

The Pesticide Properties Database

And its sister databases on biopesticides and veterinary substances

August 2025





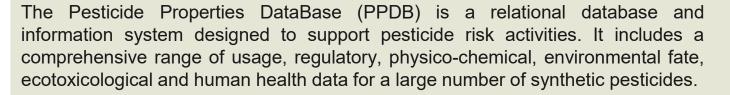
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Introduction



A related system – the Biopesticide Properties DataBase (BPDB) – holds similar data for biopesticides which includes plant- and insect-derived chemicals, semiochemicals, beneficial viruses and bacteria, as well as micro- and macro-organisms.

There are two other related data sets. Firstly, the Veterinary Substance DataBase (VSDB) holds similar data to the PPDB and BPDB for substances used in veterinary medicine. Secondly, our dataset on 'Other related substances' includes data for biostimulants, synergists and safeners, adjuvants, wood preservatives, bactericides and other biocides.

All four datasets have a similar structure and presentation format. They share the same website and user facilities. This presentation focuses on the PPDB but will also briefly describe the data differences.



PPDB history

The PPDB began in 1994 as part of a research project to develop an environmental management system for agriculture (EMA). EMA was released as a CD-ROM and included a simple database of pesticide properties to support the pesticide risk module within it.

Over time, due to requests to share, the database grew in terms of the number of active substances it contained data for, and the range of parameters stored. Eventually, EMA was retired but certain aspects, including the pesticide database, were retained and moved on-line.

This opened up the database globally and significant demand coupled with the ever more demand for data by pesticide risk assessments the database continued to expand. To ease data management the database was sub-divided into the four data sets we now have.

Some 30 years later we are going from strength to strength, still developing and expanding and our user-base grows year on year.



02 Data content

The PPDB holds data related to the following broad categories:

- I. Substance overview, usage and regulation
- II. Substance identification
- III. Physico-chemical properties
- IV. Environmental chemistry and fate plus quality judgements
- V. Terrestrial and aquatic ecotoxicology plus quality judgements
- VI. Human health
- VII. Handling, storage, waste and transport



(i) Substance overview, usage and regulation

- □ Brief summary of data in the record
- General description of the substance
- ☐ Simple colour-coded data alerts based on data within the record
- □ Information on types of applications including crops, pests and diseases, brands & formulations.
- □ EU, UK and other country regulatory status
- Availability status and key dates
- □ Regulatory and environmental status of the chemical including for example: PFAS, VOCs, PIC substances, marine pollutants.

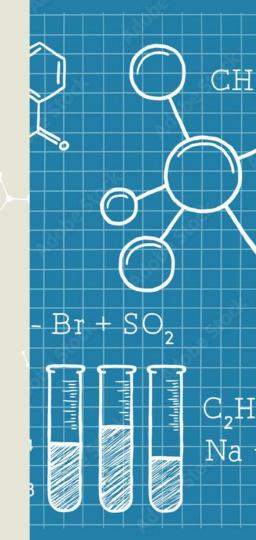


(ii) Substance identification

In this section of the database there is the following information:

- ☐ Chemical/pesticide class
- □ IUPAC and CAS chemical name
- □ Common names and synonyms
- □ CAS number, EU number & other numerical ID's and codes
- □ Chemical formula & molecular mass
- □ SMILES and InChI
- □ 2D and 3D structures
- □ Regulatory and environmental status of the chemical including for example:

PFAS, VOCs, substances subject to PIC regulations, marine pollutants



(iii) Physico-chemical properties

- ☐ Physical state & appearance
- □ Solubilities in water & organic solvents
- Melting, boiling & decomposition points
- □ Flammability, Flashpoint
- □ Vapour pressure, Henry's constant & volatilisation
- ☐ Chemical formula & molecular mass
- □ Surface tension
- □ Refractive index
- UV-vis absorption



(iv) Environmental chemistry & fate

- ☐ Soil adsorption & mobility data
- □ Degradation rates for soil, water, air & plants
- ☐ Hydrolysis and photolysis
- ☐ Metabolites for surface waters, groundwater
- ☐ Embedded links to separate metabolite pages
- □ Environmental fate indices including
 - □ GUS & SCI-Grow
 - □ Particle-bound transport
 - □ Bioconcentration
- □ Data quality assessments (Quality Barometer, QB)



(v) Ecotoxicity

- Acute and chronic terrestrial ecotox data
 - □ Mammals & birds
 - ☐ Bees (honeybees, bumblebees, mason bees)
 - ☐ Earthworms & soil micro-organisms
 - ☐ Beneficial insects & terrestrial plants
 - □ Data interpretations
- □ Acute and chronic ecotox data
 - ☐ Fish (temperate & tropical species)
 - ☐ Invertebrates & sediment dwellers
 - ☐ Higher & lower aquatic plants
 - Marine bivalves
 - □ Data interpretations
- □ Data quality assessments (Quality Barometer)





(vi) Human health

- ☐ Oral, dermal and inhalation toxicity data
- □ Other toxicity endpoints
- □ Weight of evidence-based health issues including:
 - □ Carcinogenicity & genotoxicity
 - □ Developmental & reproduction toxicity
 - Neurotoxicity
 - □ Irritancy
- ☐ Health-based guidance values: ADI, ARfD, AOEL, AAOEL
- □ CPL hazard warnings
- WHO classification



(vi) Handling, storage, waste & transport

- □ Dangerous properties e.g. explosive, oxidising
- ☐ Incompatible substances
- ☐ Transport information & UN number
- ☐ Waste disposal & packaging information
- ☐ Storage information, shelf-life
- □ Chemical stability



System formats

Database access is available via two main ways:

Firstly, our online databases are free to use subject to compliance with our terms and conditions of use. These web pages contain no adverts and no links to third-parties except where we have a formal collaboration agreement and we actively share data. No login or user profile are needed. The website displays about 80% of the pesticide data we hold.

Secondly, we offer our data in MS Access or MS Excel formats for a fee under time-limited usage licences. This format allows the data to be used off-line and linked to 3rd-party applications and systems. The fee payable depends on the data required, licence length, number of users and update requirements. In addition to the data provided online, licence holders can opt to also receive additional, more indepth data, for example, on degradation rates and soil adsorption.

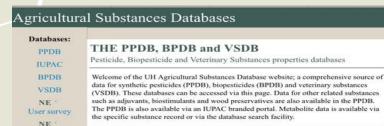


PPDB home page

Newsletter Aug

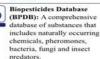
Screen shots of the online system.





Pesticide Properties Database (PPDB): The main PPDB website that includes chemical identity, physicochemical, human health and ecotoxicological

Click here to access this database



Click here to access this database

comprehensive database of Mancozeb

(Also known as: manzeb)

database

IUPAC PPDB: The

the PPDB. This contains the

delivery pages.

IUPAC-branded version of

same information as the

main PPDB website but

Click here to access this

Veterinary Substances

DataBase (VSDB): A

using IUPAC-branded

SUMMARY

These databases have been developed and are manager Environment Research Unit (AERU) at the University Mancozeb is a fungicide that was once commonly used. It has a users to support risk assessments and risk management to leach to groundwater. It is not persistent in soil systems but nMammals - Acute oral LD₁₀₀ (mg > 5000

Database home page

Macrocystis integrifolia extract Macrocystis pyrifera extract Magainin 2 peptide Magnesium phosphide Malathion Maleic hydrazide

Maleic hydrazide choline

Maleic hydrazide potassium Maleic hydrazide sodium

Malic acid

Malonoben

Mancopper Mancozeb

Mandestrobin

Mandipropamid

Maneb

Mazidox MCPA

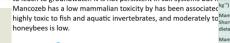
MCPA-butotyl MCPA-butvl

Snippit of the PPDB A-Z index.



Pesticide profile pages.

A5 Rat Mammals - Chronic 21d NOAEL 70 A5 Rat Reproductive Moderate (mg kg⁻¹ bw d⁻¹) Birds - Acute LDso (mg kg-1 A5 Anas platyrhynchos A4 Colinus virginianus Birds - Chronic 21d NOEL (mg A5 Anas platvrhvnchos Moderate kg⁻¹ bw d⁻¹) Ecotoxi Earthworms - Acute 14 day LCso > 299.1 A5 Eisenia foetida Moderate (mg kg⁻¹) Earthworms - Chronic NOEC, A5 Eisenia foetida Moderate



Data alerts

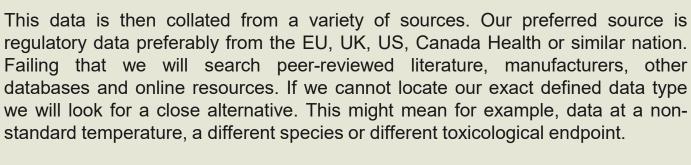
The following alerts are based on the data in the tables below. A Birds - Short term dietary implications for human health, biodiversity or the environment b

Environmental fate

Data sources and choices



Firstly, we define each data parameter in terms of meta-data. For physicochemical and environmental fate data this might be in terms of, for example, measurement conditions and reporting metrics. For ecotoxicity it is in terms of the tested species, toxicological end point and reporting metric.



The result is that our datasets are as complete as they can be, but they are not 'pure' – meaning that the data type may not be identical for each pesticide. This information is communicated to the user via an associated text description and our unique Quality Barometer (QB). The QB is a two-part code which conveys the broad data source type and our confidence in the data quality. Data quality is allocated via a simple rule-base assigning a number 0-5 (low-high).

Data management



- ☐ The core database has been developed in an off-line MS Access format. This database consists of 20+ tables and hundreds of parameters.
- □ To aid data management, a bespoke Data Management Software system has been developed in-house which allows data to edited, added, searched and displayed off-line. It also allows us to keep tract of updates, data sources and other management data.
- □ Data is updated regularly using our data protocols. These describe each parameter, its meta data and preferred reporting format. This helps ensure data integrity and uniform data presentation.
- □ The Data Management System validates data entry, checks for erroneous entries and ensures embedded links function. It calculates indices, the data alerts and applies the interpretation rules. It then automatically writes the hundreds of HTML pages for the PPDB website.
- ☐ The Data Management system can also export data selected from the core database for external clients in MS Access or MS Excel files.

The <u>next slide</u> provides a schematic of the data management system.





Data collated from scientific publications, regulatory documents & databases. Data is reformatted, interpreted & used to populate the core PPDB.





Data management protocols & data quality assessments ensure data integrity. Data is updated regularly.

CORE PPDB



PPDB Core system is a MS Access database.



Data is stored, updated and maintained off-line using AERU-UH in-house developed management software.



Management software checks the data, external links and writes static HTML pages for uploading to the public free-to-use PPDB website.



Data exports to MS Access or MS
Excel sold under time-limited
licences to UH external clients.
Data also used by AERU to
support research contracts.

Behind the scenes



Our collaborators

We collaborate with various organisations. This enables us to offer additional data and facilities on the website. For example, the 3D chemical structure diagrams are provided by the Cambridge Crystallographic Data Centre. We also have good working relationships with the pesticide industry who provide data and help validate our data sets.



Art of presentation

We try to present our data in a logical and structured manner. Our clients are varied from laypersons to risk assessment professionals and regulators. The pesticide profile pages include data interpretations, pop-up windows to provide additional information and help icons for understanding the data.



Tracking usage

Whilst our online users do not need login names or accounts to use the PPDB, we do have a data tracker which helps us keep track of the broad user location and how they access and use the data. It also tells us the most population pages and when our documents are downloaded.

BPDB, **VSDB** & Other substances



Biopesticides

- □ Same structure as PPDB.
- Includes plant- & insectderived chemicals, pheromones, beneficial bacteria and virus's, micro- and macroorganisms.
- Some additional data.
- ☐ Separate web-pages and substance index.



Veterinary

- □ Same structure as PPDB.
- Stores data for veterinary pharmaceuticals.
- Some additional data.
- Some additional data sources.
- ☐ Separate web-pages and substance index.



Other substances

- □ Same structure as PPDB.
- □ Stores data for biostimulants, synergists, safeners, adjuvants, wood preservatives, bactericides & other biocides.
- Some additional data sources.
- □ Included as a sub-index to the PPDB.

User support facilities

Various user support facilities are available on the website including:

- A search facility which allows specific pesticides to be identified by various names, codes and identifiers.
- □ Each database has a main A-Z index to help identify specific substances quickly.
- ☐ There are a number of useful documents on the website giving detailed information on the databases and how they should be used.
- Other documents are also available including newsletters, posters, presentations, videos and associated publications.
- □ Licensing details and fees.
- □ Error reporting form.
- You can print out individual records for reference.
- ☐ Or email us aeru@herts.ac.uk





Hints and tips



- ☐ Can't find a pesticide in our system? Pesticides are often known by many different names. Use the search facility which works using chemical names, common names, synonyms and the CAS number.
- ☐ Metabolites are best found using the link from the parent page.
- Pesticide data, especially that for ecotoxicity. is notoriously variable. Different data from different sources doesn't necessarily mean one is wrong. It might just be from a different study. We try and give the worse case data for ecotoxicity.
- Our data records are rarely complete for a number of reasons. The data might not exist, we might not have found it or we may have rejected it. We don't guarantee we have all the data or that our data is error-free. Talk to us if something is missing or doesn't look right.
- Remember our data sets are not 'pure' and so it's important to take careful note of the supporting associated text fields.
- Remember data is not fixed. It can and does change regularly as new data emerges and risk assessments evolve. Data on the website is the most up to date. Data issued under licence as Access or Excel are snapshots of the data on the issue date. It might contain different data to that online.

Licensing, T&Cs and services

- Data on our websites are free to use subject to compliance with our <u>Copyright</u> and <u>Terms and Conditions of Use</u>.
- □ Data is issued as MS Access and MS Excel subjected to payment of a fee for a time-limited licence.
- ☐ The fee is based on the amount of data required, what you intend to use the data for and how many people will access the data. Discounts are given for multi-year licences. Full information can be found on the PPDB website.
- ☐ We can create bespoke data sets for you.
- We can develop datasets for you.
- We will consider adding your data to our system for public dissemination talk to us.



Example applications



Policy & monitoring

- □ Development evidencebased pesticide policies.
- □ Policy support for food and water companies.
- Development of water quality monitoring programmes.
- Screening studies.



Research

- □ Development of risk assessment models and similar tools.
- □ Chemical discovery applications.
- ☐ In silico property predictions
- Exposure mapping



Risk assessments

- Data sets for models and decision support systems
- □ Indicator development
- □ Al applications
- ☐ Grower exposure assessments.
- Species specific studies (e.g. bees, beneficial arthropods)

PPDB & Pesticide Indicators

- UK Pesticide Load Indicator (PLI): The UK PLI consists of 20 load metrics: 4 environmental fate metrics (incl. persistence and mobility) and 16 ecotoxicity metrics (incl. toxicity to non-target wildlife species) from the PPDB. These metrics are combined with estimates of the mass of application (based on the UK PUS) to examine patterns in load across space and time. The PLI is being used to support a national target to reduce pesticide load by at least 10% by 2030, using 2018 as a baseline year (as outlined in the UK Pesticides National Action Plan 2025). The work is funded by the Defra and undertaken in collaboration with Fera Science.
- Pesticide risk indicator for the Convention on Biological Diversity: The PPDB team are contributing to an expert group convened by the FAO to help develop a methodology for Headline indicator 7.2 under the monitoring framework of the Kunming-Montreal Global Biodiversity Framework (GBF)...
- □ **FEAST:** The Farmland Ecosystem Assessment Support Tool (<u>FEAST</u>) software (developed by AERU as part of their H2020 <u>FrameWORK</u> project) has been adapted to include the metrics within the UK PLI and GBF to facilitate the calculation of farm level pesticide load.



10 Contact details

Do you have any questions?

For licensing & purchasing email Dr Andy Green: a.green@herts.ac.uk

For website, technical, and other issues email: aeru@herts.ac.uk





Thanks

CREDITS: This presentation template was created by <u>Slidesgo</u>, and includes icons by <u>Flaticon</u>, and infographics & images by <u>Freepik</u>

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