

SC 11: Experimenting new tools to support read across for environmental and toxicity endpoints

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Abstract

Read across is gaining more and more attention, and is used to assess properties of chemicals and to register substances to REACH. However, currently it is only based on the expert judgment. Within this subjective framework, it is expected that different results are obtained for the same chemical. Conversely, there are toxicity rules, structural fragments, and toxicity pathways that may provide a valuable resource to assist the expert with the identification of suitable similar compounds in read across process.

This course will operatively introduce ToxRead (www.toxgate.eu), a new free software providing a unified view of the toxicological features associated to the target chemical. After entering the chemical and property of interest, similar chemicals are extracted from the database, ordered according to similarity, and graphically shown with experimental values, presence of relevant features, their statistics.

The course will focus on fish acute toxicity and BCF, and show other endpoints. We will compare the read across results with QSARs, giving access to the free models in VEGA-QSAR (www.vega-qsar.eu), and finally discuss how to integrate them within a weight-of-evidence approach.

The course is intended for people working in industry, regulators, scientists; some background in toxicology will be valuable.

Course objectives

- Understand the present methods for read across and their new needs;
- Learn a new software tool;
- Being able of making read across exercises with the help of a dedicated software;
- Integrate results from read across and QSAR within a weight-of-evidence approach;
- Give indications to the developers about new needs and desiderata

Course level

Introductory

Note

Participants should bring their own laptop in order to follow this course