

QSAR APPLICATION TOOLBOX, v 4.4
BASIC TRAINING WORKSHOP

BARCELONA, SPAIN

7-8 SEPTEMBER 2020

AGENDA

Monday, 07 September 2019 (09:00 – 17:00)

Two coffee breaks: 11:00-11:30; 15:30-16:00

Lunch: 13:00-14:15

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 # 66251)
 - 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

- Identifying alerts that could be assumed as SARs
- Category formation in case of multiple mechanisms in parent
- 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

- Three layers of the report – only prediction layer to be shown (CAS # 98-01-1)
- Table with experimental mutagenicity data

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I. Filtering by test conditions. Fish sensitivity

Example:

- 1) Predicting acute aquatic toxicity (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. Export data

VI. Effective use of EChA_Chem data (IUCLID 6.2)

- a. BOD: 301F - CAS # 99-71-8
- b. CA: CAS 95-64-7