Course title: Computational toxicology for regulatory purposes

Language: English

Modality: Online

Duration: 60 hours of dedication, including video sessions, test sessions, practical exercises and final exercise.

Module 1: Regulatory aspects for the registration of chemical products

Teacher: Arthur Luttenauer

- **Part 1: Introduction, definitions and basic concepts**
- **Part 2: REACH regulation**
  - Overview of REACH
  - Safety Data Sheet
  - Evaluation, authorization and restriction
- **Part 3: CLP regulation**
  - Overview of CLP
  - CLP classification
  - Labelling and packaging
  - Practical exercises *(Classification of a substance)*
- **Part 4: Other regulations**
  - ICH
  - Cosmetics

Module 2: Computational methods in regulatory chemistry

- **Part 1: Introduction to computational methods**
  Teacher: Eva Serrano Candelas
  - Overview of computational toxicology
    Concepts and alignment with regulations
  - Application of computational methods for the prediction of molecular properties
    General workflow, managing molecular structures, basic concepts, introduction to gap-filling methods
  - Specific regulations for (Q)SAR predictions
    Requirements of computational methods for regulatory applications

- **Part 2: Methods based on structural alerts**
  Teacher: Eva Serrano Candelas
  - Understanding SAR
  - Software for SAR analysis
  - Practical exercises with Toxtree

- **Part 3: Read across and trend analysis with QSAR Toolbox**
  Teacher: Martina Palomino Schätzlein
  - Introduction to QSARToolbox
    Traditional interface and brief explanation of the different sections
  - Analogs determination with QSARToolbox
    Workflow, demonstration and practical exercise
  - Read across with QSARToolbox
    Workflow, demonstration and practical exercise
  - Trend analysis with QSARToolbox
    Workflow, demonstration and practical exercise

- **Part 4: QSAR prediction with different platforms**
  Teacher: Enrique Llobet Serra
  - QSAR building workflow
    Data curation, training and validation set generation, descriptor calculation and selection, model building, and validation.
  - QSAR prediction in a regulatory context
    QMRF, QPRF, applicability domain
  - Overview of QSAR prediction tools
  - ProtoPRED
    Overview and practical exercises for human toxicity
  - VEGA
    Overview and practical exercises for mutagenicity
  - OPERA
    Overview and practical exercises for endocrine disruption and environmental
  - ECOSAR and EPISUITE
    Overview and practical exercises

Module 3: Final exercise

- **Course participants will perform a final practical exercise where they will have to apply the knowledge obtained throughout the course. These exercises will be corrected by the course teachers. Questions and doubts can be solved in individual tutorial sessions.**