# QSAR TOOLEOX

The OECD QSAR Toolbox for Grouping Chemicals into Categories

## OECD (Q)SAR Toolbox v.4.4.1

Tutorial on how to predict ecotoxicological endpoint by automated workflow

### **Outlook**

- Background
- Keywords
- Objectives
- Automated workflow
- The exercise
- Report

## Background

This is a step-by-step presentation designed to take the user of Toolbox through the automated workflow for ecotoxicity prediction.

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### **Keywords**

**TARGET CHEMICAL -** chemical of interest

**MODULE –** a Toolbox module is a section dedicated to specific actions and options

**WORKFLOW** – the use, in combination, of the different modules (e.g. prediction workflow: from input to report)

**PROFILER** - algorithm (rule set) for the identification of specific features of the chemicals. Several types of profilers are available, such as structural (e.g. Organic functional groups), mechanistic (e.g. Protein binding by OECD) and endpoint-specific (e.g. in vitro in vitro mutagenicity (Ames test) alerts by ISS) profilers.

**ALERT** - the profilers consist of sets of rules or alerts. Each of the rules consists of a set of queries. The queries could be related to the chemical structure, physicochemical properties, experimental data, comparison with the target or list with substances and external queries from other predefined profilers (reference queries).

**CATEGORY** – "group" of substances sharing same characteristics (e.g. the same functional groups or mode of action). In a typical Toolbox workflow, it consists of the target chemical and its analogues gathered according to the selected profilers

**ENDPOINT TREE** – Endpoints are structured in a branched scheme, from a broader level (Phys-Chem properties, Environmental Fate and transport, Ecotoxicology, Human health hazard) to a more detailed one (e.g. EC3 in LLNA test under Human health hazard-Skin sensitization)

**DATA MATRIX** – Table reporting the chemical(s) and data (experimental results, profilers outcomes, predictions). Each chemical is in a different column and each data in a different row

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### **Objectives**

#### This presentation demonstrates how to:

• Fill data gaps for a single chemical or batch of chemicals by automated workflow for ecotoxicological endpoint

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### Automated workflow (AW) for ecotoxicity Mechanistic understanding

According to **McFarland**, the toxicity to aquatic organisms depends on penetration (log  $K_{OW}$ ) of the chemical, followed by interaction with cellular biomolecules.

### **Ecotoxicological endpoint is:**

- Sub-hazard *Aquatic toxicity*
- Effect *Mortality*
- Endpoint *LC50 (EC50)*
- Test duration 96 h
- Test species **P. promelas**

#### **Workflow components:**

• Except *Input* and *Reporting*, the rest of the Toolbox modules are part of the automated workflow (AW).



### **Workflow components: Profiling**

- The aim is to collect structural and mechanistic information about the target
- Profilers collecting information for the target are organized in two groups:
  - Primary grouping profilers (PGPs):
    - US EPA, Verhaar,
    - MOA,
    - ECOSAR,
    - OFG (without nested)
  - Profilers for subcategorization (PS):

Substance type, Protein binding (OASIS/OECD), Chemical elements, Str. Similarity (ACF-first neighbors, Dice > 50%)



#### **Workflow components: Data**

- Data used in this workflow is for acute aquatic toxicity endpoint (e.g. LC50)
- Databases used in AW are:
  - Aquatic OASIS
  - ECOTOX
  - ECHA REACH
- Endpoint data for LC50 used in AW:
  - *P. promelas* ~ 5400 data for ~ 2400 chemicals
  - O. mykiss ~ 6000 data for ~ 2000 chemicals



### Workflow components: Category building

- The aim is to collect analogues based on global molecular features
- Profilers suitable for primary categorization:
  - US EPA,
  - Verhaar,
  - MOA,
  - ECOSAR,
  - OFG,
  - OFG US-EPA,
  - OFG, Norbert Haider
- The most populated group with data based on the above mentioned profilers is used for data gap filling



### Workflow components: Data Gap Filling

- The aim is to fill the data gap by
  - Read-across (RA), or
  - Trend analysis (TA)
- Trend analysis is the default approach
- Read across is applied if

   Prediction by Trend analysis is not acceptable, or
   The number of analogues is < 10</li>
- Gap filling and subcategorizations are sequence of logical operations (if, then), combined with criteria for acceptance.



#### Workflow components: Subcategorization

- The aim is to increase the similarity of analogues with the target
- It is consecutive process of application of primary grouping profilers (PGPs) and profilers for subcategorization (PS)
- Hierarchy of application of PGPs and PS depends on the number of analogues they have collected
- Sub-categorization process is based on:
  - Sequence of subcategorization steps
  - Criteria for acceptance of subcategorization steps



### Workflow components: Subcategorization

#### Sequence of subcategorization steps:

Mandatory:

- 1. Substance type eliminates not discrete chemicals
- 2. Water solubility (WSKOWWIN + WATERNT)
  - eliminates chemicals with LC50 > WS

Not mandatory:

- 3. Consecutive sub-categorization based on PGPs:
  - US EPA,
  - Verhaar,
  - MOA,
  - ECOSAR,
  - OFG (without nested)
- 4. Consecutive sub-categorization based on PS:
  - Substance type,
  - Protein binding (OASIS + OECD),
  - Chemical elements,
  - Str. Similarity



#### Workflow components: Subcategorization

**Criteria for acceptance of subcategorization step:** 

- Depends on the specific statistical and structural criteria (e.g, experimental error, 95% of residuals, log  $K_{OW}$ , range of variation of the analogues etc.)
- Criteria are different for RA and TA



### Workflow components: Subcategorization

Criteria for acceptance of subcategorization for **Trend** analysis

#### **1.** Sub-categorization by PGPs

**IF** Interpolation **AND** ( $R^2 \uparrow OR 95\%$  of residuals  $\downarrow$ ) **AND**  $NA \ge 10$  **THEN** accept the subcategorization and continue with the next PGP,

**ELSE** reject subcategorization and continue with the next PGP

#### 2. Sub-categorization by PSs

**IF** Interpolation **AND** ( $R^2 \uparrow \mathbf{OR} 95\%$  of residuals  $\downarrow$ ) **AND**  $NA \ge 10$ **THEN** accept sub-categorization and continue with the next PS, **ELSE** continue with the next PS



#### **Definitions:**

Interpolation:  $\log K_{OW}$  of the target should be within the range of  $\log K_{OW}$  of analogues

Correlation coefficient  $R^2 \uparrow : R^2$ increases **OR**  $R^2 \ge 0.85$ 

95% of residuals  $\downarrow$ : 95% of residuals decreases **OR** 95% of residuals  $\leq 1.0$ 

*NA* – Number of analogues

### **Workflow components: Subcategorization**

Criteria for acceptance of subcategorization for **Read** across

#### 1. Sub-categorization by PGPs

**IF** Interpolation **AND** ( $LC50 \downarrow$  **OR** log  $Kow \downarrow$ ) **AND**  $NA \ge 5$ **THEN** accept sub-categorization and continue with the next profiler

**ELSE** reject sub-categorization and continue with the next profiler

#### 2. Sub-categorization by PSs

**IF** Interpolation **AND** ( $LC50 \downarrow$  **OR** log  $Kow \downarrow$ ) **AND**  $NA \ge 5$ **THEN** accept sub-categorization and continue with the next profiler

**ELSE** reject sub-categorization and continue with the next profiler



#### Definitions

Interpolation: log  $K_{OW}$  of the target should be within the range of log  $K_{OW}$  of analogues

 $LC50 \downarrow$ : for the 5 closest analogues the range of variation of LC50decreases **OR** range of variation is  $\leq 2 \log units$ 

log  $K_{OW}$ ↓: for the 5 closest analogues the range of variation of log Kow decreases **OR** range of variation is ≤ 2 log units

NA – Number of analogues

#### **Workflow components**

Criteria for acceptance of **prediction for Trend** analysis:

 After the subcategorization step is accepted then the prediction could be accepted if the criteria are met:



#### After sub-categorization by all PGPs and PS

**IF**  $R^2 \ge 0.7$  **and**  $NA \ge 10$ **THEN** accept the prediction and generate report, **ELSE** switch to Read across

#### **Workflow components**

Criteria for acceptance of **prediction for Read across**:

 After the subcategorization step is accepted then the prediction could be accepted if the criteria are met:

#### After sub-categorization by all PGPs and PS

**IF** Interpolation **AND**  $LC50 \le 2 \log \text{ units } \mathbf{OR} \log Kow \le 2 \log \text{ units } \mathbf{AND} NA \ge 5$ **THEN** accept prediction and proceed with Report

#### Definitions

Interpolation: log  $K_{OW}$  of the target should be within the range of log  $K_{OW}$  of analogues

 $LC50 \le 2$ : for the 5 closest analogues the range of variation of LC50 is  $\le 2 \log units$ 

log  $K_{OW} \le 2$ : for the 5 closest analogues the range of variation of log  $K_{OW}$  is  $\le 2$  log units

#### NA – Number of analogues

The OECD (Q)SAR Toolbox for Grouping Chemicals into Categories



### Workflow algorithm - illustration



The OECD (Q)SAR Toolbox for Grouping Chemicals into Categories

#### Algorithm of Ecotoxicological workflow



### Automated workflow for skin sensitization Summary

- The automated workflow for ecotoxicological endpoint is based on LC50 experimental data only;
- The AW follows the implemented logic and finishes with a prediction;
- The automated workflow (AW) is designed to apply data gap filling for discrete chemicals only;
- The AW does not allow interactions during the workflow process;
- Analogous sets of chemicals are selected based on the hypothesis that the toxicological effects of each member of the category will show a common behaviour;
- AW can be executed for one chemical as well as for a batch of chemicals.

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### **The Exercise**

- In this exercise we will predict the ecotoxicity for:
  - Single chemical CAS# 111-86-4;
  - Batch of chemicals

• This prediction will be accomplished by using of the automated workflow for ecotoxicity prediction.

#### **Chemical Input**

- This module provides the user with several means of entering the chemical of interest or the target chemical.
- Since all subsequent functions are based on chemical structure, the goal here is to make sure the molecular structure assigned to the target chemical is the correct one.

#### **Chemical Input Ways of Entering a Chemical**

- I. Single target chemical
  - Chemical Name
  - Chemical Abstract Services (CAS) number (#)
  - SMILES (simplified molecular information line entry system) notation
  - Chemical with defined composition
  - Drawing chemical structure
  - Select from User's List/Inventory/Databases

#### II. Group of chemicals

- User's List
- Inventory/Database

#### Chemical Input: Single target chemical

- Open the Toolbox.
- Click on "Input" (see next screen shot).

#### Chemical Input Single target chemical



1. Click on <u>Input</u>

2. Differ ways of entering the chemical

#### **Input Single target chemical** by CAS RN



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Location of the Automated workflow for Ecotoxicity



- 1. A dialogue window gives the user a choice to select the endpoint (1);
- 2. Then select OK (2);
- 3. A documentation is available (3).



A workflow controller window is displayed throughout the automated workflow procedure. It includes:

- 1) Workflow name (1);
- 2) General task (2);
- Active task (this is subtask of the general task, which is currently being performed)(3);
- 4) Navigation options (4);
- 5) Activity log (5).

Workflow Controller     Workflow name Ed	r [Automated mode] cotoxicological Endpoi	1		-		×
General task	Defining category	with profile	er [US-EPA New Chemical Categories] $\sim 2$			
Active task Pause Show action log	Gathering data	3		Doc	umenta	tion
AGE 1: INITIAL Retrieving t Subcategoriz Retrieving a Retrieving a Retrieving a Retrieving a Retrieving a	DATA COLLECTION A target ation by profiler all categories for all categories for all categories for all categories for all categories for	AND CHECKS [Substanc profiler profiler profiler profiler profiler	:e type] [Substance type] [Protein binding by OECD] [Organic functional groups (US EPA)] [Acute aquatic toxicity MOA by OASIS] [Organic functional groups, Norbert Haider	(checkmo	1)]	^
Retrieving a Retrieving a Retrieving a Retrieving a Retrieving a Setting sele	all categories for all categories for all categories for all categories for all categories for ected databases to	profiler profiler profiler profiler profiler [Aquatic	[Protein binding by 0ASIS] [Organic functional groups] [Acute aquatic toxicity classification by V [Aquatic toxicity classification by ECOSAR] [US-EPA New Chemical Categories] OASIS,ECOTOX,ECHA CHEM,Aquatic ECETOC] and	erhaar (i inventor	Modifie ies to	ed [
< Copy Log		Ĺ			1	>

- 1) When the workflow finishes a message is displayed that the prediction is accepted (1).
- 2) Also the progress bar is completely filled (2).
- The user has to press **OK** (3).
- 4) Then close the workflow window by pressing X button (4).



#### Data Gap Filling Automated workflow: Single chemical

QSAR TOOLBOX	► Input	Profiling	← Data	► Category definition	01010 01 0 10100 • Data Gap Filling	► Report									• • • × • • ×	
Gap Filling	Workflow														The OECD QSAR To for Grouping Chem into Categories Developed by LMC	olbox icals , Bulgaria
<ul> <li>Documents</li> </ul>	Filter endpoint tree		Ŷ	1 [target]	2	3	4	5	6	7	8	9	10	11	12	13 ^
cument 1 : [C: 1]:Md: 0;P: 1] CAS: 111864 []: [C: 1517;Md: 234;P: 1] Aliphatic Amines (L []: [C: 1560;Md: 234;P: 1] Aliphatic Amine 	Structure			H3C~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~		Ja	~~	nju O	***	-922		Je of	Ŷ.×	No State	NS-	
▼         [C: 88M4 2348: 1] Filter by W           ▼         [C: 88M4 2388] 1] Filter b           ▼         [C: 88M4 2388] 1] Filter b           ▼         [C: 88M4 1569: 1]           □         [C: 68M4 1569: 1]           □         [C: 15M           □         [C:	Structure info     Parameters     Physical Chemical P     Ecotoxicological Inf     Aquatic Toxicity     Mortality     ECS0 <0F     Coto Coto     Coto	roperties and Transport formation R> LC50 alia (animals) hordata (chordates) 2 Actionatesonii (cm	AW SW ,													
		- Pimephales pr	omelas													
<ul> <li>Data Gap Filling Settings</li> </ul>		96 h	118/265	M: 5.15 mg/L M: 5.19 (4.73+5.7) mg/L M: 5.19 mg/L M: 5.19 mg/L T: 6.61 (2.53÷17.3) mg/L	M: 25 mg/L M: 25 (22.6÷27.6) mg/L M: 25.1 mg/L			M: 102 mg/L M: 102 (97.9÷106) mg/L M: 102 mg/L								
✓ Only endpoint relevant	Seament Toxici	ty														-
At this position:	Terrestrial Toxici     Human Health Haza	ity ards		•												
QSARs 0 Automated workflows 0 Standardized workflows 0	Profiling			Discrete shemical												
In nodes below:	Substance ty	ipe.		and the chemical	-											
QSARs 0 Automated workflows 0 Standardized workflows 0																
The prediction	is disp	laved	on	the ma	trix lab	eled	with `	`T″. whi	ch sta	ands f	for tre	end a	nalvs	is:		

The prediction is displayed on the matrix labeled with "T", which stands for trend ana
 "M" stands for measured data.

#### Document 1

# [C: 1;Md: 0;P: 1] CAS: 111864

- IC: 1517:Md: 234:P: 11 Aliphatic Amines (US-EPA New Chemical Categories).
- 🔲 [C: 1680;Md: 264;P: 1] Aliphatic Amines (Aquatic toxicity classification by ECOSAR)
  - 🔺 🌐 [C: 97;Md: 234;P: 1] Enter GF (AW by trend analysis)
    - 🔺 回 [C: 89;Md: 215;P: 1] Subcategorized: Substance type
      - ▲ 〒 [C: 88;Md: 214;P: 1] Filter by WS Exp Water Solubility
        - ▲ ▼ [C: 85;Md: 203;P: 1] Filter by WS Water Solubility
          - T [C: 84;Md: 198;P: 1] Filter by WS Water Solubility (fragments)
            - 🔺 回 [C: 74;Md: 176;P: 1] Subcategorized: Aquatic toxicity classification by ECOSAR
              - 🔺 回 [C: 62;Md: 158;P: 1] Subcategorized: US-EPA New Chemical Categories
                - Ic: 59;Md: 154;P: 1] Subcategorized: Acute aquatic toxicity MOA by OASIS
                  - 4 🔯 [C: 15;Md: 45;P: 1] Subcategorized: Organic functional groups
                    - 🔯 [C: 12;Md: 33;P: 1] Subcategorized: Structure similarity
- C: 537;Md: 94;P: 1] Amine, primary<AND>Aliphatic amine, primary (Organic functional groups)
- 🔲 [C: 264;Md: 65;P: 1] Aliphatic Carbon [-CH3]<AND>Aliphatic Carbon [-CH2-]<AND>Aliphatic Carbon [CH]<AND>Amino, aliphatic attach [-NI-
- 🔲 [C: 523;Md: 94;P: 1] Amine < AND > Primary amine < AND > Primary aliphatic amine (Organic functional groups, Norbert Haider (checkmol))
- C: 627;Md: 190;P: 1] Narcotic Amine (Acute aquatic toxicity MOA by OASIS)

- The steps executed in the AW are listed in the Documents panel;
- Grey highlighted level indicates that at this level a prediction is accepted
- AW always finishes at the level of primary grouping.

In case the prediction does not answer the criteria for acceptance of the prediction (1) or not enough data is collected for primary grouping then the corresponding messages appears, such as: "No enough data to build primary group" or Couldn't find a valid answer"(1)



Click **OK** (1);
 Then close the work

Then close the workflow controller window (2)

### **The Exercise**

- In this exercise we will predict the ecotoxicity for:
  - Single chemical CAS# 111-86-4;
  - Batch of chemicals

• This prediction will be accomplished by using of the automated workflow for ecotoxicity prediction.

#### Data Gap Filling Automated workflow: Batch mode

- There are several ways to load a batch of chemicals amongst which:
- Selection of chemicals from databases/inventories;
- Loading of chemicals from user's file.

(see next slide)

#### List with chemicals (batch work)

**Input:** Ways of Entering a Chemical List



- 1) Database
- 2) Inventory
- 3) List: Last used files/ From examples folder

Data Gap Filling Automated workflow: Batch mode

In this tutorial, <u>Query tool</u> functionality is used to load chemicals with known CAS RNs.

#### Data Gap Filling Automated workflow: Batch mode

| QSRR TOOLBOX   | Delete<br>ase Inventory  | Category definition   | 01010<br>01 0<br>10100<br>ta Gap Filling 		 Re       | eport                    |                       |  |      |      |                   |      |
|--|--|---|--|--------------------------|-----------------------|--|------|------|-------------------|------|
| Documents  | Filter endpoint tree   | 1 [target]  | 2  | 3                        | 4                     | 5  | 5    | 7    | 8                 | 9 10 |
| Databases Databases Defect All De | зта 2  | H3C~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~   |  | Janapoo                  | ~~j£~                 | rgti   | Sec. | -922 | ing D<br>ing Cong | a at |
| Environmental Fate and Transport     Second Social Information     Aquatic ECETOC     Aquatic ECETOC     Aquatic DASIS     ECOTOX     Food TOX Hazard EFSA     Human Health Hazards  | Structure info Parameters Physical Chemical Properties Convincemental Fate and Transport Cookicological Information Aquatic Toxicity Mortality Mortality Coordata (chordates) Chordata (chordates) Chordata comperences) |   |  |                          |                       |  |      |      |                   |      |
|  | 96 h 118/265   | M: 5.15 mg/L<br>M: 5.19 (4.73÷5.7) mg/L<br>M: 5.19 mg/L<br>M: 5.19 mg/L<br>T: 6.61 (2.53÷17.3) mg/L | M: 25 mg/L<br>M: 25 (22.6+27.6) mg/L<br>M: 25.1 mg/L |                          |                       | M: 102 mg/L<br>M: 102 (97.9+106) mg/L<br>M: 102 mg/L |      |      |                   |      |
|  | Sediment Toxicity<br>— Terrestrial Toxicity<br>Human Health Hazards<br>Profiling<br>— Predefined   |   |  |                          |                       |  |      |      |                   |      |
| ✓ Inventories  | Substance type   | 1. Go to<br>2. Then<br>3 <i>. Selec</i>   | go to Data<br>go to Da<br>ct Aquat                   | anel(1<br>ataba<br>ic OA | .)<br>se (2)<br>SIS d | )<br>atabase   | (3)  |      |                   |      |

The OECD (Q)SAR Toolbox for Grouping Chemicals into Categories





- Go to **CAS** tab(1);
   Type in the empty
- field the CAS #: 5428546 (2)
- Click on Add (3) to add CAS #. Repeat steps 2 and 3 to add the next 3 CAS #: 90017; 62533; 110407;
- 4) Click on **Add** (4)to create the query (5);
- 5) Click on **Execute** button(6).



- 1) Select *Data gap filling* tab (1);
- 2) Click on Automated (2);
- 3) Select **Ecotoxicological endpoint** (3) from the pop-up window (4);
- 4) Click on **OK** (5).

|    |   | 💽 Select one - 🗆 🗙   |
|----|---|--|
| 1) | A dialogue window gives<br>the user a choice to<br>select the endpoint (1); | Aquatic toxicity<br>Which data do you want to use?<br>I<br>Fish, LC50(EC50) at 96h for Pimephales promelas (mortality) |
| 2) | Then select <b>OK</b> (2).  |  |
|    |   | Documentation OK Cancel  |
|    |   | 2  |

- A <u>Workflow</u> <u>controller</u> window appears, which is not active(1);
- The pop-window <u>Select range (2)</u> is displayed where the user has to select the range of chemicals from the set, which has to be predicted;
- 1) Finally press <u>OK (</u>3).

| y 💽 Workflow Controller [Automated mode  | 2]  | ×             |
|--|---|---------------|
| Workflow name Ecotoxicological En<br>General task<br>Active task<br>Pause Stop | Select the range on which to execute the wor X >= 1 <= 4 Ok | Documentation |
| Show action log  | 3   |               |

- When the workflow finishes, there is an indication in the title of workflow controller(1).
- Also the progress bar is completely filled (2).
- The predictions are displayed on the matrix(3). There is also an indication that 4 out of 4 chemicals are predicted
- 4) Finally close the workflow window by pressing X button (4).

| Filter endpoint tree           | <b>Y</b> 1                    | 2                     | 3                            | 4                      |
|--------------------------------|-------------------------------|-----------------------|------------------------------|------------------------|
| Structure                      | 🖉 Workflow Controller [Finish | ed workflow]          | 0                            |                        |
| 1                              | Workflow name                 |                       |                              |                        |
| Structure info                 | General task                  | Retrieving diff       | erent analogues for profiler | [Structure Similarity] |
| Parameters                     | Active task                   |                       |                              |                        |
| Physical Chemical Properties   | Pause Sto                     | op                    |                              | Documentation          |
| Environmental Fate and Transpo | Charles and the second        | 1                     |                              |                        |
| Ecotoxicological Information   |                               | /                     |                              |                        |
| Aquatic Toxicity               | AW S Z                        |                       |                              |                        |
|                                |                               |                       |                              |                        |
| └────── EC50 <or> LC50</or>    |                               |                       |                              |                        |
| Animalia (animals)             |                               |                       |                              |                        |
| Chordata (chord                | ates)                         | 3                     |                              |                        |
| Actinoptery                    | gii (ray-finned               | 5                     |                              |                        |
| Pimepha                        | les promelas                  |                       |                              |                        |
| 96 h                           | 4/4 R: 28                     | .4 (0.621÷1 T: 253 (4 | 13.1÷1.4 T: 2.85 (0.2        | 13÷3 R: 65.1 (11.5÷36  |
| Sediment toxicity              |                               |                       |                              |                        |
| — Terrestrial Toxicity         |                               |                       |                              |                        |
| 🕀 Human Health Hazards         |                               |                       |                              |                        |

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#### List with chemicals (batch work)

#### Report: Generation of report

An this stage, it is not possible to generate a report for chemicals predicted in batch mode.

The system kindly informs you that *Predictions from batch mode cannot be reported.* 

### **Congratulations!**

- You have completed the tutorial on the automated workflow for ecotoxicological endpoint.
- You have been introduced to the automated workflow in a single and in a batch mode.
- You have now been introduced to the consecutive steps of the AW for ecotox and the rationale behind each step.
- Note, proficiency comes with practice!