QSAR APPLICATION TOOLBOX, v 4.4.1
BASIC VIRTUAL TRAINING WORKSHOP

AGENDA

Day 1

Two breaks – 15` every hour and half

I. Introducing basic definitions and demonstrating general functionalities

- **Simplified User Interface**
- **Classical User Interface**
  - Document tree
  - Endpoint tree
  - Selecting target endpoint
  - Coloring of profilers/databases
  - Profiling – three layers of the hierarchical profilers; explain profiling result
  - Collecting data
  - Forming categories
  - Data gap filling (relevant subcategorizations)

a. Predicting Acute aquatic toxicity to Tetrahymena pyriformis, IGC50 (CAS # 66-25-1)

b. Predicting fate and ecotox (CAS # 120-82-1)

- Bioconcentration factor - BCF; Cyprinus carpio, 56 days;
- Biodegradation (BOD, 301C, 28d)
- Acute aquatic toxicity (Pimephales promelas, LC50, 96 h)

II. Alert performance and its application – Part I

a. Identifying alerts that could be assumed as SARs

b. Category formation in case of multiple mechanisms in parent

c. Identifying conservative alerts

Examples:

1) Identification of "SAR" alerts - SS, EC3 - CAS # 3934-20-1

2) Multiple mechanisms in parent

– Skin Sensitization - CAS # 366448-53-5

- Ames +S9 - CAS# 60784-46-5

- Identification of "conservative" profilers - Gene mutation - CAS # 98-01-1

III. Prediction report

a. Three layers of the report – only prediction layer to be shown (CAS # 98-01-1)

b. Table with experimental mutagenicity data

Day 2

Two breaks – 15` every hour and half

I. Filtering by test conditions

Example:

1) Predicting acute aquatic toxicity. Fish sensitivity (CAS # 120-83-2)
2) Predicting Ames mutagenicity +S9 (CAS # 9002-92-0)

II. Automated and standardized workflows

a. Aquatic toxicity
b. Skin sensitization
c. Batch mode implementation

Examples:

1) Predicting acute aquatic toxicity (CAS # 120-83-2) – execution of AW and SW
2) Predicting Skin sensitization (CAS # 366448-53-5) - execution of AW and SW

III. Predicting carcinogenicity (CAS # 60784-46-5)

IV. Collecting weight of evidences (WoE)

V. Exporting data. "Unlocking" of ECHA REACH database

VI. Effective use of ECHA REACH data (IUCLID 6.3)

a. BOD: 301F – analysis of the data