

## QSAR - A TOOL TO FILL (ECO)TOXICOLOGICAL DATA GAPS

### Introduction to the OECD QSAR Toolbox

More and more emphasis is put on the prediction of (eco-)toxicological properties of chemicals from non-testing methods, such as QSAR modelling, to minimise time and cost. The aim of this one-day course is to make you familiar with the OECD QSAR Toolbox to be able to fill data gaps and screen chemicals for harmful properties without new tests.

The OECD QSAR Toolbox has been developed within the OECD chemical programme in collaboration with the European Chemicals Agency (ECHA) to support industry and minimise unnecessary testing. During the course we will use the most recently released version of the Toolbox.

After the course you may be able to use the Toolbox to perform the below tasks:

- To group chemicals into categories (when physiochemical, human health, ecotoxicological and/or environmental fate properties or their modes of action are similar).
- To fill (eco-)toxicological data gaps based on read-across or trend analysis.
- To search for published experimental results in approx. 40 databases.
- To find out if a target chemical substance is included in national regulatory inventories.
- To evaluate the toxicity of pharmaceutical impurities or of chemicals in medical devices.

#### COURSE TOPICS

- Basic theory of QSAR
- Explaining the steps of the OECD QSAR Toolbox workflow
- How to search for data on a chemical in the OECD QSAR Toolbox databases
- How to predict skin sensitisation, AMES mutagenicity potential, etc. of a chemical
- How to use the OECD QSAR Toolbox for REACH registrations

#### TARGET GROUP AND PREREQUISITES

Anyone who wants to explore the possibility of filling data gaps on a scientifically sound basis to save time and money but without having to carry out new laboratory tests. Preferably, you should have good knowledge of chemistry and/or biology, including the various types of toxicity testing and hazard classification end-points.

You are requested to bring your own laptop and the latest version of the Toolbox must be downloaded prior to the course. When you register, you will receive further instructions on how to download the Toolbox.

#### THE ACADEMY BY DHI

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**MIKE Powered by DHI** courses focus on practical skills, hands-on exercises and teaching you how to get the most out of your software. These courses also enable you to understand the power of the MIKE tools for building decision support systems.

**Thematic courses** allow you to apply concepts, applications and decision support principles to the entire business process within current areas: aquaculture and agriculture, energy, climate change, flooding, coast and marine, surface and groundwater, urban water, industry, environment and ecosystems, product safety and environmental risk, etc.

**Our trainers** are experienced professionals, many of whom are recognised international experts in their fields. The use of highly skilled trainers guarantees the quality of THE ACADEMY courses.

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