

SC 1: Transparent and reproducible communication of QSARs

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Abstract

Quantitative Structure-Activity Relationship (QSAR) models are used for understanding chemical processes in toxicology, biomedicine, biotechnology, etc., not mentioning their use for predictive purposes in decision support scenarios. Unfortunately many of the knowledge included in models is not accessible or is in difficult way. QsarDB initiative is about making this knowledge in models transparent, reproducible and accessible. The proposed course is intended for all levels of QSAR practitioners. The course gives detailed insights and guidelines on how one can electronically publish QSAR models so that they are dynamic and interactive and predictions are properly reported. A novel approach is demonstrated and hands-on education is provided for the QSAR data organization in QDB archive format and archival in the QsarDB.org (www.qsardb.org) repository. As a result of the course, the participants will have better knowledge about organizing QSAR data and will be able to make their own models accessible via the web in a transparent and reproducible way. They will know how to use the models in QsarDB repository and retrieve prediction reports.

The course is addressing all four major user groups at different levels of QSAR model development and use: academics, governmental institutions, companies, and consulting organizations.

Course objectives

The main objective is to introduce different user groups to QsarDB concept. In more detail: (a) to give knowledge how to present and archive published QSAR data; (b) how to use and upload models into the QsarDB repository and what functionality is available for the decision support (including reporting predictions).

Course level

Introductory

Note

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