Led by the developers:

Organized by:

QSAR APPLICATION TOOLBOX
BASIC VIRTUAL TRAINING WORKSHOP
AGENDA

Day 1

I. Basic definitions and general functionalities

At the beginning of the course we cover the core features and terminology of QSAR Toolbox, including document and endpoint trees, data matrix, profilers, target endpoint and more. Explore each of the Toolbox modules - Input, Profiling, Data, Category definition, Data Gap Filling, Reporting and learn the possibilities they offer.

II. Example case studies on predicting ecotoxicological and environmental fate hazards endpoints

In this section, the principles of building category approach hypothesis will be demonstrated with several case studies. Our goals are: (1) to introduce the main information which could be obtained in each of the modules in the system and (2) to demonstrate the process of building and refining chemical categories.

III. Alert performance and its application

A very simple and useful functionality is available in QSAR Toolbox, allowing to estimate performance of functional groups and alerts with respect to a target endpoint. The information obtained from this functionality prove to be crucial in various practical scenarios, such as: (1) evaluating reliability of identified alerts for read across applications; (2) comparing alerts in multifunctional chemicals based on their performance to resolve cases when there are no analogues; (3) identifying alerts with low performance illustrating their inadequacy for searching analogues and read across prediction purposes.

IV. Empirical structural similarity

The main purpose of this topic is to fully understand the importance of accurately applying the calculated empirical structural similarity. When and how to apply it effectively. You will learn about the settings that influence the structural similarity estimation, including the method of estimating similarity according to Tanimoto, Dice, etc., the equation and molecular features used for their calculation. The different measures and setting demonstrate the operation character of similarity. This will be demonstrated with example chemicals.

V. Prediction report

Report of the prediction follows simple templates which are developed in accordance with ECHA requirements. Specific sections of the report will be demonstrated related to reporting AMES mutagenicity data according to TG 471.

Day 2

I. Grouping chemicals based on custom criteria

Functionalities allowing to define a chemical category based on custom criteria such as user-defined fragment or phys-chem property will be introduced. The goal of this topic is to demonstrate how to collect analogues or refine a chemical group in case of lacking appropriate profiler for the endpoint of interest. This will be demonstrated with case studies.

II. Metabolism – simulation and use: Introduction

Consideration of the metabolic activation is an essential component of every toxicological assessment concerning especially human health hazards. In general, the usage of metabolism for read across purposes is a key component of the advanced training. In this context, we introduce straightforward examples to illustrate the importance of metabolic activation in the toxicological evaluation of chemicals and for building the read across hypothesis. Two case studies will be presented demonstrating the assessment of skin sensitization accounting for the metabolic activation.

III. Automated and standardized workflows

Manual read across using the information in the Toolbox sometimes is a time-consuming process, isn't it? What if instead of manual work, the data gaps could be automatically filled in by read-across? Would you say it sounds amazing? The good news is that you'll find out about that very option in Toolbox right here. Our main goal is to present the conceptual algorithms used to build the so-called automated workflows for predicting skin sensitization and acute aquatic toxicity and exemplify them. Key component here is the development of an automated workflow for the purposes of OECD TG 497 which is associated with the defined approaches on skin sensitization (DASS). The DASS automated workflow is in QSAR Toolbox and will be introduced and demonstrated with a few case studies.

IV. Export of data

The system provides a lot of functionalities to export results from QSAR Toolbox, including experimental and predicted data, profiling results, calculated 2D/3D parameters. Additional settings in the exporting functionality allows to filter and select specific information which to be exported.

V. Toolbox Repository

Are you aware that QSAR Toolbox has its own repository and its own collection of plug-ins? It could be accessed directly from QSAR Toolbox or through internet browser, allowing to select and install the plug-ins you are interested in. One of them is the unlocking plug-in of ECHA REACH database which will allow to export data from ECHA REACH database (otherwise you are not allowed to do it).