Typical actions performed by the Toolbox

- Describes the structure of a chemical.
- Indicates if a chemical is included in national/regional regulatory inventories or existing chemical categories.
- Searches for available experimental results for the chemical of interest.
- Explores a chemical list for possible similar chemicals.
- Groups chemicals based on mechanism of action and/or structural similarity.
- Groups chemicals based on a common metabolite.
- Enables exclusion of different chemicals from the group.
- Extracts experimental data for similar chemicals.
- Fills data gaps for chemicals using read-across, trend analysis or QSAR models, where applicable.
- Designs a data matrix of a chemical category for printing/exporting results.
- Connects to IUCLID software for direct data exchange.
- Generates reports.

The QSAR Toolbox

- Facilitates the practical application of grouping of chemicals and read-across approaches for data gap filling.
- Serves as a platform that incorporates various modules and databases from other sources.
- Is applicable to discrete organic chemicals.
- Is available free of charge. Download instructions and free training material are available online at: **www.qsartoolbox.org**

In cooperation:

OECD

ECHA
European Chemicals Agency

ECHA-11-L-08-EN

QSAR TOOLBOX

The OECD QSAR Toolbox for Grouping Chemicals into Categories

http://www.qsartoolbox.org

QSAR TOOLBOX

What is the Toolbox?

The Toolbox is a software application to identify and fill (eco)toxicological data gaps for chemicals hazard assessment. Grouping chemicals into chemical categories is crucial to the workflow of the Toolbox.

What tools are available?

The Toolbox contains:

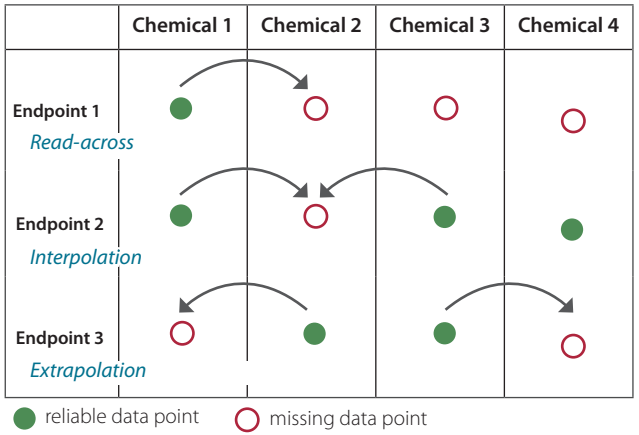
- databases with results from experimental studies;
- accumulated knowledge for structural characteristics (alerts) that can indicate the presence of hazards and other properties, and
- tools to estimate missing experimental values by read-across, by trend analysis (i.e. interpolating (preferred) or extrapolating from a trend (increasing, decreasing, or constant) from tested to untested chemicals within a category) and/or by (Q)SAR models.

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. It allows a quick evaluation of 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?

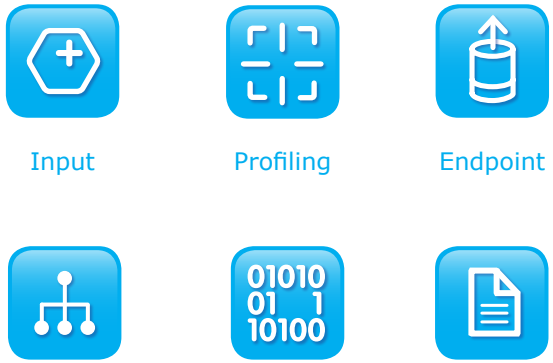
A chemical category is a group of chemicals with physical-chemical, toxicological and/or ecotoxicological properties and/or environmental fate properties that are likely to be similar or follow a regular pattern because of their similar chemical structure. Using this category approach, not every chemical 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 category members occupy different columns, and the category endpoints occupy different rows. Data gaps may be filled by read-across from a tested to an untested chemical or by trend analysis.

Why the chemical category approach?

- It uses an identified mechanism or mode of action of chemicals to justify similarity within the category.
- It allows for entire categories of chemicals to be assessed when only a few members have been tested, saving animals and costs.
- It enables robust hazard assessment through mechanistic comparisons.
- It facilitates the optimisation of testing strategies for members in a category.



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