

TYPICAL ACTIONS PERFORMED BY THE TOOLBOX

With the Toolbox a user can

- Describe the structure of a chemical.
- Find out if a chemical is included in national/regional regulatory inventories or existing chemical categories.
- Find out if a chemical has already been assessed by other agencies/organizations.
- Search for available experimental results.
- Explore a chemical list for possible analogues.
- Group chemicals based on mechanism or mode of action or structural similarity.
- Group chemicals based on a common metabolite.
- Identify chemicals with anomalous metabolic pathways or toxicity mechanisms.
- Fill data gaps for chemicals in a category using read-across, trend analysis or QSAR models.
- Fill data gaps for individual chemicals using a QSAR model library.
- Design a data matrix of a chemical category for printing/exporting results.

VERSION 1.0

The first version of the Toolbox was publicly released in March 2008.

WHAT DO I NEED TO INSTALL THE TOOLBOX?

The Toolbox is a stand-alone software designed to work in a Windows® environment on a PC. It requires a processor running at 2GHz or faster, 8 Gigabytes of hard disc space for storage and 1 Gigabyte of RAM to operate. It comes with an easy to use installation Wizard.

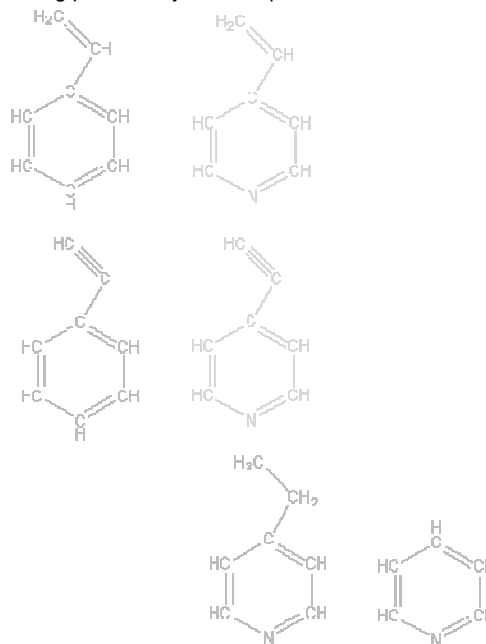
WHERE CAN I GET THE TOOLBOX?

The Toolbox is available free of charge. For download instructions, visit

www.oecd.org/env/existingchemicals/qsar



The OECD QSAR Application Toolbox was developed with funding provided by the European Union.



The OECD QSAR Application Toolbox

- Fills data gaps by read-across and trend analysis
- Groups chemicals into categories
- Gives access to a library of QSAR models



www.oecd.org/env/existingchemicals/qsar

WHAT IS THE TOOLBOX ?

The OECD QSAR Application Toolbox is a software application intended to be used by governments, the chemical industry and other stakeholders to fill gaps in (eco)toxicity data needed for assessing the hazards of chemicals. The Toolbox incorporates information and tools from various sources into a logical workflow. Grouping chemicals into *chemical categories* (see overleaf) is crucial to this workflow.

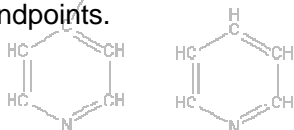
WHAT TOOLS ARE IN THE TOOLBOX ?

The Toolbox contains:

- databases with results from experimental studies,
- a library of QSAR models,
- tools to estimate missing experimental values by read-across, i.e. extrapolating results from tested chemicals to untested chemicals within a category, and
- tools to estimate missing experimental values by trend analysis, i.e. interpolating or extrapolating from a trend (increasing, decreasing, or constant) in results for tested chemicals to untested chemicals within a category.

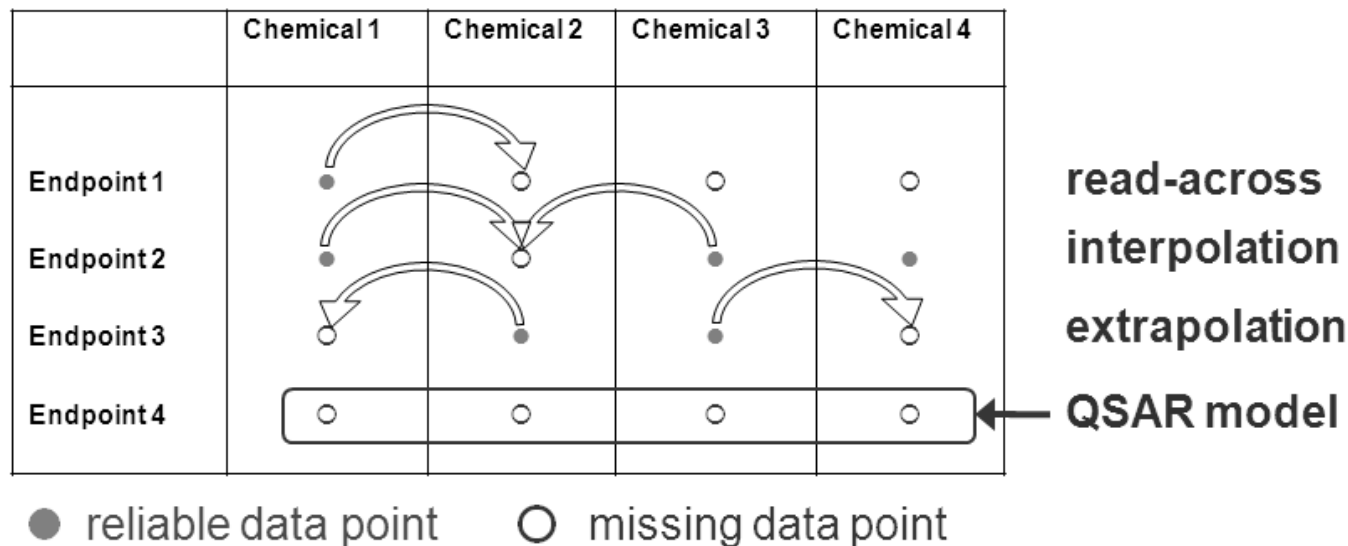
KEY FEATURES OF THE TOOLBOX

The Toolbox allows a user to systematically group chemicals into categories according to the presence or potency of a particular effect for all members of the category. The Toolbox is able to quickly evaluate chemicals for common mechanisms or modes of action as well as for common toxicological behaviour or consistent trends among results related to regulatory endpoints.



WHAT IS A CHEMICAL CATEGORY ?

A chemical category is a group of chemicals whose physical-chemical and toxicological and/or ecotoxicological properties and/or environmental fate properties are likely to be similar or follow a regular pattern because of their similar chemical structure. Using this so-called category approach, not every chemical needs to be tested for every endpoint because the available test results for the members of the category allow an estimation of the results for the untested endpoints.



As illustrated above, a chemical category can be represented graphically as a two-dimensional matrix in which different category members occupy different columns, and the different category endpoints occupy different rows. Data gaps may be filled by read-across from a tested chemical to an untested chemical, trend analysis (interpolation or extrapolation) or related QSAR methods.

WHY THE CHEMICAL CATEGORY APPROACH ?

The category approach used in the Toolbox:

- Focuses on intrinsic properties of chemicals (mechanism or mode of action, (eco)toxicological effects).
- Allows for entire categories of chemicals to be assessed when only a few members are tested, saving costs and animals.
- Enables robust hazard assessment through mechanistic comparisons without testing.

