Below the search bar is a grid of tool cards. Each card displays a logo (e.g., PBT ECHA, VEGA, KATE), a title, a category, and a star rating. The tools shown include: ECHA P screening (BETA) (Profilers, 5 stars), ECHA B screening (BETA) (Profilers, 5 stars), ECHA T (ENV) screening (BETA) (Profilers, 5 stars), NIES\_JAPAN KATE Addin (QSARs, 5 stars), VEGA addin (QSARs, 5 stars), ECHA REACH Unlock Plugin (System Extensions, 5 stars), LMC Oral absorption (Profilers, 5 stars), and LMC Blood brain barrier (Profilers, 5 stars).

## What's new ? OECD launches the QSAR Toolbox version 4.5

The OECD Hazard Assessment programme is actively working to increase the regulatory acceptance of QSARs methods, tools and approaches such as the QSAR Toolbox and to make these technologies more accessible and transparent.

The [QSAR toolbox](#) is a software application intended for use by governments, chemical industry and other stakeholders for filling gaps in (eco)toxicity data needed for assessing the hazards of chemicals. It has been developed in close collaboration with the European Chemicals Agency. The Toolbox incorporates information and tools from various sources into a logical workflow. Crucial to this workflow is grouping chemicals into chemical categories.

### New features include:

- Workflow editor allows automated and standardized workflows for predicting or grouping of chemicals to be developed by the users
- IUCLID Plug in allows users to enter target chemical by IUCLID ID, use composition search in IUCLID databases, and import from IUCLID.
- Pilot version of web client available as part of the standard installation provides basic features from the Simplified UI along with a dedicated module for searching in imported IUCLID databases
- Automated Workflow for Skin sensitization for Defined approaches (DASSAW) was updated based on the protocol of the DASS guideline ([OECD Guideline No. 497](#)).

### New databases:

- Human skin sensitisation NICEATM/BfR - New: 1 377 substances and 2 277 data points
- Photosensitivity database - New: 73 substances and 563 data points



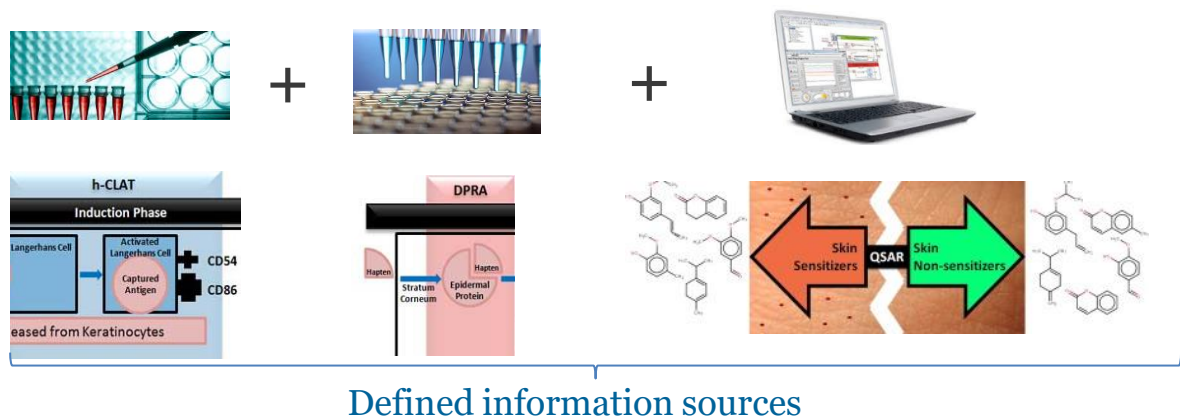
For more information on the QSAR Toolbox, please consult our [website](#).

---

For additional information please contact : [ehs.contact@oecd.org](mailto:ehs.contact@oecd.org)  
[patience.browne@oecd.org](mailto:patience.browne@oecd.org)  
[tomoko.aoyagi@oecd.org](mailto:tomoko.aoyagi@oecd.org)



# Defined Approaches for Skin Sensitisation Guideline



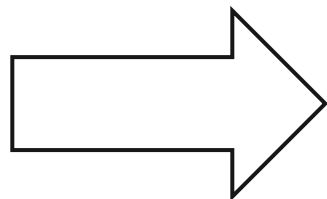
Score	h-CLAT MIT	DPRA depletion	QSAR TB
3	≤10 µg/mL	≥42.47%	-
2	>10, ≤150 µg/mL	≥22.62, <42.47%	-
1	>150, ≤5000 µg/mL	≥6.376, <22.62%	Alert
0	not calculated	<6.376%	No alert

Potency: Total battery score	Strong :	Weak :	Not classified :
	6-7	2-5	0-1

Defined data interpretation



Methods A + B + C



Predict the mouse!

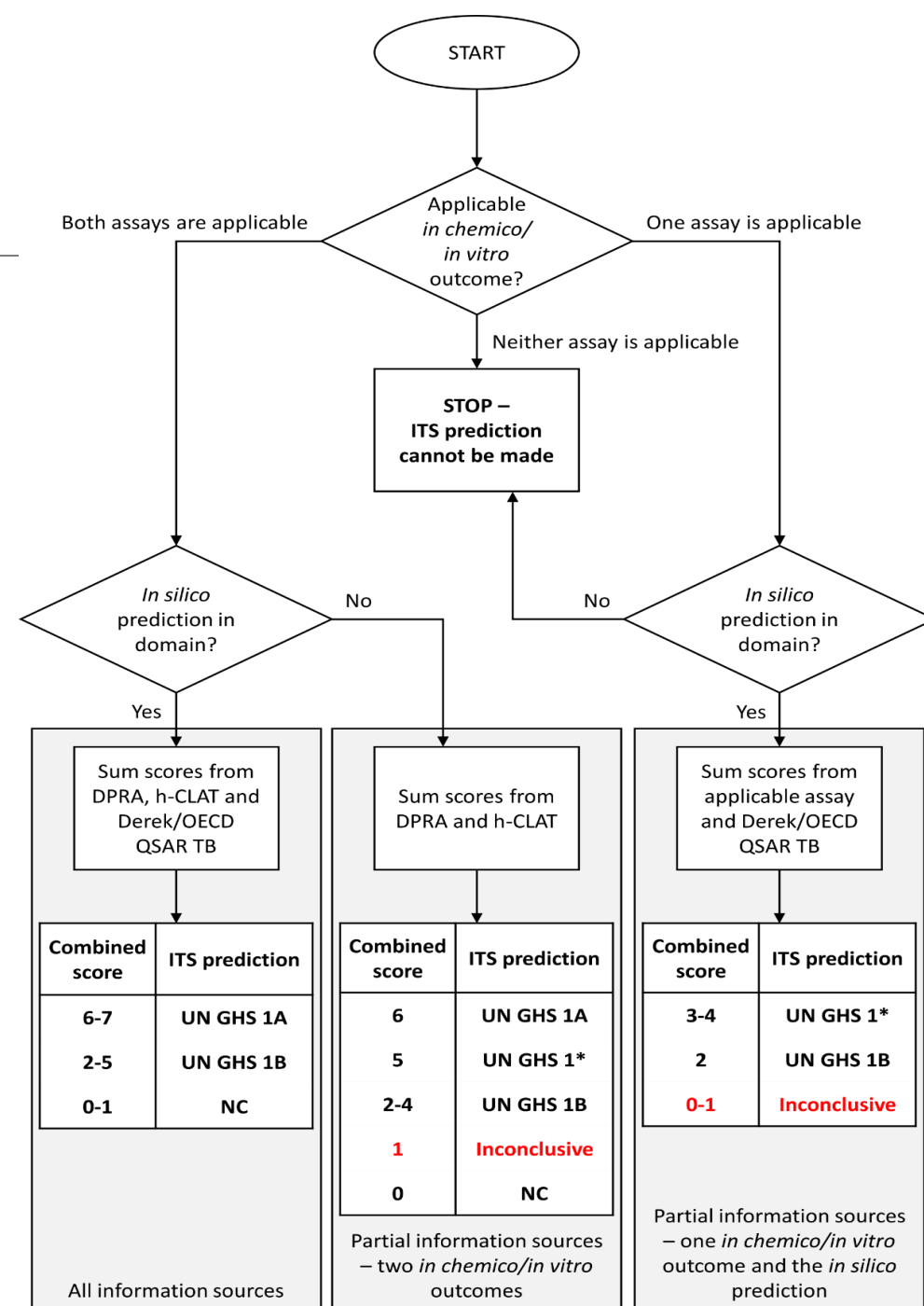
[OECD iLibrary | Guideline No. 497: Defined Approaches on Skin Sensitisation](#)





# QSAR TB prediction in DASS

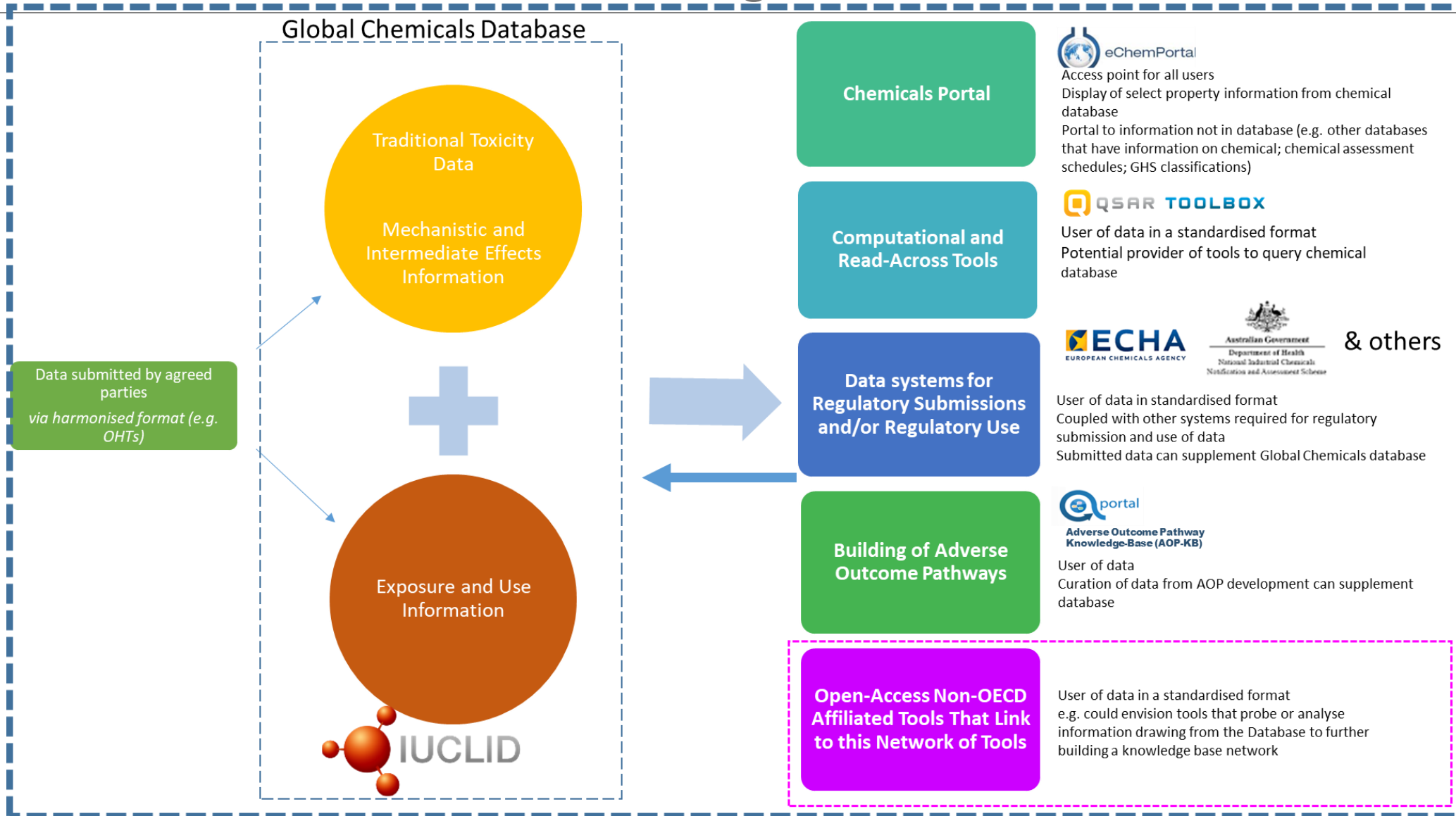
- OECD Expert Groups provided input on:
  - Assuring stability of predictions across versions of Toolbox
  - Including QSAR prediction in report submitted to regulators
  - Defining domain (e.g. based on physical-chemical properties, structure, mechanism)
  - Scoring in silico information source in DASS
  - Consideration of in silico predictions under MAD



\*Conclusive for hazard, inconclusive for potency



# OECD Electronic Ecosystem: Global Chemical Knowledge Base







# Global Use by Regulators



 Environment and Climate Change Canada

 Health Canada



## QSAR TOOLBOX



# Projects ongoing and forthcoming

---

- Continued updates to QSAR Toolbox
  - Version 4.6 expected Q1 2022
  - Near-term planned updates
    - Further alignment and integration between the QSAR Toolbox and IUCLID
      - E.g. improved data filtering and searches
    - Improved Reporting
    - Continued improvements, maintenance and user support
- QSAR Assessment Framework
  - Led by Italy (Istituto Superiore di Sanità)
  - Project under the OECD Working Party on Hazard Assessment
  - Review (and possible update) OECD Guidance Documents
    - [GD 49](#): Principles for the validation of QSARs
    - [GD 69](#): Guidance for Validation of (Quantitative) Structure-Activity Relationship [(Q)SAR] Models