

QsarDB repository: transparent and reproducible communication of QSARs

This course is not about making QSAR models, but it is about making them transparent, reproducible and accessible. It is intended for all levels of QSAR practitioners. The course gives detailed insights and guidelines on how one can make her/his static published QSAR dynamic and interactive. A solution is demonstrated for the quantitative structure-activity relationship data organization and archival in an extensible format called the QSAR DataBank (QsarDB for shorter, or QDB for shortest) and for the repository, i.e. the collection of the QsarDB archives. The course is divided into the following sections:



9:30 – 10:00 Introduction to QsarDB

Introduction is given on why and how QsarDB has been developed. The first lecture provides detailed description of the QsarDB data schema and data format, and the QsarDB archive layout conventions.

10:00 – 10:30 QsarDB repository

The second lecture introduces the QsarDB repository, i.e. the collection of the QsarDB archives, and the unique digital identifier for the predictive models. Also, various visualization options are presented and how they can be used in everyday application of QSARs.

10:30 – 10:50 Break

10:50 – 13:00 Demonstrations & hands-on experience

- Part 1: Demonstration of the web interface and functionality, practical examples of use
- Part 2: Exploration of the QsarDB archive content
- Part 3: Making a QsarDB archive with command-line tools
- Part 4: Making a QsarDB archive with graphical user interface
- Part 5: Uploading a QsarDB archive into repository

Course outcome: As a result of the course the participants will have greater knowledge about organizing QSAR data and will be able to make their own models accessible via the web in a transparent and reproducible way. Models users will know how to use the QsarDB repository and models therein.

Important: For the hands-on part participants need to provide their own internet enabled laptop computer for use on the course. Wi-Fi will be available at the training venue. Materials for the hands-on part will be delivered for the registered participants.