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
  - Registration with REACH
  - Evaluation with REACH
  - Practical exercises (*FDS and REACH dossier*)
- **Part 3: CLP regulation**
  - Overview of CLP
  - CLP classification
  - Practical exercises *(Classification of a substance)*
- **Part 4: Other regulations**
  - ICH
  - Cosmetics
  - Other
  - Practical exercises

Module 2: Computational methods in regulatory chemistry

- **Part 1: Introduction to computational methods**
  Teacher: Eva Serrano Candelas
  - Basic concepts
    Compound identification, analogs, similarity, categorization, profiling, applicability domain.
  - Overview of computational methods
    Characteristics of computation methods for toxicity prediction
  - Software options
  - Application of computational methods in regulations
  - Practical exercises

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

- **Part 3: Read across and trend analysis with QSAR Toolbox**
  Teacher: Martina Palomino Schätzlein
  - Read across
    Theoretical background. Software options.
  - Trend analysis
    Theoretical background. Software options.
  - Introduction to QSAR Toolbox
    Data handling, grouping, profiling, input.
  - Practical exercises with QSAR Toolbox
    Analogs identification and categorization, trend analysis and read across

- **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
  - ProtoPRED
    Overview and practical exercises in the context of ICH
  - VEGA
    Overview and practical exercises for ecotoxicology
  - OPERA
    Overview and practical exercises for endocrine disruption
  - 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.**