Modeling Regulatory Threshold Levels for Pesticides from Effect Databases

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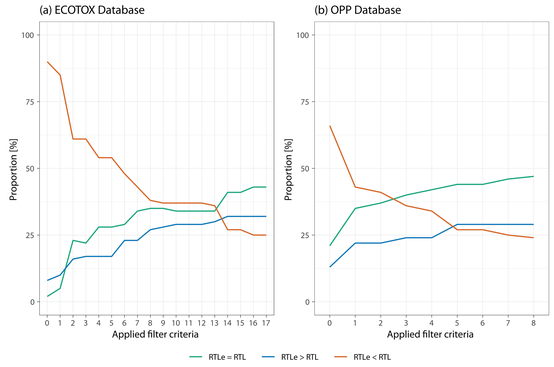
1. Problem

The **manual** compilation of **regulatory threshold levels** (RTL) for pesticides from U.S. EPA regulatory documents is very **time-costly** and especially for a **large number** of pesticides **not feasible.**

Consequently, **scientific risk evaluations** [1-2] were **restricted** to a small number of RTL (n=27 [1], n=32 [2]) such that only a small proportion of actually occurring **pesticides in surface waters** could yet be evaluated in terms of their **risk potential** for aquatic ecosystems.

To enable **comprehensive**, scientific risk evaluations, **solutions** are urgently needed.

Methods



Influence of the consecutive application of formulated filter criteria on the proportion of substances for which **RTLe** were correct, underestimated or overestimated the **RTL** (a) in the ECOTOX and (b) OPP database.

2. Solution

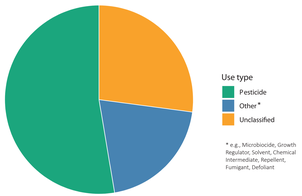
Develop a model, that estimates RTL (RTLe) from available effect data relevant to U.S. EPA pesticide regulation

Use two large databases containing pesticide effect data:
- ECOTOX database [3]
- OPP database [4]

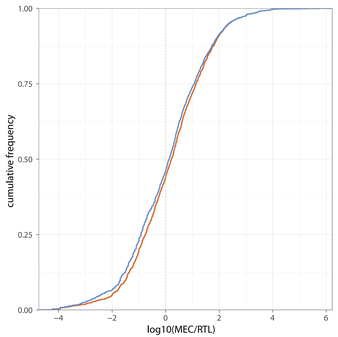
Translate quality criteria into SQL to exclude invalid endpoints following official (test) guidelines [e.g., 5-9]

Calculate thresholds based on selected, remaining effect data

Receive 1,284 acute freshwater RTLe



3. Case study



Exceedance rates of measured environmental concentrations (MEC, n=3001, 1962 -2017, [2]) for 27 pesticides were calculated for RTL and RTLe:
- mean difference: 3.6 percentage points (95%-CI 2.2 - 5.4)
- mean exceedance rates:
  - RTL: 55.8% (95%-CI 51.8 – 59.8)
  - RTLe: 52.0% (95%-CI 48.0 – 56.0)

→ No statistically significant difference between the exceedance rates was observed, underlining the model's usability for scientific risk evaluations.

Data quality

Validation. Model precision was determined by comparing RTLe to a set of manually retrieved RTL (n=143; calibration dataset: n= 94, validation dataset: n=49). There was no significant difference in model precision between calibration data estimates and validation data estimates (Wilcoxon rank sum test, ECOTOX: p=0.63; OPP: p=0.47).

Deviation. 96% of RTLe deviated +/- 1 order of magnitude from the RTL, 88% of RTLe lay within +/- 0.5 orders of magnitude.

Bootstrapped model precision. Mean ratio RTLe/RTL: 1.21 (1.04– 1.42 95%-CI; median=1)

→ Model precision is high with a tendency to slightly overestimate the RTL resulting in liberal thresholds

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[4] US Environmental Protection Agency (2017) OPP Pesticide Ecotoxicity Database, updated 03/16/2017. Available: https://www.epa.gov/pesticide-science-and-assessing-pesticide-risks/ecotox-database (03/2018)
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[6] US EPA (2016), Ecological Effects Test Guidelines OCSPP 850.1210 Acuatic Invertebrate Acute Toxicity Test, Freshwater Daphnids. Available: https://www.regulations.gov/document?D=EPA-HQ-OPP-2009-0314-0041 (12/2019) pp. 1–17.
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