

# Short-term toxicity to fish example

## **Introduction to OECD QSAR Toolbox**

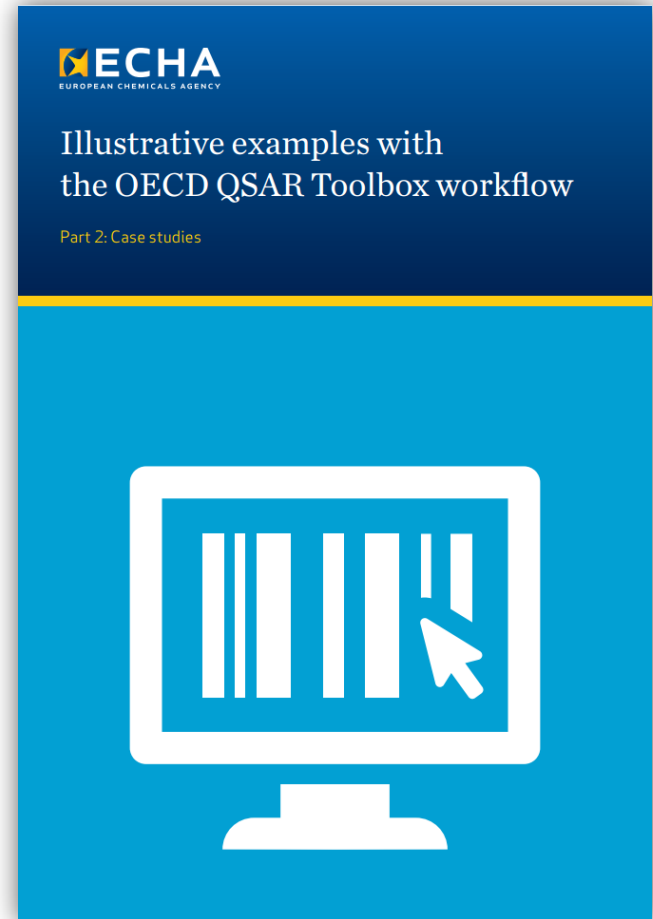
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# Content

- Illustrative example on short-term toxicity to fish of propriophenone
  - What to consider for a reliable and adequate prediction using the Toolbox
  - Not a tutorial on how to use the software



# Endpoint: short-term toxicity to fish

- Relevant for REACH 2018 registration deadline
- Recommended OECD test guidelines require testing on vertebrate animals

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Illustrative examples with the OECD QSAR Toolbox workflow

## 2.6 EXAMPLE 4. PROPIOPHENONE

The fourth example illustrates the workflow for a quantitative assessment of fish short-term toxicity for propiophenone (CAS number 93-55-0, SMILES: C(-O)(c1ccccc1)CC).

### 2.6.1 Input

The structure can be introduced in the Toolbox using the drawing tool, the CAS number or the SMILES notation. A structure could also be selected by a database, inventory, or user list.

### 2.6.2 Profiling

The outcomes of the endpoint specific profilers for aquatic toxicity are:

- Class 5 (Not possible to classify) (Acute aquatic toxicity classification by Verhaar)
- Basesurface narcotics (Acute aquatic toxicity MOA by OASIS)
- Neutral organics (Aquatic toxicity classification by ECOSAR)

Figure 23 shows the results of the profiling for the target chemical (black font indicates no alert; while red font highlights the presence of alerts; yellow indicates parameters which have not been calculated in the Toolbox).

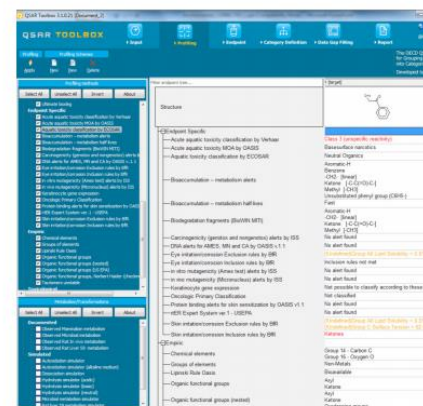


FIGURE 23. PROFILING RESULTS FOR THE TARGET CHEMICAL.

# Hands-on exercise



# Thank you!

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