Agricultural Substances Databases
Instructions for Using the Web Versions

The document aims at providing basic information on how to use the Pesticide Properties DataBase (PPDB) and its sister products: the BioPesticide DataBase (BPDB) and Veterinary Substance DataBase (VSDB). Information on the Terms and Conditions of Use can be found in the document 'Conditions of Use'. Support information can be found in the document 'Background and Support Information'. Common questions are answered in the Q&A document. These documents are available on the website as PDF downloads, in the 'Support' section.

Contents

Accessing the databases

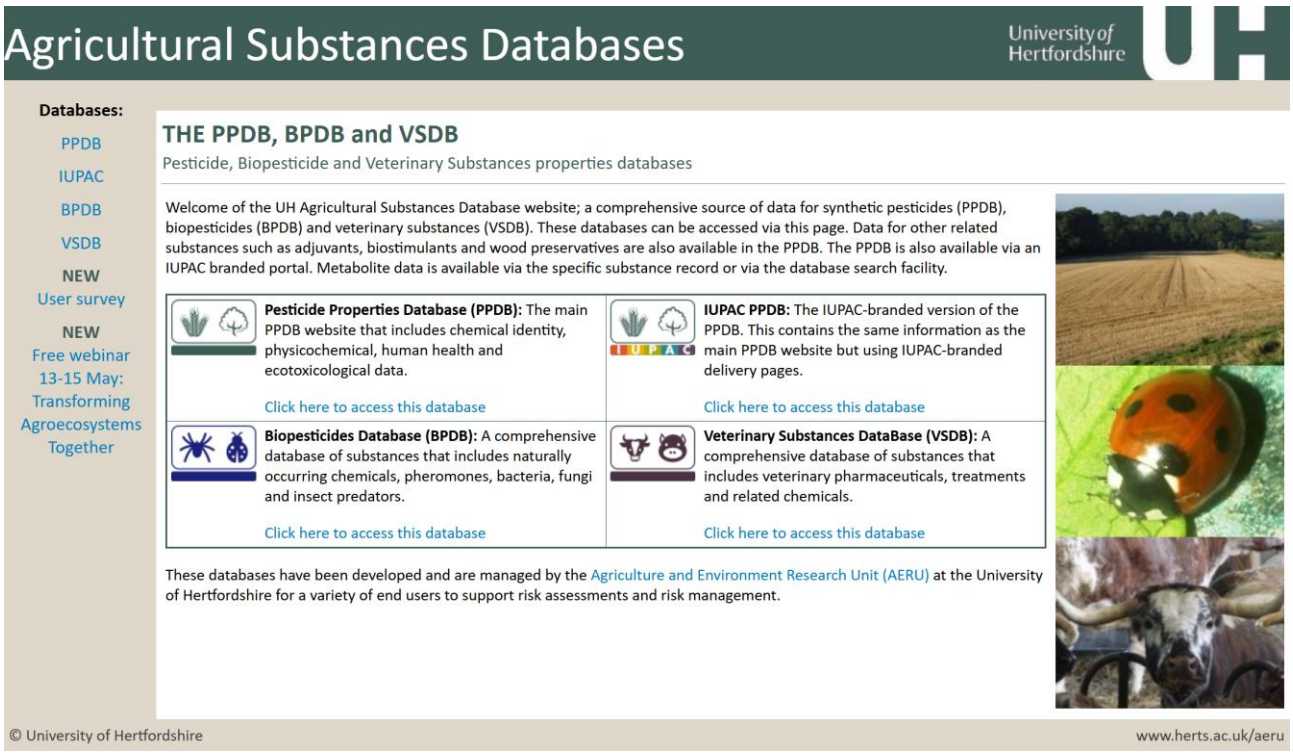
The main landing page is available at:

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

This gives access to all four databases or they can be accessed directly from:

- For the PPDB online go to https://sitem.herts.ac.uk/aeru/ppdb/index.htm.
- For the IUPAC version of the PPDB go to https://sitem.herts.ac.uk/aeru/iupac/index.htm.
- For the BPDB online go to https://sitem.herts.ac.uk/aeru/bpdb/index.htm.
- For the VSDB online go to https://sitem.herts.ac.uk/aeru/vsdb/index.htm.

The Landing page



The databases landing page gives access to all four databases.

- **The Pesticide Properties DataBase (PPDB):** The PPDB includes data for chemical identity, physicochemical properties, human health and ecotoxicology. There is also regulatory and commercial information, and broad information on use. This database also contains information on other related substances including biostimulants, adjuvants, solvents and wood preservatives.

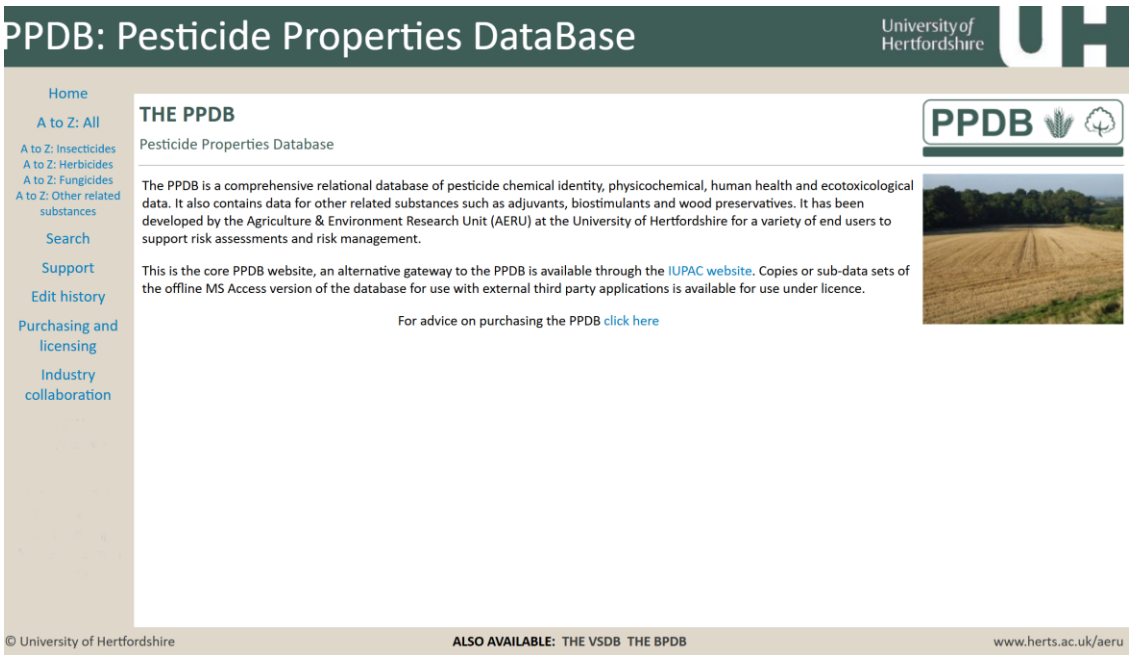
- **The IUPAC PPDB:** The IUPAC-branded version of the PPDB contains the same information as the main PPDB website but using IUPAC-branded delivery pages.

- **The BioPesticides DataBase (BPDB):** A The BPDB contains data for substances and organisms that are naturally occurring or which originate from a natural source, and that have a plant protection application. The data presented is identical to the PPDB although some of the parameter are not relevant (e.g. degradation data for living organisms).

- **The Veterinary Substances DataBase (VSDB):** The VSDB contains data for veterinary pharmaceuticals, treatments and related chemicals. Data is similar to that in the PPDB but environmental and ecotoxicological data is somewhat scarce.

All four databases are operated and navigated in the same manner so only the PPDB is described herein.

The Home page

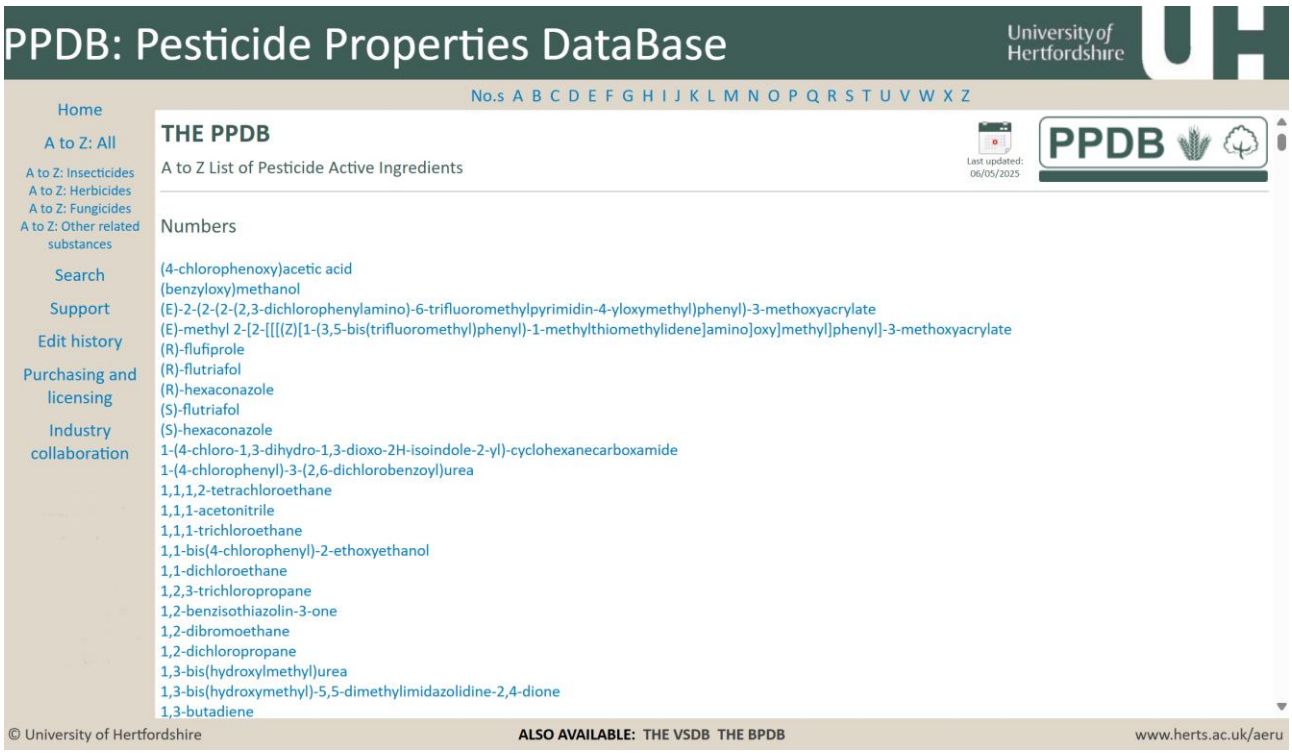


The Home page of the PPDB (https://sitem.herts.ac.uk/aeru/ppdb/en/) is shown above. Minor changes are made from time to time to the left-hand side menu. This menu provides a number of different options and remains constant on the left-hand-side regardless of where you are in the database. The core options are:

- Home page - this returns you to the introductory page of the database;
- The A to Z of the database contents. This may include sub-sections of data. This provides access to individiual data records;
- A search facility;
- Support information;
- Edit history;
- Purchasing and Licensing information.

This menu may change from time to time adding in new facilities (e.g. user surveys, industry collaboration portal). The core options are described below.

The A-Z index page

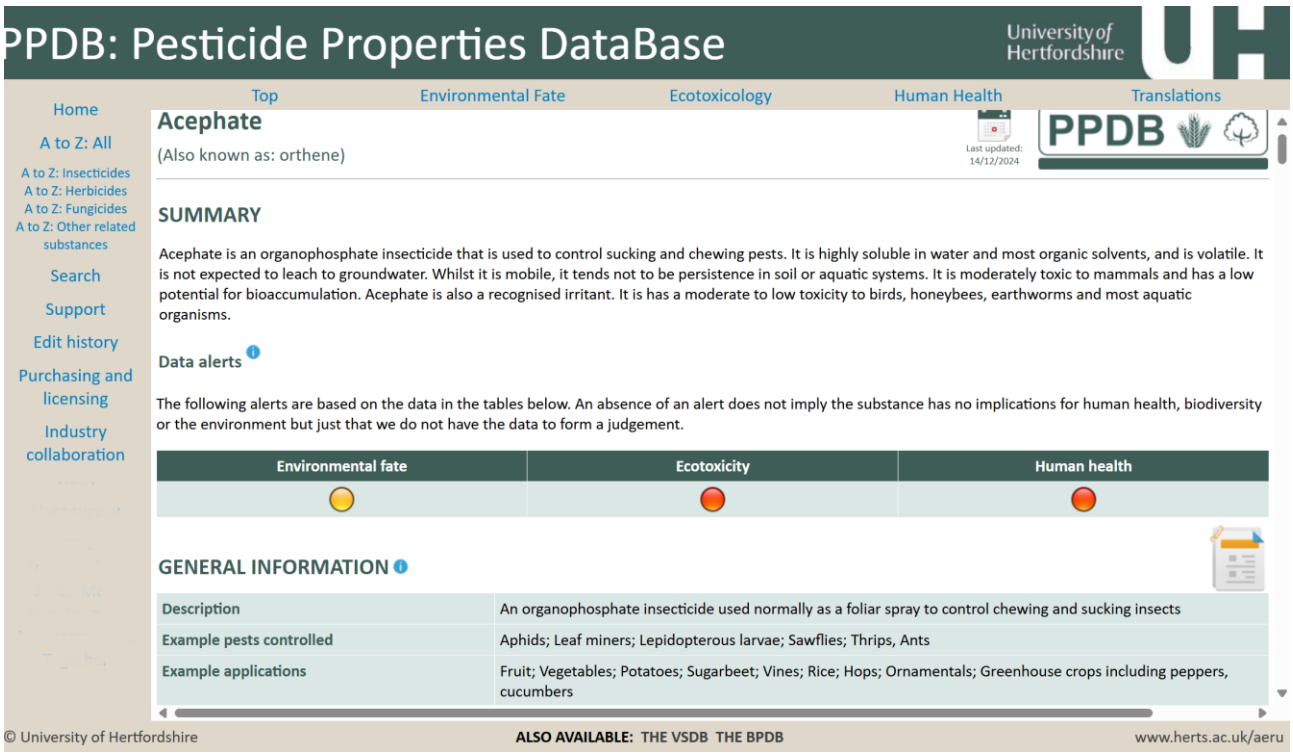


A list of the substances for which data is available in the database are given in the central area arranged in an A to Z format. Click on the selected substance to open that record. Navigation up and down the list can be done either by selecting the starting letter of the substance (top of page) or by scrolling up and down using the scroll bar on the right hand side together with the mouse or computer controls.

Please note:

- Metabolites are only accessible via the parent record or via the search facility – see below.
- Pesticides often have multiple alias's if you cannot find the substance you are looking for try searching using the CAS number.
- Not all data sets will be complete. There may be data gaps for a number of reasons including (a) the data may not exist, (b) the data is not relevant in the context of plant protection, (c) we may not have found any useful information.
- The database is updated regularly, often daily. The date the website was last updated online can be seen at the top of the page below the title banner. Due to the frequency of updating the online version of the database may not be exactly the same in terms of content/data as off-line versions of the database. The online version will always be the most up to date. Users with off-line licences will be issued with quarterly updates as part of the agreement. If more frequent updates are required this can be arranged for a small additional fee.

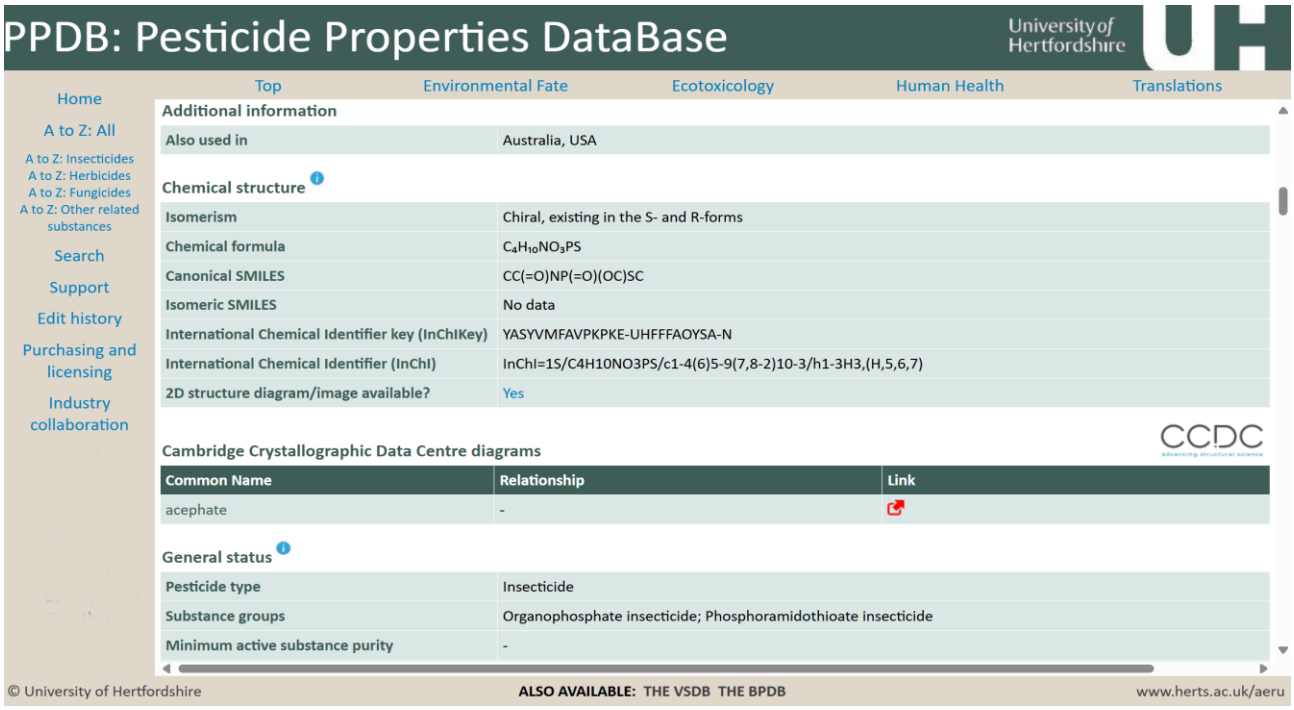
The data record



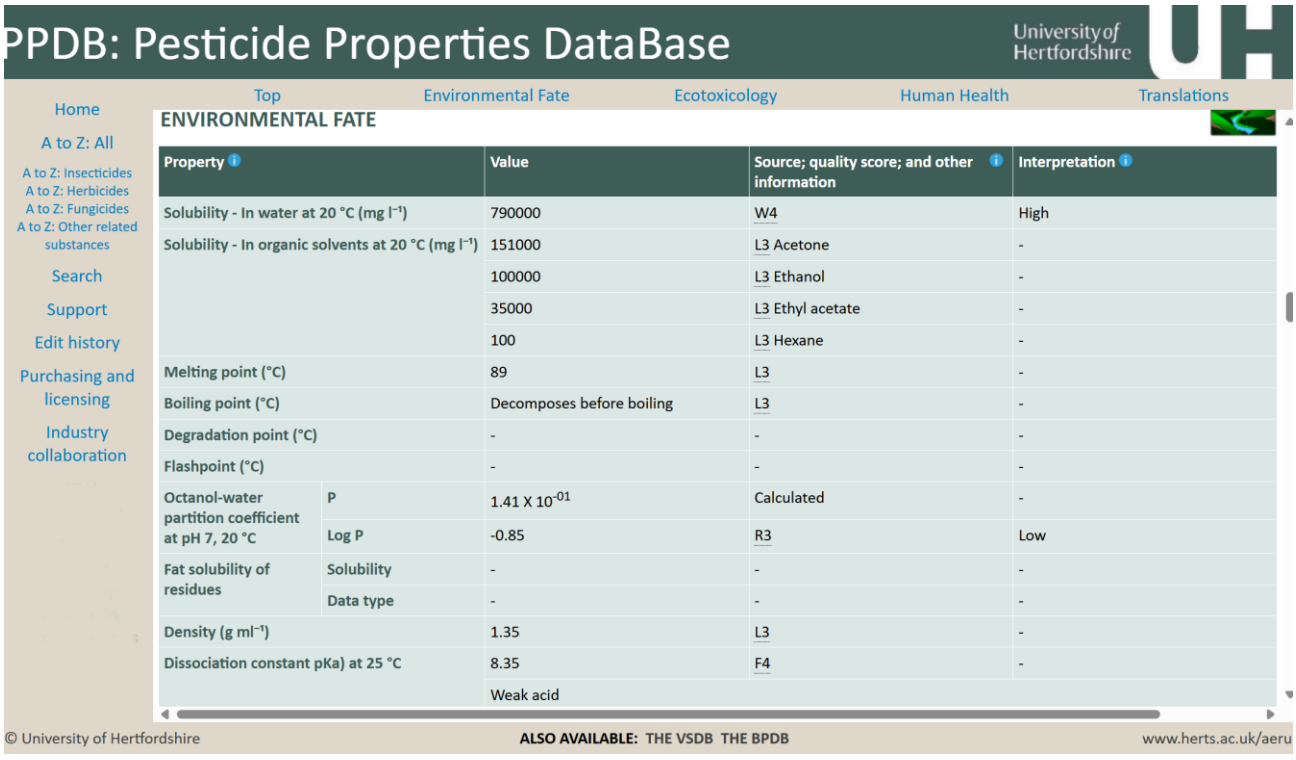
The selected record will be displayed in a standard PPDB format. New parameters may be added from time to time. At the top of the record other names in common use are displayed. A short summary of the data may also be provided. The data the record (rather than the online system) was last updated can also be seen. Links to the various data sections are also given at the top of the page.

Data is divided into the following broad sections:

- Data alert system – PPDB only. This is 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.
- General information: including examples of pests treated, substance type, chemical formula, structures etc., as well as regulatory and commercial information.
- Environmental fate: this section includes information on physico-chemical properties, degradation, soil adsorption, mobility and metabolites. There are also a number of auto-calculated environmental indices.
- Ecotoxicological data: this includes endpoints/interpretations for a range of fauna and flora. Data for terrestrial and aquatic species are in separate sub-sections.
- Human health data: this includes toxicological endpoints and descriptive text, as well as health and handling issues.
- Translations of the main common name into several European languages.



As shown in the image above, at various places on the record the information icon can be seen. Clicking this icon will provide access to the appropriate section within the support and information document. In various places a warning icon may also be shown. Clicking on this will open a new window containing cautionary notes for the relevant data item. We also include links to associated third-party sites with relevant information. For example, in the image above a link is given to the 3D structure of the molecule on the CCDC website.

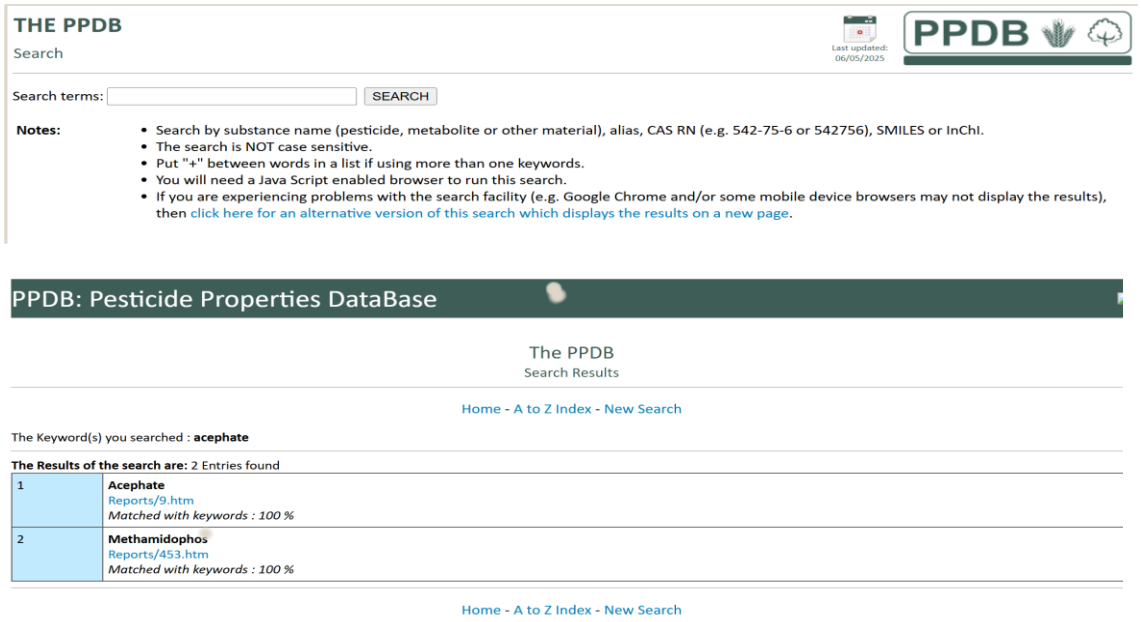


As shown above, many of the parameter values in the database have accompanying information fields. This information is vitally important in understanding the data. It will show the Quality Barometer (see below) alongside the parameter value. Environmental fate and ecotoxicological data may include a general interpretation based on regulatory thresholds and commonly used rules-of-thumb given to help laypersons understand the data. Other information may also be included such as if the data is non-standard in anyway (e.g. non-standard metrics or species).

In addition, environmental fate and ecotoxicological data items are tagged with a code (Quality Barometer) that has an alphanumeric format (e.g. A5, Q1). The character part of this code allows the broad source of the data to be identified. Information on these codes can be found in the 'Background and Support' document available on the database 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 as the published data will have been heavily scrutinised and peer reviewed by experts. 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 quality assessment 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.

More details regarding the individual parameters within each record can be found in 'Background and Support information' which is available through the link in the 'Support' section on the left of the screen. You will also find information relating to the data in the relevant Q&A document. A glossary document, also found in the Support section, will also give information on various parameters in the database.

Search



Selecting the search option will take the user to the search page. Data can be searched for by:

- Full chemical name (IUPAC or CAS name) for the substance, metabolite or additive.
- Common name, alias or code.
- Common name in any of the PPDB operating languages.
- CAS number.
- Structural descriptor (e.g. SMILES or InChI).

Many substances have similar names and alias and many different ways in which the chemical can be identified. Ideally a unique identifier (e.g. the CAS number) should be used. Metabolites may be found using this option or via links in the paraent record.

Identifying metabolites can be difficult. Ideally select the parent substance from the A-Z Index and follow the links. Alternatively, try the manufacturers development code, CAS number or chemical name.

Type the search term in the box and click the Search button. Results of the search will be displayed. Select the item you wish to view.

Support

This option provides access to a number of documents that provide more detail on using the database, its data and conditions of use as well as other relevant documents. Some of these have been produced in-house but others are useful documents produced by third parties and provided as reference materials. Please check these documents before you contact us. We do not normally provide support to users of the free of charge online system. A small amunt of support time is included to licenced clients. The core set of support documents includes:

- Terms and Conditions.
- Copyright statement.
- Background and Support Information.
- Instructions for Use (this document).
- Q&A section: this provides brief answers to common questions.
- Glossary of Terms.
- Using the Database Offline.
- What are CIPAC Code Numbers?
- The IUPAC International Chemical Identifier.
- EU Risk and Safety Phrases. Summary of Hazard Phrases - CLP Classification.
- The Global Harmonised System (GHS) - Aldrich summary.
- The Global Harmonised System (GHS) - Allocation of Label Requirements.
- A form to return to us for reporting suspected errors.
- Newsletters, Posters & Publications.

Edit history

As the database is updated very regularly we are unable to keep a detailed record of what changes. The date the website was last updated online can be found on the database homepage. The date an individual record was last edited can be found at the top of the substance record page. On the left hand side menu the ‘Edit

history' option will provide a little more detail and provide broad information on key updating events such as when a new parameter is added or a specific data reviewed (e.g. regulation).

Purchasing & licensing

This page provides details on how to purchase the database in MS ACCESS or MS EXCEL format. More details can be found in the 'Terms and Conditions of Use' document.

Disclaimer

The various databases have been developed by collating and formatting data from a wide variety of different sources. We have taken considerable care to ensure that the information it contains is as accurate and as complete as possible and we have also attempted to provide guidance on our confidence in the data via the quality barometer. However, the University of Hertfordshire, collaborating organisations and individuals and our funders bear no responsibility for errors or omissions in the either the database or the original sources.

Information in this database in no way replaces or supersedes information provided on the pesticide product label or under other regulatory requirements. Please refer to the pesticide product label. Should you have comments about the database or suggestions for changes, please contact us (see below).

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