Session 2: Ecotoxicological Databases

Theoretical Ecotoxicology

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About me

- **Paul Ozoh** (Master in Ecotoxicology)
  - **PhD** Student
  - Ecotoxicology working group (Ecotoxicology_UDE)

- **Research interests:**
  - Large scale ecotoxicology risk analysis
  - Chemical risk assessment
  - Data analytics and visualisation

- **Current work**:

- "**Benchmarking pesticides** environmental risk assessment to support a transition towards a holistic paradigm"

Learning objective

- Understand the fundamental basis of risk assessment
- Which are the common databases to get ecotoxicological risk assessment data?
- How can we access these databases automatically?

Risk Assessment

- What is risk assessment?

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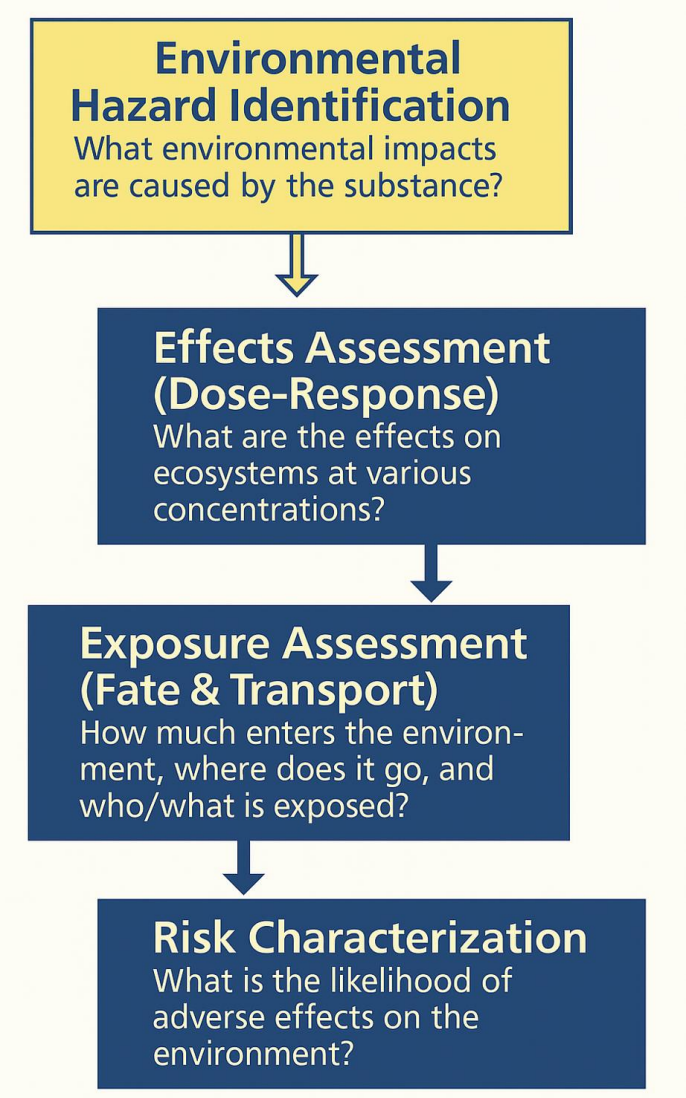
Risk Assessment

- What is risk assessment ?

- Risk assessment is a process that evaluates the likelihood of adverse **effects** that may occur due to **exposure** to one or more stressors (Tarazona and Ramos-Peralonso 2014; Damalas and Eleftherohorinos 2011; Finizio and Villa 2002).



Risk Characterisation – deterministic approach

- Most often used in environmental risk assessment

- Comparison of a point estimate of **exposure** (e.g. Predicted Environmental Concentration (PEC) value) to a point estimate of **effect** (e.g., LC_{50}, EC_{50} value, etc.)

- **Assessment (safety) factors** (AF) are often used (between 10 - 1000); applied to toxicity endpoints (e.g., LC_{50} / 100)

- Calculation of **risk quotients** (aquatic organism):
  Exposure / Toxicity (incl. AF) > 1 → **Risk**
  Exposure / Toxicity (incl. AF) < 1 → **No Risk**

➡ Output: point estimate of risk (single value; “yes or no decision“)

Risk Assessment- Types

Priori type (or prospective)**:**

- environmental releases have not yet occurred (chemical is not in use)
- e.g., **pesticide** registration
- exposure must be modelled/estimated; effects can be assessed for a few species only

➡ *Regulatory Risk Assessment of Pesticides in the EU*

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➔ *Regulatory Risk Assessment of Pesticides in the EU*

Post hoc (or retrospective):
- contamination has occurred, the chemical is in use
- e.g., mining sites, spills, pesticide application
- exposure and effects can be measured/observed; „real“ exposure and effects (but:
uncertain in space and time; measurements may be biased)

➔ *Environmental Risk Assessment of Pesticides - Global Field Data*

Pesticide Risk Assessment- EU

Goal: Ensure pesticides are safe for humans and the environment.

Who is responsible?

- The EU makes the rules: EU Regulation No. 1107/2009 (in force since 2011*).
- **EFSA** (European Food Safety Authority) checks the science.
- Each EU country (**Member State (MS)**) approves products.

How it works:

Step 1: EU approves the active ingredient.
Step 2: MS approve the actual pesticide

(*formerly: Directive 91/414 EEC: authorization of PPP and their active substances)

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How Are Risks Assessed?

Tier 1: Simple and very cautious ("worst-case" assumptions)

Higher Tiers: More detailed and realistic (uses field data, models, etc.)

Ecotoxicological risk assessment

- Mammals and birds
- Aquatic organisms
- Bees
- Arthropods other than bees
- Soil organisms
- Non-target soil micro-organisms
- Non-target plants

EU Pesticides Database

- A centralised, official EU database for pesticide safety, regulatory status, and residue levels.
- **Key Features**:
  - Active Substance Information: Approval, restrictions, classification
  - Maximum Residue Levels (MRLs): Food/feed residue limits by substance or crop
  - Regulatory Documents: EFSA opinions, legislation, peer review reports
  - Search Tools: Filter by crop, residue, product type, etc.

European Commission | EU Pesticides Database

https://ec.europa.eu/food/plant/pesticides/eu-pesticides-database/start/screen/active-substances

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EFSA OpenFoodTox

- OpenFoodTox enables structured, reproducible, and transparent risk assessments in EU food safety.
- Covers 4,800+ substances evaluated by EFSA since 2002.

Key Features:

- Includes toxicological reference values: Acceptable Daily Intake (ADI), Acute Reference Dose (ARfD), Tolerable Daily Intake (TDI), No Observed Adverse Effect Levels (NOAELs), etc.
- Hazard endpoints: genotoxicity, carcinogenicity, reproductive and neurotoxicity
- Chemical identifiers: CAS, SMILES, with links to PubChem and others.
- Available as Excel, CSV, JSON for integration and modelling

EUROPEAN FOOD SAFETY AUTHORITY

https://www.efsa.europa.eu/en/data-report/chemical-hazards-database-openfoodtox

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Other Public Databases

ECHA EUROPEAN CHEMICALS AGENCY

ECHACHEM ECHA CHEMICALS DATABASE

https://chem.echa.europa.eu/

- To access detailed information on the properties, hazards uses, and regulatory status of chemical substances registered in the EU

PPDB

https://sitem.herts.ac.uk/aeru/ppdb/

PPDB (Pesticide Properties DataBase)

- Provides information on the environmental and toxicological properties of pesticide active substances.

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Other Public Databases

https://chem.echa.europa.eu/

- To access detailed information on the properties, hazards uses, and regulatory status of chemical substances registered in the EU

https://qsartoolbox.org/

Quantitative Structure-Activity Relationship (QSAR)

- To predict the properties and potential hazards of chemicals using computational models and existing data, supporting chemical risk assessment and regulatory decision-making.

https://sitem.herts.ac.uk/aeru/ppdb/

PPDB (Pesticide Properties DataBase)

- Provides information on the environmental and toxicological properties of pesticide active substances.

https://pubchem.ncbi.nlm.nih.gov/

- A free, open-access database that provides detailed information on the chemical structures, properties, biological activities, and safety data of millions of compounds.

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Developed Packages to access Databases

Standartox

- To standardise ecotoxicity data from various sources, enabling consistent and comparable assessments of chemical toxicity across species and studies

data MDPI

Data Descriptor

Standartox: Standardizing Toxicity Data

Andreas Scharmüller [1,2,*], Verena C. Schreiner [1] and Ralf B. Schäfer [1]

Data, 5(2), 46.| **DOI**: 10.3390/data5020046

ChemLook

https://github.com/andschar/chemlook

- A GitHub project that enables users to retrieve chemical substance data from various online sources—e.g. PubChem, PubMed, and ChemSpider.

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webchem

- an R package for users to retrieve chemical information from online databases such as PubChem, ChemSpider, and EPA CompTox.
- It streamlines access to identifiers, properties, and structure data

webchem: An R Package to Retrieve Chemical Information from the Web

Eduard Szöcs, Universität Koblenz-Landau
Tamás Stirling, Independent Researcher
Eric R. Scott, Tufts University
Andreas Scharmüller, Universität Koblenz-Landau
Ralf B. Schäfer, Universität Koblenz-Landau

Journal of Statistical Software, 93(13), 1–17| **DOI:** 10.18637/jss.v093.i13

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Take note!

- Calculation of aquatic organism **risk quotients** (RQ):

  Exposure / Toxicity (incl. AF) > 1 → **Risk**

  Exposure / Toxicity (incl. AF) < 1 → **No Risk**

- Example:
  - Exposure = PEC = 0.5 mg/L
  - Toxicity = EC_{50} = 1 mg/L
  - AF = 100 (Acute Aquatic organism –Tier 1)

$$RQ = \frac{PEC}{(Toxicity\ /\ AF)}$$

RQ = 0.5/(1/100) = **50** → **Risk or No Risk?**

Questions?

➡ *Time for Exercise*

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