Predicting Fate of Plant Protection Products

Marc-Sven Roell
Bayer Crop Science
Early Environmental Safety

22th Sep 2023
EMBL-EBI Industry Programme Workshop
Environmental Fate of Plant Protection Products

Impact of Plant Protection Products on Environmental Microorganism

Predicting Fate
Environmental Fate of Plant Protection Products

Impact of Plant Protection Products on Environmental Microorganism

Predicting Fate
Environmental Fate of Plant Protection Products

All the above processes are investigated by Environmental Fate, for the active ingredient and its transformation products (metabolites), generally in studies with radio-labelled test compounds.
Environmental Fate of Plant Protection Products
Environmental Fate of Plant Protection Products

- Environmental Fate Studies
- A.I. & Metabolites
- Ecotoxicological Studies
- Substance Properties
- Effect Data (Hazard)
- Environmental Modeling
- Exposure
- Environmental Risk Assessment
Environmental Fate of Plant Protection Products

**Efate**
- **What** will be in the environment?
- **How much & how long** will be in the environment?

**Exposure Modeling**
- What will be the **exposure** in the environment?

**Ecotox**
- What will be the **effect** on organisms in the environment at the PECs?

**Effect Modeling**
- What will be the **effect** for the environment & organisms?

**Environmental Risk Assessment**
- Is there a real hazard or is the **risk** negligible?

**A.i. & metabolites**

**Kinetics & substance properties**

**Predicted environmental concentrations (PECs)**

**Acute and chronic toxicity endpoints (NOEC, ECx)**

**Effect data & Potential Hazard**

**Comparison & balance of exposure & effect**
Environmental Fate of Plant Protection Products

Impact of Plant Protection Products on Environmental Microorganism

Predicting Fate
Ecotoxicological Tests

Microorganism

“This Test Guideline describes a laboratory test method designed to investigate the long-term effects of chemicals, after a single exposure, on nitrogen transformation activity of soil microorganisms.” (1995)
Content

Environmental Fate of Plant Protection Products

Impact of Plant Protection Products on Environmental Microorganism

Predicting Fate
Defining Health – Predicting Fate

Intrinsic Chemical Properties
- PhysChem
  - logP
  - Water Solubility
  - Molecular Weight
  - Melting Point

Sorption

Environmental Physicochemistry
- pH
- CatEx Capacity
- Organic C

Biology
- Microbes?
- Enzymes?

Intrinsic Chemical Properties

Bioavailability

Biology of Environmental Compartment
Microbiomics is key to reduce environmental impact and deliver solutions to farmers

How does soil, rhizosphere and leaf biome impact product performance?
Early Environmental Safety workflow to support Safety-by-Design approach

The Design-Build-Test-Learn Cycle:

- **Rational molecule design and optimization**
- **Feed data into in silico models**
- **Develop predictive screening assays**
- **Generate data for environmental profile**
Predicting Fate of Plant Protection Products

Marc-Sven Roell

Bayer Crop Science
Early Environmental Safety

22th Sep 2023

EMBL-EBI Industry Programme Workshop