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Assessment of chemicals

Grouping of Chemicals: Chemical Categories and Read-Across

A **chemical category** is a group of chemicals whose physicochemical and human health and/or ecotoxicological properties and/or environmental fate properties are likely to be similar or follow a regular pattern, usually as a result of structural similarity.

The similarities may be based on the following:

- a common functional group (e.g. aldehyde, epoxide, ester, specific metal ion);
- common constituents or chemical classes, similar carbon range numbers;
- an incremental and constant change across the category (e.g. a chain-length category);
- the likelihood of common precursors and/or breakdown products, via physical or biological processes, which result in structurally similar chemicals (e.g. the metabolic pathway approach of examining related chemicals such as acid/ester/salt).

As a result of these similarities, data gap filling in a chemical category can be carried out by applying one or more of the following procedures: read-across, trend analysis, and (external) (Q)SARs.

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, as illustrated in the following figure.

	Chemical 1	Chemical 2	Chemical 3	Chemical 4	
Structure	xxxxxxxx	xxxxxxxx	xxxxxxxx	xxxxxxxx	
Property 1	● → ○	● → ○	● → ○	● → ○	SAR/Read-across
Property 2	● → ○	○ ← ●	○ ← ●	○ ← ●	Interpolation
Property 3	○ ← ●	○ ← ●	○ ← ●	○ ← ●	Extrapolation
Activity 1	● → ○	● → ○	● → ○	● → ○	SAR/Read-across
Activity 2	● → ○	○ ← ●	○ ← ●	○ ← ●	Interpolation
Activity 3	○ ← ●	○ ← ●	○ ← ●	○ ← ●	Extrapolation

● Existing data point ○ Missing data point

Graphical illustration of a chemical category

In the **read-across approach**, endpoint information for one chemical (the source chemical) is used to predict the same endpoint for another chemical (the target chemical), which is considered to be "similar" in some way (usually on the basis of structural similarity or on the basis of the same mode or mechanisms of action). In principle, read-across can be used to assess physicochemical properties, toxicity, environmental fate and ecotoxicity. For any of these endpoints, it may be performed in a qualitative or quantitative manner.

Qualitative read-across is similar to the use of a SAR, and the process involves:

- the identification of a chemical substructure or mode or mechanism of action that is common to two substances (which are considered to be analogues); and
- the assumption that the presence (or absence) of a property/activity for a substance can be inferred from the presence (or absence) of the same property/activity for the analogous substance.

The main application of qualitative read-across is in hazard identification.

Quantitative read-across involves:

- the identification of a chemical substructure or mode or mechanism of action that is common to two substances (which are considered to be analogues); and
- the assumption that the known value of a property for one substance can be used to estimate the unknown value of the same property for another substance.

In both cases, expert judgement is needed and some justification should be provided.

Guidance on chemical categories and read-across

The following guidance documents have been developed by OECD on chemical categories:

- [Guidance on Grouping of Chemicals](#), second edition Series on Testing and Assessment No. 194, 2014
- [Guidance Document for using the OECD \(Q\)SAR Application Toolbox to develop Chemical Categories according to the OECD Guidance on Grouping of Chemicals](#), Series on Testing and Assessment No. 102, 2009