

## The University of Hertfordshire Pesticide Properties DataBase – Common Questions & Answers

This document seeks to provide information regarding the PPDB and to answer a number of common questions regarding the terms and conditions of use, and various aspects of the data and its presentation. Information on the management and data acquisition of the database can be found in a document ‘Background and Support’ that is available on the PPDB website. A simple guide to using the database ‘PPDB Instructions for use’ is also available.

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## What is the Pesticide Properties DataBase?

The Pesticide Properties DataBase (PPDB) is a comprehensive relational database of pesticide physicochemical, toxicological, ecotoxicological and other related data.

The database has been developed by the Agriculture & Environment Research Unit (AERU) based at the University of Hertfordshire, UK. It has developed from a database that originally accompanied the EMA (Environmental Management for Agriculture) software (also developed by AERU), with additional input over the past 2 decades from various research activities.

## What data is held in the database?

The database holds data for around 2000 pesticides, 750 metabolites and 600 other related substances (including biostimulants, adjuvants, wood preservatives). Biopesticides and veterinary substances are held in separate databases (the BPDB and VSDB respectively). These two databases follow the same protocols as the PPDB. PPDB data can be broadly divided into the following areas:

1. General data including a range of identity codes, structural descriptors, chemical names, synonyms, language translations, classification systems, country registrations and broad usage information.
2. Physicochemical property data which can influence the environmental fate and transport of pesticides. Also included are a number of pre-calculated fate indices.
3. Ecotoxicological data for a comprehensive range of terrestrial and aquatic taxa both acute and chronic.
4. Human health information including risk and safety information, toxicity endpoints, exposure limits, health issues, ADI, ARfD, AOEL, AAOEL and drinking water MACs.
5. Layperson interpretations based on regulatory thresholds and commonly used rules-of-thumb. These parameters are only available on the website and NOT in the MS ACCESS or EXCEL formats as data is calculated automatically by the code generating the webpages.
6. Information on commercial products including brand names, companies using or selling the active substance (often historic data), associated substances (other actives, parent compounds, adjuvants and inert materials used within the products) and examples of formulations and application. This type of information is not intended to be exhaustive or comprehensive, just illustrative.
7. A simple data hazard alert system, generated using the interpretation of the substance properties to categorise each substance into one of three groups: high (red), moderate (yellow) or low (green) with respect to environmental fate, ecotoxicity and human health. This indicator system is only available on the website and is NOT in the MS ACCESS or MS EXCEL databases as data is calculated automatically by the code generating the webpages. However, these data can be added to these formats for a small additional fee.

## How is it different from other existing databases?

In contrast to other databases, the PPDB is rather extensive in the number of compounds it covers (ca. 3000+ records). The need for this has been three-fold. Firstly, in order to be utilised by pesticide risk systems used across the EU it has been necessary to include all active substances used in the EU and, secondly, due to considerable interest from further afield, including developing countries, we have

broadened the data further. Finally, metabolites and adjuvants added to product formulations might also cause environmental issues but very few pesticide databases include them - we have tried to fill a data gap.

Researchers and other users of pesticide data will recognise the problems of finding useful, quality data. Data are often scattered across many resources on- and off-line and data identification is often a frustrating and time consuming activity. The PPDB seeks to solve this problem by bringing the best data together in a single, harmonised dataset. Also, the PPDB is updated on a very regular basis. It is not unusual for us to update daily.

Previous databases tend to have been developed with specific goals in mind (such as a particular model, a specific discipline (e.g. aquatic risk or human health) or to support use or registration within a specific country. Therefore they have tended to cover a small number of substances in detail or have a restricted number of properties for a wide range of substances. As a result they often have limited applications. In contrast the PPDB has adopted a 'broad' and 'deep' approach ensuring application to many modelling, risk and decision support systems thus ensuring a consistent data set.

## Where does the data originate?

The best sources of information currently available for pesticide properties are the monographs/dossiers produced as part of the EU review process and published by EFSA. These documents have been used in priority for putting together the PPDB. Where EFSA documents are not available or if additional data is needed, alternative sources are used. These include:

- Regulatory dossiers from other countries e.g. UK, USA, Australia, Canada and New Zealand. These tend to follow similar structures and include similar parameters as those of the EU.
- Public domain databases and documents from various national government departments including the databases from the European Commission's DG Health & Consumers, European Chemical Agency, UK's Chemical Safety Directorate, Germany's Federal Environment Agency, Health Canada and the US Environmental Protection Agency.
- Peer reviewed scientific publications and data derived from research projects and reports.
- We have also used databases such as ESIS (European Chemical Substances Information System), TOXNET and other health related databases.
- Manufacturer's safety datasheets, technical information and environmental fact sheets, on- and off-line.

In a limited number of instances where data is scarce, it has been collated from miscellaneous on-line sources. In order to indicate our confidence in the data, all data within the PPDB is 'tagged' with a code so that its source and quality can be identified (see below).

## What is the quality of the database?

We have taken the utmost care in selecting data and transferring it correctly to the database. We have also cross-checked different datasets against each other as a means of ensuring data integrity. Several of our end users have undertaken independent quality assessments and peer reviews and we are delighted to say few issues have been reported. Still, we would be most grateful if you could let us know if you identify an error. There is a form to complete on our website and is found under the 'Support' section.

**Please note that the PPDB team cannot be held responsible for any loss or action resulting from the use of the data held in the PPDB.**

Pesticide data by its very nature can be highly variable. Just because two separate references quote different values does not mean that one is incorrect. Where different sources of data have given widely different values, we have attempted to validate them at source, going back to original publications where possible.

As mentioned previously, each data item is tagged with a code that allows the source of the data to be identified. Information on these codes can be found in the 'Background and Support' document available on the PPDB website. The tag also includes a confidence score, ranging from 1 (low) to 5 (high), which reflects the faith we have in the quality of the data. If the information is unreferenced or from a potentially unreliable source, it will have a low score. If a data item can be verified and its source identified then its quality score is increased. For EU data and those derived from national regulators, the quality score will normally be 5. In some instances, the quality score may be downgraded to 4 where there is an element of doubt such as in cases where the endpoint reported is different from our first choice. It should be remembered that the quality assessment process is a subjective process. A low score does not imply the data is incorrect and equally a high score does not mean it is accurate.

The database is actively updated as additional information is identified and new/higher quality data becomes available. You will find the date of the last update of the database on the PPDB website <https://sitem.herts.ac.uk/aeru/ppdb/>. It is normally displayed in the top left-hand corner of the A-Z Index page and at the bottom of each individual record. There is also an 'Edit history' option on the home page of the database that will provide general update information.

## How are pesticide property values selected?

The data quoted for physicochemical properties is usually a mean value of the various studies identified. Where data is particularly sensitive to climate or soil, a text field providing the data range has been added. Where data is just naturally very variable, we have attempted to select that most appropriate for temperate conditions. Additional information can be found in the 'PPDB Background & Support Information' document available as a pdf download on the website.

For biodiversity impacts we usually report the worst case value for that particular species.

Health data is somewhat different and depends on the specific issue but, because the PPDB has an international focus and different countries use different assessment and classification processes, we use a 'weight of evidence' approach considering all of the information we have identified. This might mean (in rare cases) that our data varies from that in a particular document. For example, there are multiple different classification systems that classify substances according to their potential carcinogenicity, each of which use different criteria and types of evidence. Sometimes these schemes do not agree on whether or not a substance is a carcinogen. They also tend to use different terminology making the landscape confusing. In the PPDB we consider all the available information from multiple sources (e.g. CLP data; US EPA, US NTP, OSHA, IARC, publications) and use a rule base to classify the data into four classes –

**Yes** (majority of our data sources agree the substance is carcinogenic),

**No** (majority of our data sources agree the substance is not carcinogenic),

**Possible** (data is conflicting/ambiguous or there is insufficient data to make a sound judgement),

**No data** (we have not identified any useful information).

Key data used in this interpretation can be found below the table in the 'General human health issues' text field.

For genotoxicity the majority of our data that classifies a pesticide into a specific genotoxicity type (Chromosome aberration, DNA damage/repair, Gene mutation and Genome mutation) has been taken (with EFSA approval) from the EFSA Genotox database. Other data has come from various data sources including regulatory dossiers and tends to be broader. Similar to carcinogenicity, we use a 4 point classification system:

1. Positive (the substance has been classified as a genotoxin),
2. Ambiguous (the data and information we have is inconclusive),
3. Negative (substance has not been classified as a genotoxin),
0. No data (we have not identified any useful information).

For endocrine disruption our data interpretation tends to follow Commission Regulation (EU) 2018/605 and similar regulations for US, Canada and Australia. We don't consider specific endpoints but just whether or not regulatory dossiers consider the substance an endocrine disrupter.

For endocrine disruption and all other health issues we use a four point classification system:

- ✓ (our data supports the health issue as positive)
- ✗ (our data supports the health issue as negative)
- ? (The data we have is inconclusive or ambiguous),
- No data** (we have not identified any useful information).

## Can you explain the Data Alert system?

Full details of how this system works can be found via the blue icon next to the 'Data alerts' title on each pesticide record or alternatively via [https://sitem.herts.ac.uk/aeru/ppdb/en/docs/Data\\_alerts\\_rules.pdf](https://sitem.herts.ac.uk/aeru/ppdb/en/docs/Data_alerts_rules.pdf).

## What are the interpretation thresholds and where did these originate?

A full description of the interpretation thresholds and where they originated is available on the 'Data Interpretation' page of the online database. Alternatively the same information is given in the 'PPDB Background and Support' document available as a pdf download on the website.

## How can I obtain a copy of the database to use off-line or link with our systems?

The database can also be obtained as an MS ACCESS or MS EXCEL file on request. This is useful for working off-line or for direct linking to third-party software. Please contact us if you wish to integrate the VSDB into your computerised tools as this will be subject to a modest licence fee to cover the production and updating costs. Details of this can be found in the 'Purchasing and Licensing' section of the database website. The actual cost will depend upon the intended use of the data and the amount of data required. When contacting us please provide the following information:

- Intended purpose of the data (e.g. in-house purposes, research project, commercial application, etc.).
- What data is required (all or specific sub-set?)

- Whether or not regular updates are required. Quarterly updates for the period of the licence agreement are included as standard, but updates can be provided more frequently if needed.
- Your contact details.

You will be required to sign a time-limited licence agreement. The licence will prohibit the transfer of the data to third parties and use of the database must be acknowledged (see below). Please look at our Terms and Conditions of Use document which is also available on the database website. Using our databases implies acceptance of these Terms and Conditions.

Please note that we include a small amount of support time with the licence. If you think you might need more than a couple of hours support time then you will need to contact the database administration to discuss your needs and the likely cost.

Contact information:

Email: [a.green@herts.ac.uk](mailto:a.green@herts.ac.uk) or [aeru@herts.ac.uk](mailto:aeru@herts.ac.uk)

Telephone: +44 (0)1707 284548

## Can I use the information in the database?

The information contained in the PPDB web pages can be used free of charge provided proper reference to the database is given. This reference should also be included when linking to the database from other websites. The general reference that should be used to refer to the database is as follows:

Lewis, K.A., Tzilivakis, J., Warner, D. and Green, A. (2016). An international database for pesticide risk assessments and management. *Human and Ecological Risk Assessment: An International Journal*, **22**(4): 1050-1064. DOI: 10.1080/10807039.2015.1133242

If you are using and so referencing pesticide dissipation on or in plant matrices then the following reference may be appropriate:

Lewis, K. & Tzilivakis, J. (2017). Development of a data set of pesticide dissipation rates in/on various plant matrices for the Pesticide Properties DataBase (PPDB). *Data*, **2**(3), 28. DOI: 10.3390/data2030028

When referring to wild bee toxicity data, the below may be more appropriate:

Lewis, K.A. & Tzilivakis, J. (2019). Wild bee toxicity data for pesticide risk assessments. *Data*, **4**(3): 98. DOI: 10.3390/data4030098

The data on this website and in the standalone MS ACCESS and MS EXCEL databases should be referred to as the 'Pesticide Properties DataBase (PPDB)' and not the 'FOOTPRINT' database. The FOOTPRINT database was a subset of data specifically used to support the EU Framework Programme FOOTPRINT project. The FOOTPRINT database is no longer available.

We do not permit extraction of the data in order to populate other databases without a licence. If you are using the free online PPDB we do not offer support but you will find extensive support and guidance information on our website.

## Can I link directly to the PPDB web pages?

If you would like to link to the PPDB, you may only do so on the basis that you comply with the following conditions otherwise we will consider it a breach of IPR/Copyright:

- a. You do not replicate either the PPDB Home page or A-Z page of this website without our express written permission.
- b. You do not remove, distort or otherwise alter the size or appearance of the logos.
- c. You do not rename or replace the headings or other content such that you imply wrongful ownership.
- d. You email us and inform us that you have made the link - ([a.green@herts.ac.uk](mailto:a.green@herts.ac.uk)).
- e. You do not create a frame or any other browser or border environment around this Website or any page within.
- f. You do not in any way imply that we are endorsing any products or services other than our own.
- g. You do not misrepresent your relationship with us nor present any other false information about us.
- h. You do not otherwise use any PPDB content displayed on this Website without our express written permission.
- i. Your website does not contain content that is distasteful, offensive or controversial, infringes any intellectual property rights or other rights of any other person or otherwise does not comply with all applicable laws and regulations.
- j. The PPDB owners cannot be held responsible for any loss or action resulting from the use of the data held in the PPDB.

We expressly reserve the right to revoke the right granted by this statement and take any action we deem appropriate.

## Third party links from the PPDB

Links to third party websites from this Website are provided solely for your convenience. If you use these links, you leave the PPDB. We have not reviewed these third party websites, we do not control them, nor are we responsible for their content or availability. We do not endorse or make any representations about them or their content.

## Can I get detailed support?

We do not offer support if you are using the free online version of the database. However, there is extensive information on the PPDB website. Should you wish to report an error please use the form on the website which can be accessed under 'Support'. If you would like to purchase support please contact the database administrator ([a.green@herts.ac.uk](mailto:a.green@herts.ac.uk)).

A small amount of support is given to clients who have purchased a licence to use the database off-line. All support requests will be considered on a case-by-case basis. Simple questions will, of course, be answered but more detailed and extensive queries may incur a small fee. Please contact the database administrator ([a.green@herts.ac.uk](mailto:a.green@herts.ac.uk)) for more information.

## What to do if you disagree with our data or think something is missing

If you think a data item is incorrect, by all means complete the form on our website, return to the email address below and we will investigate it for you.

If you think we should include other information or other substances please let us know and we will consider your request. Ideally email us a copy of relevant information or provide us with the reference.

## Other related services

- Provision of the database in alternative formats - e.g. MS ACCESS or MS EXCEL.
- Customised / branded portals to the database. The PPDB/IUPAC site is an example of this see: <http://sitem.herts.ac.uk/aeru/iupac/index.htm>.
- Specialised software for interfacing to the database e.g. to allow desktop off-line interrogation or customised formatting.
- Database updates and licence renewals.
- Data analysis.

Please contact us with your requirements.

## Contact details:

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