

# FOOTPRINT

Functional Tools for Pesticide  
Risk Assessment and  
Management

The Pesticides Properties Database



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## Why we need a database



- > Minimises data input
  - Essential for FOOT-FS
  - Will ensure all tools use a harmonised data set
  - Helps ensure model results are transparent
- > Existing data sets inadequate
  - Poor range of active substances
  - Too many data gaps
  - Poor evidence of validation & maintenance (*many not being updated*)
- > Will ensure data is -
  - Reliable, consistent & fit for purpose
  - Common syntax, units and semantics
  - Available for ad-hoc browsing and for integrating into software
  - Valuable to wide range of users


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## What does it contain

- > General pesticide information e.g.
  - Names - common, generic, alias's & EU registration data
  - Chemical group, pesticide type, formula, structure, CAS & molecular mass
- > Physicochemical data e.g.
  - SG/BD, Pka, solubility, VP, Hd, Log P, Koc, Kf, 1/n
  - DT50: soil, hydrolysis & photolysis, water-sediment systems
- > Ecotoxicology e.g.
  - Fish, aquatic invertebrates, algae, higher aquatic plants
  - Mammals LD50 & NOEL, birds, honeybees, earthworms (*not part of FOOTPRINT*)
- > Human health e.g. (*not part of FOOTPRINT*)
  - WHO, ADI, AOEL, exposure limits
  - General descriptions & Dangerous Substance Directive List I




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## Where has data come from

- > EU 91/414 Evaluation Dossiers
- > Country Registration Authorities & Government departments (e.g. PSD, Danish EPA, US EPA)
- > National datasets (e.g. Agritox, Exttoxnet, ChemID)
- > Environmental NGOs (e.g. FAO, PAN)
- > Manufacturers (e.g. Syngenta, Monsanto, KingTai)
- > Scientific literature (e.g. Journals, Pesticide Manual, Agrochemicals Handbook)
- > Colleague datasets, research datasets



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## How has data been chosen



- > Data confidence scoring applied to data - highest scoring data selected first. Depends on:
  - data origin
  - published date
  - adequacy of reference
  - match to desired parameter
  - fitness for purpose
- > Fate data - mean of data available
- > Ecotox data - reasonable worse case data



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## Database Access



- > Baseline data as MS Access Database
  - format allows for integrating directly into software applications
  - allows easy updating and maintenance
  - portable
  - licence fee required if database distributed to third parties with other software applications
- > On-line
  - MS Access database streamed through filters to
    - generate HTML pages and index
    - generate layman interpretations using standard regulatory thresholds or widely used ' rules of thumb ' and hazard indicators
    - translation in to European languages (*under development*)
    - search facilities, Q&A, update log
    - access free of charge



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## Comparison with other datasets



Parameter	PPDB (670 records)	AGRITOX (100/370 record subset)
General description & generic name	100%	100%
CAS RN Number	100%	99%
Chemical formula	99%	94%
Molecular mass	100%	94%
Structural picture	94%	51%
Relative density / bulk density	78%	0%
Pka (nb: data not always relevant)	48%	32%
Aqueous solubility	97%	90%
Partition Coeff Log P	95%	77%
Vapour Pressure	95%	85%
Henry's constant	87%	59%
Soil DT50	86%	64%
Sorption Coeff Koc	80%	44%
Aqueous photolysis DT50	49%	37%
Neutral hydrolysis DT50	66%	86%
Water-sediment system DT50	35%	25%
Bioconcentration data	45%	18%
Toxicity - mammals	99%	97%
Toxicity - birds	87%	82%
Toxicity - fish	93%	84%
Toxicity - aqueous invertebrates	89%	76%
Toxicity - honeybees	76%	74%
Toxicity - earthworms	56%	46%
Toxicity - algae	75%	61%
Toxicity - higher aquatic plants	31%	14%



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## Next steps



- > Continue developing language translation filters
- > Continue filling data gaps and improving data quality
- > Update as new active substances become available



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