Computational toxicology for regulatory purposes

ProtoQSAR

Module 1: Regulatory aspects for the registration of chemical products

1.1 Basic concepts in regulatory chemistry
1.2 Introduction to CLP Legislation
1.3 Key aspects of REACH Regulation
1.4 Other relevant regulations

Module 2: Computational methods in regulatory chemistry

2.1 Introduction to computational methods
- Representing chemical compounds
- Overview of computational methods
- Application of *in silico* methdos in Regulations

2.2 Analogs and read across with QSAR Toolbox
- Analog identification and categorization
- Read across and trend analysis: basic concepts
- Practical exercises *(Prediction with QSAR Toolbox)*

2.3 QSAR with different prediction platforms
- Workflow of QSAR model building
- Characteristics of different QSAR prediction tools
- Practical exercises *(Predictions with different tools)*