The University of Hertfordshire Agricultural Substances Databases - Background and Support Information

The present document (version 02/2023) aims at providing information regarding the PPDB, BPDB and the VSDB, their management and data acquisition. It seeks to answer common questions regarding these matters. Information on the Terms and Conditions of use for each database can be found in a document that is available on the database website as a PDF download.

Contents

PPDB, BDPB, VSDB
Version: April 2024

1.0. Introduction

1.1. What are the UH Agricultural Substances Databases?

The University of Hertfordshire's (UH) Agriculture & Environment Research Unit (AERU) have developed three databases relating to chemical (natural and synthetic) substances used in agriculture: pesticides, biopesticides and veterinary substances.

The Pesticide Properties DataBase (PPDB) is a comprehensive relational database of pesticide physicochemical, toxicological, ecotoxicological, human health and other related data. It contains data relating to synthetic pesticides and their metabolites. It has evolved from a database that originally accompanied the EMA (Environmental Management for Agriculture) software (also developed by AERU) and has been systematically developed further and expanded with funding from other research projects and earned income. This database has also been issued in IUPAC format.

The BioPesticides DataBase (BPDB) is similar to the PPDB but contains data for biological pesticides – those that have been derived from natural substances such as plants. This was developed when the PPDB became very large and it was advantageous from a management point of view to separate certain records out, especially as the BPDB contains data not relevant to the PPDB such as taxonomic classifications and substance source.

The veterinary Substance DataBase (VSDB) contains data relating to substances used to manage the health and welfare of animals (mostly farmed livestock). It evolved in the same way as the BPDB as it also contains data not relevant to the PPDB or the BPDB such as pharmacological data relating to the drug or treatment activity.

1.2. How do the databases work?

The data is collated and stored in an MS Access database. A Microsoft Visual Basic data management application has been developed to manage the data adhering to strict formatting and quality control protocols and to keep track of versions, literature references and record cross-referencing. Another Visual Basic application is used to filter the data, handle the translations and generate the thousands of HTML pages for the PPDB website.

1.3. Data gaps

There are several reasons why data might be missing but this is usually because:

a) The substance has not been tested and so the data does not exist;
b) The substance has been tested but the data has not been made available for the public domain and so we do not have it or do not have permission to use it;
c) The data has been tested but units of measurement are incompatible with standard risk assessments and there is no method of converting the data with any acceptable degree of confidence;
d) We just haven't found the data.

Missing data should not be interpreted as the absence of an impact or issue.

2.0. Explanation of the Terms and Parameters Used

2.1. General chemical status information – descriptors and registration

Parameter	Explanation
Reference	Additional name for the chemical, including those used during substance development and prior to formal naming.
Alias's/synonyms (below the substance name)	Other names by which the substance is known. These are enabled in the various database search facilities.
Summary	This is a short paragraph picking out the key parameters providing an overview of the pesticide substance and it chemical and (eco)toxicological properties.
Data alerts	These alerts are based on data in the tables discussed below to highlight areas of potential concern. However, the absence of an alert does not imply that a substance has no implications for human health, biodiversity or the environment, just that we do not have the data to form a judgement.
Description	General description of the major uses of the substance.
Example pests controlled	A non-exhaustive list of pests that the substance controls.
Example applications	A non-exhaustive list of application situations.
Efficacy & activity	Information on the efficacy and activity of the pesticide towards the pest the substance is intended to control.
Appearance and life cycle (BPDB only)	A brief description of the form taken by the organism and the key elements of its life cycle.
Availability status	An indication of whether the substance is currently available or obsolete (if known).
Introduction & key dates	Year (and country where known) of introduction, registration or discovery.
Taxonomic classification (BPDB only)	Taxonomic classification of the organism.
Examples of species treated (VSDB only)	Key livestock types for which the substance is used as a veterinary product.
UK regulatory status (PPDB/BPDB only)	Status of the chemical within UK approvals system.
EC Regulation 1107/2009 status (PPDB/BPDB only)	Status of the chemical in the EU peer review process EC directive 1107/2009 (repealing 91/414) of pesticide/biopesticide active substances.
Dossier rapporteur/co-rapporteur (PPDB/BPDB only)	National regulatory authority responsible for regulatory assessment.

Date EC 1107/2009 inclusion expires (PPDB/BPDB only)	Date current status expires (if appropriate).
EU Candidate for substitution (CfS) (PPDB/BPDB only)	These are pesticide active substances identified during the EU regulatory assessment process as having a less favourable toxicological or environmental profile but which still satisfy the criteria for approval. Article 24 of Regulation (EC) No. 1107/2009 states that candidates for substitution (CfS) are approved for a period not exceeding seven years. The criteria for selection includes (for example) substances which are carcinogenic, those which have negative effects on reproduction and those that are a high risk to groundwater whilst also showing a toxic effect of concern.
Listed in EU database (PPDB/BPDB only)	Whether the substance is present in the EU approvals database.
Approved for use or known to be used in the following EU-27 Member States (PPDB/BPDB only)	Provides an indication of where the active substance has been authorised for agricultural use within the EU. Please check with the relevant national authority before relying on this data.
Also used in / Additional information (PPDB/BPDB only)	Other countries where we believe the substance is used. Please check with the relevant national authority before relying on this data.
Isomerism	This is a description of the isomeric nature of the substance.
Chemical formula	This is a concise way of expressing information about the atoms that constitute the chemical.
Canonical SMILES	The **S**implified Molecular **I**nput **L**ine **E**ntry **S**pecification (SMILES) is a specification for describing the structure of chemical molecules using short ASCII strings. SMILES strings can be imported by most molecule editors for conversion back into drawings or models of the molecules. Canonical SMILES are those used by the most common applications and omits isotopic and chiral information.
Isomeric SMILES	SMILES as above but including isotopic and chiral information.
International Chemical Identifier key (InChIKey)	IUPAC **In**ternational **Ch**emical **I**dentifier. This is a textual identification for chemical substances, that provides a standard, readable way of encoding molecular information and to facilitate the search for such information in databases and on the web. This parameter is a condensed version of the InChI Identified described below.
International Chemical Identifier (InChI)	IUPAC **In**ternational **Ch**emical **I**dentifier. This is a textual identification for chemical substances, that provides a standard, readable way of encoding molecular information and to facilitate the search for such information in databases and on the web.
2D structure diagram/image available?	Either Yes or No. If Yes is stated this will be a link to a separate window displaying the structure diagram.

Cambridge Crystallographic Data Centre diagrams (PPDB only)	If appropriate a link will be provided to the Cambridge Crystallographic Data Centre structural diagram page.
Pesticide, biopesticide or veterinary substance type	The specific type of substance described according to the type of pest or disease they control e.g. Insecticide, Herbicide, Fungicide, Acaricide, Antiparasitic, Anthelmintic etc.
Metabolite type	General description of the host process that creates the metabolite e.g. soil, surface water, animal, plant, groundwater.
Other constituent type	General description of the purpose of the constituent in the formulation i.e. solvent, wetter, carrier etc.
Substance group	Chemical classification group based on the chemical structure.
Minimum active substance purity	Minimum substance purity of the active ingredient.
Known relevant impurities	Information on any relevant impurities declared for the substance.
Substance origin	Whether the substance is natural or synthetic.
Mode of action	The mechanism by which the substance performs its main function.
Molecular target (VSDB only)	This is the key molecule involved in a particular metabolic or signalling pathway that is specific to the disease condition or pathology or to the infectivity or survival of a microbial pathogen.
Substance source (BPDB only)	The origin of the organism/substance.
Substance production (BPDB only)	How the organism/substance is produced.
Uses (BPDB only)	What the organism/substance is used for.
Target pests (BPDB only)	What pests the organism/substance can be used to treat.
Target host (BPDB only)	What crops the organism/substance can be used in.
Farming system suitability (BPDB only)	Comments of the suitability of the organism/substance for use in different farming systems.
CAS RN	Chemical Abstracts Service Registry Number - a unique identify for the chemical.
Alternative/old CAS RN	Additional/old Chemical Abstracts Service Registry Number(s) for the substance.
EC number	The unique reference number for the chemical in the European Chemical Substances Information System (EINECS) or European List of Notified Chemicals (ELINCS).
CIPAC number	The CIPAC code number system is a simple approach for an unambiguous coding of chemicals. CIPAC, FAO, WHO and the EU are the main users of this system.

US EPA chemical code	The U.S. Environmental Protection Agency (U.S. EPA) assigns a unique reference number to individual pesticide active ingredients to assist in their identification. This code is sometimes referred to as the Shaugnessy Number.
PubChem CID	Identifier within the PubChem chemistry database of the National Institutes of Health (NIH).
ATCvet Code (VSDB only)	The WHO's Anatomical Therapeutic Chemical Classification System for veterinary medicinal products (ATCvet) is used to classify veterinary drugs.
Therapeutic Class (VSDB only)	The broad therapeutic grouping of the substance.
Controlled Drug? (VSDB only)	Whether the substance is a controlled drug or not under UK legislation.
Regulation 37/2010 MRL Classification (VSDB only)	EU Regulation 37/2010 classifies pharmacologically active substances according to their permitted maximum residue limits in food of animal origin.
Molecular mass	The relative molecular mass (molecular weight) of a chemical is the mass of a molecule of the chemical relative to the mass of a carbon atom taken as exactly 12.
Chemical name	Name of the chemical according to the nomenclature rules of IUPAC or CAS. Where this is not available or does not apply a generic name is given.
Other status information	This will display information relating to the status of the substance with respect to other legislation, international conventions and information regarding phase out. Including: **PIC Annex 1 chemicals**: The Rotterdam Convention on Prior Informed Consent (PIC). The Convention covers pesticides and industrial chemicals that have been banned or severely restricted for health or environmental reasons by parties and which have been notified for inclusion in the PIC procedure by those parties. One notification from each of two specified regions triggers consideration of addition of a chemical to Annex III of the Convention. Severely hazardous product formulations that present a hazard under conditions of use in developing may also be nominated for inclusion in Annex III. **POP chemicals**: The Stockholm Convention on Persistent Organic Pollutants (POP). POPs are exceedingly toxic chemicals that are extremely persistent in the environment, travel long distances on wind and water currents, and concentrate up the food chain to accumulate in our bodies. They also have serious health implications and can cause cancer, neurological and learning disabilities, and subtle changes to human reproductive and immune systems. The Stockholm Convention bans or severely restricts the most hazardous POPs, and establishes an international, science-based process for adding other POPs to the treaty. Those listed in this database also include chemicals that are new POP candidates proposed by other organisations including the WWF. **VOC chemicals: Volatile organic compounds (VOCs)** are organic chemical compounds that have high enough vapour pressures under normal conditions to significantly vaporise and enter the atmosphere. The term VOC may have special legal meanings in some countries.

	LRTAP Chemicals: The Convention on Long-range Transboundary Air Pollution (LRTAP): The aim of the Convention is that Parties seek to limit and, as far as possible, gradually reduce and prevent air pollution including long-range transboundary air pollution. Chemicals considered to be the most serious problem are assigned to Annex 1. **PAN Dirty Dozen / PAN Bad Actor**: The Pesticide Action Network (PAN) have identified these chemicals as being particularly harmful. **OSPAR**: OSPAR Convention for the Protection of the Marine Environment: pfa - priority substances for action, soc - substances of concern. **WFD**: Water Framework Directive 2000/60/EC: phs - priority hazardous substance, pps - possible priority substance, other - other substance of concern. **Groundwater contaminant**: substance is known to have polluted groundwaters and is a substance of concern.
Relevant environmental water quality standards	This field gives an indication of the quality standards in place for the protection of aquatic life.
Resistance code (HRAC, WSSA, IRAC, FRAC) (PPDB/BPDB only)	This is the HRAC, WSSA, IRAC or FRAC code that denotes their resistance classification and can be used in resistance management programmes.
Examples of recorded resistance	Information on any known resistance issues for the substance.
Physical state	Provides an indication of the physical state of the material – solid, liquid or gas and its general appearance. This normally applies to the active substance in its pure state unless stated otherwise.
Related substances & organisms (BPDB only)	Any known related substances and organisms and links to their pages if appropriate.
Can be a metabolite of	Information on the substances of which the relevant substance can be a metabolite and links to their pages if appropriate.

2.2. Formulations

Example manufacturers &/or suppliers	Examples of companies that have manufactured, supplied or used the substance in their products currently or historically.
Example products using this active	Non-exhaustive list of examples of products that include the substance. These products may be historical and no longer available.
Formulation and application details	This provides brief information on the main types of formulation and aspects relating to their application.

2.3. General chemical properties related to environmental fate

NB: where the stored parameter differs significantly from the information stated below this will be described in the accompanying text field.

Parameter	Explanation
Solubility in water (mg l^{-1})	The mass of a given substance (the solute) that can dissolve in a given volume of water. Value reported is at 20°C. Note for some chemicals solubility may be pH sensitive.
Solubility in organic solvents (mg l^{-1})	The mass of a given substance (the solute) that can dissolve in a given volume of solvent. Value reported is at 20°C. Note for some chemicals solubility may be pH sensitive.
Melting point (°C, at 1 atmosphere pressure)	The temperature at which the given substance changes its physical state from solid to liquid.
Boiling point (°C, at 1 atmosphere pressure)	The temperature at which the vapour pressure of the substance in its liquid state equals the environmental pressure surrounding the liquid i.e. it boils
Degradation temperature (°C, at 1 atmosphere pressure)	The temperature at which the substance is no longer stable and begins to break down.
Flash point (°C)	The flash point of a flammable substance is the lowest temperature at which it can form an ignitable mixture in air.
Octanol-water partition coefficient (as LogP)	LogP is the logarithm (base-10) of the partition coefficient between n-octanol and water. It is used in environmental fate studies and large values (+4 or higher) are regarded as an indicator that a substance will bio-accumulate. For some substances LogP will be very sensitive to pH.
Fat solubility of residues	Fat-soluble pesticides are those that can be stored in the liver or in fatty tissues. Consequently, they may bioaccumulate and can be environmentally persistent. As a guide the value of Log P can be used. Where log P is greater than 3 the pesticide residue is likely to be soluble in fat but there are exceptions to this rule and so assessment using metabolism and farm animal feeding studies provides the most accurate guide. This information can be important for oil extraction processes as fat solubility will influence the concentration of a pesticide in the processed products.
Density	Parameter given depends on the physical state (solid or liquid) of the chemical (g ml^{-1}).
Dissociation constant pKa	Strengths of acids and bases can be indicated on a common scale at 25°C. Defined as the negative logarithm of the acidity constant Ka. The lower the pKa the stronger the acid. For example, acetic acid has a pKa of 4.75 whilst sulphuric acid has a pKa of -3.0. pKa is used here as an indicator of the potential of a compound to form ions in water. Many chemicals are either permanently ionic or will change ionic state somewhere in the range of the pH of environmental soils and water. Knowing the ionic sate of a chemical provides important information on its potential mobility and persistence in the environment.

Vapour pressure (mPa)	The pressure at which a liquid is in equilibrium with its vapour at 20°C. It is a measure of the tendency of a material to vaporise. The higher the vapour pressure the greater the potential. The short-range air transport exposure assessment scheme uses a vapour pressure trigger to identify substances of potential concern. The trigger is 10-2 mPa (at 20°C) if a substance is applied to plants and 10-1 mPa (at 20°C) if the substance is applied to soil. Substances that exceed these triggers, ideally require drift mitigation.
Henry's law constant Dimensional	A Gas Law states that the amount of gas absorbed by a given volume of liquid at a given temperature is directly proportional to the partial pressure of that gas in equilibrium with that liquid. As such it provides an indication of the preference of a chemical for air relative to water i.e. its volatility. Henry's Law Constant is usually quoted in $Pa.m^3/mol$.
Volatilisation as max % of applied dose lost (from plant surface & from soil surface)	The percentage of the applied dose lost from the plant and soil surface due to volatilisation at 20°C in the stated timeframe, which is normally 24 hrs. The trigger for concern is >= 20%[1]. For pesticides with volatilisation rates below 20% volatilisation is not considered as critical.
Max UV-Vis absorption ($L\ mol^{-1}\ cm^{-1}$)	Different compounds may have very different absorption maxima and intensities. The wavelength of maximum absorbance is a characteristic value and so can be used for identification purposes.
Surface tension ($mN\ m^{-1}$)	The tendency of the surface of to resist an external force.
Refractive index (VSDB only)	This is an optical term and is a dimensionless number that describes how light, or any other radiation, propagates through that medium.
Environmental release (VSDB only)	Main mechanisms of entry into the environment.
General biodegradability (PPDB only)	Short text giving comment on the general biodegradability of the pesticide in the environment.
Soil degradation DT50 Typical/Laboratory/Field - days	DT50 is the time required for the chemical concentration under defined conditions to decline to 50% of the amount at application. In many cases chemicals show "half-life" behaviour, in which subsequent concentrations continue to decline by 50% in the same amount of time. In such cases several or more four half-lives (in which the concentration declines to 1/8 or 1/16, e.g.) are a measure of the persistence on the chemical. Three parameters are given. Typically, data is derived from laboratory studies, but where the substance is persistent in soil under laboratory conditions, field studies may be carried out. 'Typical values' quoted are those given in the general literature and are often a mean of all studies field and laboratory.

[1] BBA - Biological Federal Institute for Agriculture and Forestry. (1990). *Study of the Volatilisation Behaviour and Fate of Plant Protection Products in the Air - Guidelines for the Official Testing of Plant Protection Products, Part IV, 6-1, Braunschweig*. [BBA - Biologische Bundesanstalt fur Land- und Forstwirtschaft (Juli 1990) Priifung des Verfluchtigungsverhaltens und des Verbleibs von Pflanzenschutzmitteln in der Luft. Richtlinien fur die amtliche Prufung von Pflanzenschutzmitteln, Teil IV, 6-1, Braunschweig.]

Notes: ***(i) Similar data is given for the DT90 i.e. the time in days for the pesticide to decline by 90%.*** ***(ii) Where the pesticide has been assessed by the EU and where data is available the DT50 used in the modelled risk assessment is also provided.*** ***(iii) More detailed data where DT50 is available by soil type, pH, organic carbon for both lab and field studies is available in the off-line MS Access database available under a licence agreement.***	
Manure DT_{50} - days (VSDB only)	The time required for the chemical concentration to decline to 50% in livestock manures.
Dissipation rate RL50 on plant matrix - days (PPDB/BPDB only)	The RL50 (Residual Level) is the rate in days for which the pesticide declines by 50% on the surface of the specified plant matrix (leaves, fruit, roots, seeds, grain etc.).
Dissipation rate RL50 on and in plant matrix - days (PPDB/BPDB only)	The RL50 (Residual Level) is the rate in days for which the pesticide declines by 50% on and in the specified plant matrix (leaves, fruit, roots, seeds, grain etc.).
Note: ***More detailed data where DT50 is available by crop/plant/tree type and matrix (fruit, leaves, foliage, rind, peel, tuber) studies is available in the off-line MS Access database available under a licence agreement.***	
Aqueous photolysis DT50 (days at 20°C pH 7)	Photochemical processes may be important in determining the fate of organic pollutants in aqueous environments. This is the rate of chemical decomposition in the aquatic environment induced by light or other radiant energy expressed as a DT50. Other information regarding, for example, pH sensitivity is also given in accompanying notes.
Aqueous hydrolysis DT50 (days at 20°C and pH 7)	This is the rate of chemical decomposition induced by water at pH 7 expressed as a DT50. Other information regarding, for example, pH sensitivity is also given in accompanying notes.
Water sediment study data - Water-sediment & Water phase only DT50s	This is the rate of chemical decomposition in water-sediment systems expressed as a DT50. Data is given for the system as a whole and for the water phase only.
Soil sorption K_{oc} / K_{foc}	Sorption coefficient data is a measure of the tendency of a chemical to bind to soils, corrected for soil organic carbon content. Values can vary substantially, depending on soil type, soil pH, the acid-base properties of the pesticide and the type of organic matter in the soil. Where data is available both the linear (K_{oc}) and non-linear (K_{foc}) parameters are given. Three summary parameters are given for K_{foc} and two for K_{oc}.
Note: (i) ***More detailed data where K_{oc}/K_{foc} plus related parameters are available by soil type (sand/silt/clay distribution as well as structure type), pH, organic carbon is available in the off-line MS Access database available under a licence agreement.***	
GUS leaching potential index **NOTE: THIS IS AN INDICATOR & NOT A RISK ASSESSMENT**	The GUS index (Groundwater Ubiquity Score) is a very simple indicator of a chemical potential for leaching into groundwater. It is based on the environmental fate properties of the chemical and takes no account of environmental conditions. It is not a substitute for modelling and risk assessment studies.

<table>
<tr><td></td><td>Calculated from the soil degradation rate (DT50) and the Organic-carbon sorption constant (koc) where:
GUS = log(DT50) x (4 - log (koc))
If GUS > 2.8 = likely to leach
If GUS < 1.8 = unlikely to leach
If GUS 1.8 - 2.8 = leaching potential is marginal
(Reference: Gustafson, D.I. (1989) Groundwater Ubiquity Score: A Simple Method for Assessing Pesticide Leachability Environmental Toxicology and Chemistry, 8, pp339-357).</td></tr>
<tr><td>SCI-Grow groundwater index
NOTE: THIS IS AN INDICATOR & NOT A RISK ASSESSMENT</td><td>This is an indicator, used by the USEPA, to crudely estimate chemical (mainly pesticide) concentrations in vulnerable groundwater. It is based on environmental fate properties of the chemical, the application rate and existing data from small-scale monitoring studies. It is not a substitute for modelling and risk assessment studies.
(Ref: www.epa.gov/oppefed1/models/water/scigrow_description.htm)
Calculated from the soil degradation rate (DT_{50}) and the Organic-carbon sorption constant (K_{foc} or K_{oc}) where:
Step 1:
<table>
<tr><td colspan="3">CO = $\log_{10}(K_{foc} + 5.0)$ OR C = $\log_{10}(K_{oc} + 5.0)$</td></tr>
<tr><td>if DT_{50} < 6.0 then</td><td>DT = $\log_{10}(DT_{50}/6.0)$</td><td>RILP = DT * CO</td></tr>
<tr><td>if DT_{50} 6.0 - 1500 then</td><td>DT = $\log_{10}(DT_{50} - 5.0)$</td><td rowspan="2">RILP = DT * (4 - CO)</td></tr>
<tr><td>if DT_{50} > 1500 then</td><td>DT = $\log_{10}(1500) = 3.17609$</td></tr>
<tr><td colspan="3">Step 2:</td></tr>
<tr><td colspan="2">If K_{foc} or Koc <= 9995 then</td><td>SCI-GROW = $0.892 * 10^{(-2.241 + (0.61 * RILP))}$</td></tr>
<tr><td colspan="2">If K_{foc} or K_{oc} > 9995 then</td><td>SCI-GROW = 0.892 * 0.006</td></tr>
<tr><td colspan="3">Note: US developed SCI-GROW assumes an application rate of 1lb a.i/acre, therefore the 0.892 is included to convert it to kg a.i./ha.</td></tr>
</table></td></tr>
<tr><td>Potential for particle bound transport index</td><td>An indicator of the general potential for particle bound transport index.</td></tr>
<tr><td>Potential for loss via drain flow</td><td>An indicator of the general potential for the loss of a substance via drain flow (derived from k_{oc}/k_{foc})</td></tr>
<tr><td>Photochemical oxidative DT_{50} (hrs) as indicator of long-range air transport risk</td><td>Photo-oxidative processes (indirect photolysis) and light-induced reactions (direct photolysis) are the main transformation pathways for pesticides in the atmosphere. Long-range air transport of pesticides will occur when compounds have a significant lifetime in air[2]. Reactions with hydroxy (OH^-) radicals are considered to be the major degradation process for most air pollutants, including pesticides due to the reaction with double bonds, the H abstractive power of hydroxyl and its high electrophilicity[3]. Due to issues of practicality, cost and unreliability the rate of degradation in air due to photochemical oxidation for pesticide risk assessments tends to be calculated using the method proposed by[2]. The EU FOCUS working group recommend a trigger of a</td></tr>
</table>

[2] Atkinson, R., Guicherit, R., Hites, R.A., Palm, W.-U., Seiber, J.N. and de Voogt, P. (1999). Transformation of pesticides in the atmosphere: a state of the art. *Water, Air and Soil Pollut.*, 115: 219-243.

[3] Atkinson, R., Darnall, K.R., Lloyd, A.C., Winer, A.M. and Pitts, J.N. Jr. (1979). Kinetics and mechanisms of the reaction of the hydroxyl radical with organic compounds in the gas phase. *Advances in Photochemistry*, 11: 375-488.

	DT50 in air of 2 days (48 hrs) to identify substances of potential concern for long-range transport[4]. In order to standardise the input parameters for the Atkinson calculation the Focus working group propose that a 12-hr day is used with a hydroxyl radical concentration of 1.5 x 106 OH radicals/cm^3.
Bio-concentration factor	The concentration of the chemical in tissue per concentration of chemical in water. This describes the accumulation of pollutants through chemical partitioning from the aqueous phase into an organic phase, such as the gill of a fish.

2.4. Metabolite/Parent information

Parameter	Explanation
Metabolites	A chemical degradation product - a chemical product formed upon the breakdown of a chemical. Metabolites are displayed in three tables: (i) known soil metabolites (2) known groundwater metabolites and (3) other metabolites (e.g. plant, surface water, sediment, animal). '**Known**' in this context refers to metabolites known to the PPDB team. These tables may not include all metabolites formed. Links cross-referencing to the metabolites are supplied.
Parent	The parent substance that has degraded to produce the metabolite.
Estimated Maximum Occurrence (PPDB/BPDB only)	The maximum amount of the named metabolite identified (via soil degradation studies) in soil expressed as a fraction of the chemical applied.
Soil Metabolite Relevancy	This refers to soil metabolites which may have toxicological or environmental concerns. Please note that some 1107/2009 dossiers pre-date the introduction of 'relevant metabolites' and, instead, declared metabolites as 'Major' if their estimated maximum formation fraction >10%. The difference between a major metabolite (which means one needing assessment) and a relevant metabolite is that a toxicological/ecotoxicological assessment has been made and a decision come to as to whether it is a relevant or a non-relevant soil metabolite.
Groundwater Metabolite Relevancy	Within 1107/2009 a groundwater metabolite is considered to be 'relevant': • if there is reason to believe that it has comparable intrinsic properties to the parent chemical in terms of its biological target activity, or • if it has toxicological properties that are considered severe, or • if it poses a higher or comparable risk to organisms than the parent substance. Therefore 'relevant' groundwater metabolites may need to so be taken into account within any risk assessment process.
Metabolite ADI	Acceptable Daily Intake - The amount of metabolite in food or drinking-water that can be ingested daily over a lifetime without appreciable health risk to the consumer, on the basis of all the known facts at the time of the evaluation.

[4] FOCUS. (2008). *Pesticides in Air: Considerations for Exposure Assessment.* Report prepared by the FOCUS Working Group on Pesticides in Air. European Commission report. SANCO/10553/2006 Rev 2 June 2008.

Safe Drinking Water Fraction	The amount of metabolite in drinking-water that can be ingested daily over a lifetime without appreciable health risk to the consumer, on the basis of all the known facts at the time of the evaluation. Determined as 20% of the ADI.

2.5. Ecotoxicology

Parameter	Explanation
Fauna and flora ecotoxicological endpoint data	Data used to measure the adverse effects on living organisms that chemicals can have when released into the natural environment. See **Endpoint Glossary and Key Species data** below.
Mesocosm study data	Mesocosm studies are a useful tool for higher-tier aquatic risk assessment. They are widely used in the regulatory assessment processes to evaluate the effects of chemical pollutants on aquatic communities at the ecosystem level.

2.6. Human health

Parameter	Explanation
Threshold of Toxicological concern (Cramer class) **NOTE: THIS IS AN INDICATOR & NOT A RISK ASSESSMENT**	Applies to non-cancer health issues and uses a decision tree approach classifying and ranking chemicals according to their expected level of oral systemic toxicity. The decision tree categorises chemicals, mainly on the basis of chemical structure and reactivity, into three classes indicating a high (Class III), medium (Class II) or low (Class I) level of concern. It is a simple toxicity indicator and should not be used if experimental data is available. See Lapenna & Worth, 2011 for more information. (Reference: Lapenna & Worth, 2011 - https://eurl-ecvam.jrc.ec.europa.eu/laboratories-research/predictive_toxicology/doc/EUR_24898_EN.pdf).
Toxicity endpoints for mammals	Oral, dermal and inhalation (and other) values provided.
Acceptable Daily Intake (ADI mg kg^{-1} bw day^{-1})	The amount of chemical in food or drinking-water that can be ingested daily over a lifetime without appreciable health risk to the consumer, on the basis of all the known facts at the time of the evaluation.
Acute Reference Dose (ARfd) (mg kg^{-1} bw day^{-1})	The amount of chemical that can be ingested over a short period of time, usually during one meal or one day, without appreciable health risk to the consumer - as far as evidence suggests.
Acute Acceptable Operator Exposure Level (AAOEL) (mg kg^{-1} bw day^{-1})	This is similar to the AOEL and is the health-based limit for exposure that could occur in a single day. It is comparable with the ARfD for consumption.
Acceptable Operator Exposure Level (AOEL) (mg kg^{-1}bw day^{-1})	This is a health-based limit that is established on the basis of the full toxicological assessment required for regulatory purposes. The risk for operators can be quantified by comparing this value with exposure level during application.
Dermal penetration studies (%)	Mean value of known studies reported. Default value in the absence of further evidence is normally taken as 10%.

Dangerous Substances Directive	This Directive concerns pollution caused by certain dangerous substances discharged into the aquatic environment and aims to regulate potential aquatic pollution. The Directive covered discharges to inland surface waters, territorial waters, inland coastal waters and groundwater. The protection of groundwater is now regulated under a separate Council Directive. Directive 76/464 introduced the concept of list I and list II chemicals. Where the chemical concerned appears on these lists it is given here.
Exposure routes public and occupational	Where identified risks to the public (e.g. bystanders and consumers) and operators/workers are identified. This list is not exhaustive but given for guidance only.
EU MRLs (mg kg^{-1})	MRLs are defined as the maximum concentration of chemical residue likely to occur in or on food, drink and feeding stuffs after the use of chemicals according to Good Practice (GP). GP is defined as the substance being applied in accordance with current regulations, product label recommendations and in keeping with local environmental and other conditions. The values listed here are for guidance only and are often those proposed within regulatory documents. More precise information on pesticides and biopesticides can be found in the EU Database.
Drinking water quality standards	This field gives an indication of the quality standards in place for the protection of drinking water quality and human health.
Drinking water MAC	The Maximum Acceptable Concentration of the chemical in drinking water.
Mammalian dose excretion route and rate	The rate at which a substance is lost from the body and the route of that loss.
Specific health issues	Summary of the main human health concerns across a number of issues. Note this is somewhat subjective as literature is not universally uniform in the way issues are addressed. We have used a 'weight-of-the-evidence' approach erring on the side of caution.
General health issues	Summary of main issues relating to human health. This list is not exhaustive and for guidance only.
Carcinogenicity	There are multiple different classification systems for carcinogenic substances, each of which uses different criteria and types of evidence. Often 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 use a 'weight of evidence' 'worse-case' approach taking 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, No, Possible and No data.
Genotoxicity	The data in the PPDB for genotoxicity is a summary and simplified interpretation of the information in the EFSA genotox database available at: https://data.europa.eu/euodp/data/dataset/database-pesticide-genotoxicity-endpoints. Data has been coded into a 4 x 2-character code; The first character refers to one of four data types are: A: Chromosome aberration; B: DNA damage/repair; C: Gene mutation and D: Genome mutation and the second character is a number 0-3 where 0=No data; 1=a significant majority of the test

	records (75%+) are positive; 2=the test results have given mixed or ambiguous results; 3= a significant majority of the test records (75%+) are negative. In addition to the EFSA data some less specific data has been collated from other sources. This is coded as 'E' and uses the same numerical coding as given above.
General handling issues	General description of any hazards that should be addressed when handling the substances.
CLP classification	The 'CLP' Regulation (EC) No 1272/2008 on the classification, labelling and packaging of substances and mixtures, or simply 'CLP', introduces the United Nations globally harmonised system (UN GHS) for classification and labelling of chemicals into Europe. For further information on this please see other documents available on the PPDB website under Support Information/Other Information.
WHO classification	Toxicity hazard class given by the World Health Organisation (WHO). • Class Ia: extremely hazardous • Class Ib: highly hazardous • Class II: moderately hazardous • Class III: slightly hazardous • O: Obsolete substance • NL: Not listed The system is based on the LD50 endpoint for rats. An ingested solid with a LD50 5mg or less/kg bodyweight is Class Ia, at 5-50 mg/kg Class Ib, at 50-500 mg/kg Class II, and at more than 500 mg/kg Class III. Values may differ for liquid oral agents and dermal agents.
UN Number	Number used world-wide in international commerce and transportation to identify hazardous chemicals or classes of hazardous materials.
Waste disposal & packaging	UN Packing Group and other relevant transport information.

2.7. Translations

Language translations for the common name by which the substance is now is provided (where known) in English, French, German, Danish, Italian, Spanish, Greek, Slovenian, Polish, Swedish, Hungarian and Dutch within each substance record. The entire PPDB database is also currently available in a range of European languages.

3.0. The primary data sources used to populate the databases

We use mainly public domain sources (mainly that of regulatory bodies), peer reviewed literature and private databases with copyright/IPR permission where required.

Note: This list is non-exclusive and just provides an example of the sources utilised.

A	EU Regulatory & Evaluation Data as published by EC, EFSA (RAR, DAR & Conclusion dossiers), EMA (e.g.) EU Annex III PIC DGD (For example see http://ec.europa.eu/sanco_pesticides/public/index.cfm or EFSA Scientific Publications https://www.efsa.europa.eu/en/publications)
AA	IOBC Database on classification of side effects to beneficial organisms, 2005
AC	EC Joint Research Centre ESIS European Chemical Substance Information Systems including ECHA (See https://echa.europa.eu/information-on-chemicals)
AE	Joint Assessment of Commodity Chemicals ECETOC (See http://www.ecetoc.org)
B	UK CRD and ACP Evaluation Documents / and other DEFRA (UK) documents (See http://www.pesticides.gov.uk/publications.asp?id=202); Also Chemicals Regulation Division, Health and Safety Executive (HSE), UK
C	AGRITOX (See http://www.agritox.anses.fr/).dataset. Dataset is no longer available.
D	Agricultural Research Information System (ARIS) Database. Dataset is no longer available.
DW	Don Wauchope personal database for Pka data: Wauchope, R. D. and Edwards, J. Dissociation constants for pesticide active ingredients: a database and comparison with predicted values. Dataset is no longer available.
E	Manufacturers Safety Data Sheets
F	U.S. EPA ECOTOX database / U.S. EPA pesticide fate database / Miscellaneous WHO documents (See https://www.epa.gov/pesticide-science-and-assessing-pesticide-risks/databases-related-pesticide-risk-assessment). FAO data, IPCS INCHEM data.
G	Extension Toxicology network Database EXTOXNET (See http://extoxnet.orst.edu/ghindex.html) Available online but no longer updated.
H	The US ARS Pesticide Properties Database (See http://www.ars.usda.gov/Services/docs.htm?docid=14199) Dataset is no longer available.
J	Pesticide Action Network Database (See http://www.pesticideinfo.org/)
K	Research Datasets (e.g. Pandora, Demetra these datasets no longer available). Norman Ecotoxicology database (See https://www.norman-network.com/nds/susdat/)
L	Pesticide manuals and hard copy reference books / other sources
M	GLEAMS Model database (Groundwater Loading Effects of Agricultural Management Systems). (See http://www.cpes.peachnet.edu/sewrl/Gleams/gleams_y2k_update.htm). Dataset no longer available.
N	Various Trusts, NGOs & Charities Data
P	Other non-EU, UK or US Governments and Regulators
Q	Miscellaneous Data from On-line Sources
R	Peer Reviewed Scientific Publications
S	Expert Judgement
T	UN EPFA Database. Dataset no longer available.
U	US Dept of Agriculture National Resources Conservation Service - various datasheets, databases and online sources

V	ChemID Online Databases (See https://chem.nlm.nih.gov/chemidplus/); Chemspider; PubChem
W	French database provided by ARVALIS-Institut du Végétal. Dataset no longer available.
X	WINPST Database (See http://www.ipm.ucdavis.edu/TOX/winpstdoc.html). Dataset no longer available.
Y	Germany's Federal Environment Agency (UBA) (See http://www.umweltbundesamt.de/index-e.htm)
Z	Kingtai Chemials Website (See http://www.kingtaichem.com/)

4.0. Quality Control and Management

Data management activities involve trawling for new or previously unidentified data. Evaluating its fitness-for-purpose, undertaking quality control activities and adding it to the database. The database and website are updated several times each week.

Data is sourced globally from published scientific literature and databases, manuals, registration databases and dossiers, company technical datasheets and research projects as described above.

Prior to entry into the databases data is subject to quality control. This is involves peer review, cross checking against other databases and data sources and, where doubt exists and the original reference is known, the original source is revisited and possibly the quality score (see below) adjusted.

Fitness for purpose is evaluated based on experimental conditions being appropriate for Europe, scientific protocols utilised, quality control findings and how recent the data is.

Data is then weighted 1 (low) to 5 (high) according to the confidence we have in that data. A low score does not necessarily indicate incorrect data but indicates we have not been able to obtain verification. Generally, as a guide the weighting scores are assigned according to the following:

1	Estimated data with little or no verification
2	Unverified data of unknown source
3	Unverified data of known source
4	Verified data
5	Verified data used for regulatory purposes.

However, confidence weightings may be adjusted if reason to doubt verified data exists or there is reason for greater confidence in an unverified value.

Once data has been accepted for inclusion into the database, data is extracted and transformed with respect to units. References are recorded and hardcopies filed.

5.0. Data Interpretation

5.1. Environmental fate

Parameter	Source	Thresholds
Solubility in water (mg l^{-1})	Arbitrary system in common use	<= 50 = Low 50 - 500 = Moderate > 500 = High
Vapour pressure at 25°C (mPa)	Based on that used within EFSA Guidance documents e/g/ 'Guidance on the assessment of exposure of operators, workers, residents and bystanders in risk assessment for plant protection products, EFSA journal 2014;12(10):3874.	< 5.0 = Low volatility 5.0 – 10.0 = Moderately volatile > 10 = Highly volatile
Henry's Law Constant (Pa m^3 mol^{-1})	Rule of thumb in wide, general use.	> 100 = Volatile 0.1 - 100 = Moderately volatile < 0.1 = Non-volatile
Octanol-water partition coefficient (Log P):	Used by the US EPA. Widely used rule of thumb.	< 2.7 = Low bioaccumulation 2.7 – 3 = Moderate > 3.0 = High
Soil degradation (days)	See note 1.	< 30 = Non-persistent 30 - 100 = Moderately persistent 100 - 365 = Persistent > 365 = Very persistent
Aqueous photolysis DT50 (days at pH 7)	See note 5.	< 1 = Fast 1 - 14 = Moderately fast 14 - 30 = Slow > 30 = Stable
Aqueous hydrolysis DT50 (days at 20°C and pH 7)	See note 5.	< 30 = Non-persistent 30 - 100 = Moderately persistent 100 - 365 = Persistent > 365 = Very persistent
Water-sediment degradation (days)	Same thresholds as soil degradation utilised. See note 1.	< 30 = Fast 30 - 100 = Moderately fast 100 - 365 = Slow > 365 = Stable
Water phase only degradation (days)	See note 5.	< 1 = Fast 1 - 14 = Moderately fast 14 - 30 = Slow > 30 = Stable
K_{oc}/ K_{foc} (ml g^{-1})	PSD Pesticide Data Requirement Handbook (2005). SSLRC Mobility	< 15 = Very mobile 15 - 75 = Mobile 75 - 500 = Moderately mobile

	Classification System. Also See note 5.	500 - 4000 = Slightly mobile > 4000 = Non-mobile
Freundlich equation	See note 9.	
GUS Index	Gustafson, DI (1989) Groundwater Ubiquity Score: a simple method for assessing chemical leachability. Environ. Toxicol. Chem 8, 339-357.	> 2.8 = High leachability 2.8 - 1.8 = Transition state < 1.8 = Low leachability
SCIGROW indicator	See note 8.	
Particle bound transport indicator	Goss & Wauchope (1990). See note 3.	
Bio-concentration factor	General rule of thumb and that used by the US EPA.	< 100 = Low potential 5000 – 100 = Threshold for concern > 5000 – High potential

5.2. Ecotoxicology

The ecotoxicological data interpretations given in the PPDB records are highly simplistic and should be used with care. Interpretations are based on a simple comparison with the 'thresholds' given below and take no account of other data which may affect the interpretation such as aquatic solubility, other related toxicological endpoints or the highest concentration tested. In addition, some of the thresholds given below are simple 'rules of thumb' and are not necessarily based on scientific observations.

5.2.1. Terrestrial ecotoxicology

Parameter	Source	Thresholds
Mammals - Acute oral LD50 (mg kg^{-1})	See note 5.	> 2000 = Low 100-2000 = Moderate < 100 = High
Mammals - Short term dietary NOEL (mg kg^{-1})	See note 5.	> 2000 = Low 100-2000 = Moderate < 100 = High
Mammals - Chronic toxicity as mg kg^{-1} d^{-1}	See note 5.	> 200 = Low 10-200 = Moderate < 10 = High
Birds - Acute LD50 (mg kg^{-1})	Consistent with US EPA Guidelines. See note 5.	> 2000 = Low 100 - 2000 = Moderate < 100 = High
Birds - Chronic toxicity as mg kg^{-1} d^{-1}	See note 5.	> 200 = Low 10-200 = Moderate < 10 = High

Earthworms - Acute 14 day LC50 (mg kg^{-1})	See note 10.	> 1000 = Low 10 - 1000 = Moderate < 10 - High
Earthworms - Chronic 14 day NOEC, reproduction (mg kg^{-1})	See note 10.	> 100 = Low 0.1 - 100 = Moderate < 0.1 = High
Soil micro-organisms	Nitrogen / carbon mineralisation.	<= 25% change is considered insignificant.
Collembola acute LC50 mg/kg	See note 11.	No interpretation
Collembola chronic reproduction 28d NOEL mg/kg	See note 11.	No interpretation
Honeybees (*Apis* spp.) - Acute LD50 (µg bee^{-1}) (contact, oral mode and unknown mode), worst case value from 24, 48 & 72hr values)	See note 5.	> 100 = Low 1 - 100 = Moderate < 1 = High
Honeybees (*Apis* spp.) - Chronic LDD50 or LC50 (µg bee^{-1} d^{-1}), 10 day	See note 11.	No interpretation
Bumblebees (*Bombus* spp.) - Acute LD50 (µg bee^{-1}) (contact and oral mode), worst case value from 24, 48 & 72hr values)	See note 5.	> 100 = Low 1 - 100 = Moderate < 1 = High
Mason bees (*Osmia* spp.) - Acute LD50 (µg bee^{-1}) (contact and oral mode), worst case value from 24, 48 & 72hr values)	See note 5.	> 100 = Low 1 - 100 = Moderate < 1 = High
Other pollinators - Acute LD50 (µg $insect^{-1}$) (contact and oral mode), worst case value from 24, 48 & 72hr values)	See note 5.	> 100 = Low 1 - 100 = Moderate < 1 = High
Beneficial insects (Ladybirds) (variable units and parameters)	See note 11.	No interpretation
Beneficial insects (Lacewings) (variable units and parameters)	See note 11.	No interpretation
Beneficial insects (Springtails) (variable units and parameters)	See note 11.	No interpretation
Beneficial insects (Parasitic wasps) (variable units and parameters)	See note 11.	No interpretation
Beneficial insects (Predatory mites) (variable units and parameters)	See note 11.	No interpretation

Beneficial insects (Ground beetles) (variable units and parameters)	See note 11.	No interpretation

5.2.2. Aquatic ecotoxicology

Parameter	Source	Thresholds
Fish - Acute 96 hour LC50 (mg l^{-1})	See note 5.	> 100 = Low 0.1 - 100 = Moderate < 0.1 = High
Fish - Chronic 21 day NOEC (mg l^{-1})	See note 5.	> 10 = Low 0.01 - 10 = Moderate < 0.01 = High
Aquatic invertebrates - Acute 48 hour EC50 (mg l^{-1})	See note 5.	> 100 = Low 0.1 - 100 = Moderate < 0.1 = High
Aquatic invertebrates - Chronic 21 day NOEC (mg l^{-1})	See note 5.	> 10 = Low 0.01 - 10 = Moderate < 0.01 = High
Aquatic crustaceans - Acute 96 hour LC50 (mg l^{-1})	See note 5.	> 100 = Low 0.1 - 100 = Moderate < 0.1 = High
Sediment dwelling organisms - Acute 96 hour LC50 (mg l^{-1})	See note 5.	> 100 = Low 0.1 - 100 = Moderate < 0.1 = High
Sediment dwelling organisms - Chronic 28 day NOEC, static, water (mg l^{-1})	See note 5.	> 10 = Low 0.01 - 10 = Moderate < 0.01 = High
Sediment dwelling organisms - Chronic 28 day NOEC, sediment (mg kg^{-1})	See note 5.	> 100 = Low 0.1 - 100 = Moderate < 0.1 = High
Aquatic plants - Acute 7 day EC50, biomass (mg l^{-1})	See note 6.	> 10 = Low 0.01 - 10 = Moderate < 0.01 = High
Algae - Acute 72 hour EC50, growth (mg l^{-1})	See note 6.	> 10 = Low 0.01 - 10 = Moderate < 0.01 = High
Algae - Chronic 96 hour NOEC, growth (mg l^{-1})	See note 6.	> 1 = Low 0.001 - 1 = Moderate < 0.001 = High

5.3. Human health

Parameter	Source	Thresholds
ADI (mg kg^{-1} bw)	The acceptable daily intake is the amount of a substance that can be ingested every day of an individual's entire lifetime, in the practical certainty, on the basis of all known facts, that no harm will result. SF – refers to the safety factor applied.	
AOEL (mg kg^{-1})	The acceptable operator exposure level is the maximum amount of active substance to which the operator may be exposed without any adverse health effects. SF – refers to the safety factor applied.	
Dangerous substances directive	This Directive requires Member States to introduce measures to eliminate (List I) or to reduce (List II) pollution of the aquatic environment from certain listed substances identified in its Annexes.	
MRL's - maximum residue limits	These limits can change and the data given here is usually that proposed by EFSA. Data may not be complete. See EU database for further information.	
Drinking water MAC	Maximum Admissible Concentration of the chemical in drinking water. The MAC for a chemical is derived from its ADI. The EU Drinking Water Directive imposes a maximum admissible concentration (EU MAC) for any individual pesticide compound of 0.1 mg l^{-1}.	
Who Toxicity class	WHO Guidelines 2004. Based on rat LD50 & physical state of the pesticide. See note 4.	See note 2.

Notes

1. Consistent with EU Guidance. (9188/VI/97 rev. 8.) and

   I. Kerle EA, Jenkins JJ & Vogue PA (1996), Understanding pesticide persistence and mobility for groundwater and surface water protection. Oregon State University. EM 8561.

   II. Rao PSC & Hornsby AG (2004) Behaviour of pesticides in Soils and water. University of Florida. See http://edis.ifas.ufl.edu/SS111.

   III. See also Note 3 below.

2. Several relevant references which include:

   I. Van der Werf , HMG (1996) Assessing the impact of pesticides on the environment. Agriculture, Ecosystems & Environment, 60, 81-96.

   II. Jury WA, Spencer WF, & Farmer WJ (1984) Behaviour assessment model for trace organics in soil. III Application of screening model. J. Environ Qual. 13, 573-579.

   III. Kerle EA, Jenkins JJ & Vogue PA (1996) Understanding pesticide persistence and mobility for groundwater and surface water protection. Oregon State University. EM 8561.

3. Table below has been extracted from:

I. Goss, D & Wauchope RD (1990) The SCR/ARS/CES Pesticide Properties Database. II using it with Soils data in a screening Procedure. In D.L. Weigmann Ed., Pesticides in the next decade: the challenge ahead, Virginia Resources Research Centre, Blacksburg, VA, USA pp471-493.

Potential for Particle-bound transport	Criteria
High	DT50 >= 40 days & Koc >= 1000 DT50 >= 40 days, Koc >= 500 & solubility <= 0.5 mg/l
Low	DT50 <= 1 day DT50 <= 2 days & koc <= 500 DT50 <= 4 days, Koc <= 900 & solubility >= 0.5 mg/l DT50 <= 40 days, Koc <= 500 & solubility >= 0.5 mg/l DT50 <= 40 days, Koc <= 900 & solubility >= 2 mg/l
Medium	All other

4. Classification given below has been extracted from the WHO Guidelines document: The WHO recommended classification of pesticides by hazard & guidelines to classification. (2004). See http://www.who.int/publications/en/

   - Class Ia: extremely hazardous
   - Class Ib: highly hazardous
   - Class II: moderately hazardous
   - Class III: slightly hazardous
   - O: Obsolete
   - NL: Not listed

5. Thresholds used have been selected to be consistent with industry guidelines, were developed, and are consistent with regulatory thresholds used in both the UK and EU. Alternative classification systems are in use. In particular, that published by the FAO (https://www.fao.org/3/X2570E/X2570E06.htm) may be useful.

6. The EU (Uniform Principles) (Annex VI of Directive 91/414/EEC) guidelines have been adopted have set toxicity:exposure (TER) ratios for algae and aquatic plants at 1/10th of those for fish and daphnids. The same ratio has been applied here.

7. In EU pesticide regulatory risk assessments 'hazard quotients' are used to determine the need for additional studies to assess risk to beneficial arthropods. Hazard quotients (HQ) are determined by dividing the Predicted Environmental Concentration (PEC) of the active substance by the median lethal rate (LR50). HQ values less than 2.0 are considered to be low risk to beneficial arthropods and additional (higher tier) data are not required. Values greater than 2.0 trigger additional data requirements. As the PEC is not known we are unable to provide an interpretation.

8. SCI-GROW is a screening model used by the US EPA to estimate pesticide concentrations in vulnerable groundwater. The model provides an exposure value that can be used to determine the potential risk to the environment and to human health from drinking water contaminated with the pesticide. The SCI-GROW estimate is based on environmental fate properties of the pesticide (aerobic soil degradation half-life and linear adsorption coefficient normalised for soil organic carbon content), the maximum application rate, and existing data from small-scale prospective ground-water monitoring studies at sites with sandy soils and shallow ground water.

SCI-GROW estimates represent worse case estimates. For this reason, it is not appropriate to use SCI-GROW concentrations for national or regional exposure estimates. Nor is this indicator an alternative to a scientific risk assessment. Values given are based on a standard 1 kg ha^{-1} or 1 L ha^{-1} application rate and should be adjusted to the actual application rate used

For more information see: http://www.epa.gov/oppefed1/models/water/scigrow_description.htm.

9. The distribution of a pesticide between the solution and absorbed phases can often be described by the "Freundlich equation", an equation that is used to describe a wide variety of adsorption data from every area of science. The equilibrium concentration and adsorbed pesticide amounts are determined experimentally. The Log10 of the quantity of adsorbed pesticide is plotted against the equilibrium concentrations. Often the relationship obtained is approximately linear and can be described by the Freundlich equation: Q=KC1/n, where Q is the adsorbed amount of pesticide (µg kg-1), C is the equilibrium concentration (µg l-1), and kf and n are the experimental parameters unique to the isotherm. The parameter n is greater than 1, the larger it is the more non-linear the equation becomes.

10. The availability of the pesticide in the soil can depend on the amount of soil organic carbon (SOC). The toxicity endpoint value may therefore be corrected for the difference in SOC of the test soil and the reference soil. This means that the toxicity endpoint value is divided by the percentage organic matter in the standard test soil and multiplied by the percentage organic matter in the reference soil. Uncorrected values are quoted herein unless otherwise stated e.g. '(corr)'.

11. Data is very limited and is presented in the literature in a variety of formats. Therefore, neither a standard format nor interpretation can be provided.

6.0. Key Species and Endpoint Glossary

Parameter	Explanation
EC_{50}	The concentration of a chemical that can be expected to cause a defined non-lethal effect in 50% of the tested population. In some cases, other percentages may be displayed (e.g., EC_{10} or EC_{15}).
LD_{50}	Used in toxicology this is the median lethal dose (LD_{50}, abbreviation for 'Lethal Dose, 50%'), of a toxic substance and is the dose required to kill half the tested population. LD_{50} figures are frequently used as a general indicator of a substance's acute toxicity.
NOEL/NOEC	'No Observed Effect Concentration'/'No Observed Effect Concentration' - greatest level or concentration of a substance, found by observation or experiment, which causes no detectable effect.
NOEAEC	'No Observed Ecologically Adverse Effect Concentration' - the highest concentration that causes no observed adverse effect on fauna or flora.

Species	Explanation
Given below are the first-choice species for ecotoxicological endpoints. However, if these are not available data for other species may be given instead. This will be indicated in the accompanying notes. Where data for several species are available, data for the most sensitive is given.	
Mammals	Rat, Mice, Dog (Mainly used for the human health studies)
Birds	Mallard duck (*Anas platyrhynchos*) Bobwhite quail (*Colinus virginianus*)
Soil micro-organisms	Various
Soil macro-organisms	Common brandling worm (*Eisenia foetida*)
Non-target plants	Various
Honeybees	European honeybee (*Apis mellifera*)
Bumblebees	*Bompus* spp. (typically *Bombus terrestris*).
Mason bees	*Osmia* spp.
Other pollinators	For example: *Megachile rotundata*, *Trigona spinipes*
Beneficial insects (Ladybirds)	Seven-spot ladybird (*Coccinella septempunctata*)
Beneficial insects (Lacewings)	Common green lacewing (*Chrysoperla carnea*)
Beneficial insects (Springtails)	*Folsomia* spp. (typically *Folsomia candida*)
Beneficial insects (Parasitic wasps)	Aphid parasitoid (*Aphidius rhopalosiphi*)
Beneficial insects (Predatory mites)	Predatory mite (*Typhlodromus pyri*)

Beneficial insects (Ground beetles)	*Poecilus* spp. (*Poecilus cupreus*)
Fish	Rainbow trout (*Oncorhynchus mykiss*) Bluegill sunfish (*Lepomis macrochirus*) Zebra fish (*Brachydanio rerio*)
Aquatic invertebrates	Daphnids (*Daphnia magna, Daphnia pulex*)
Aquatic crustaceans	Mysid shrimps (*Americamysis bahia*)
Sediment dwelling organisms	Chironomid midges (*Chironomus riparius*)
Higher aquatic plants	Duckweed (*Lemna gibba, Lemna minor*)
Algae	Green algae (*Pseudokirchneriella subcapitata, Scenedesmus subspicatus*)
For ecotoxicological data the 'worst case' data has been selected unless it appears wildly out of character with the majority of studies published. We have chosen specific species and endpoints wherever possible to ensure a harmonised and balanced data set. In some cases, endpoints other than these may be used, where this is the case the accompanying text will provide additional information.	
Mammals	Acute oral LD_{50}, short term 90-day NOEL as mg kg^{-1} and reproductive toxicity as mg kg^{-1} d^{-1}
Birds	Acute oral LD_{50} as mg kg^{-1} and reproductive toxicity as mg kg^{-1} d^{-1}
Soil micro-organisms	Various endpoints depending on availability, including information on N & C mineralisation (% effects)
Soil macro-organisms	14-day LC_{50} and chronic reproduction NOEC as mg kg $soil^{-1}$ dry weight
Non-target plants	Various endpoints depending on availability
Honeybees	Reasonable worse case of the 24, 36 and 72hr values (where available)
Bumblebees	Reasonable worse case of the 24, 36 and 72hr values (where available)
Mason bees	Reasonable worse case of the 24, 36 and 72hr values (where available)
Other pollinators	Reasonable worse case of the 24, 36 and 72hr values (where available)
Beneficial insects (Ladybirds)	Various mortality endpoints depending on availability (incl. LR_{50}, ER_{50}, % mortality, qualitative)
Beneficial insects (Lacewings)	Various mortality endpoints depending on availability (incl. LR_{50}, ER_{50}, % mortality, qualitative)
Beneficial insects (Parasitic wasps)	Various mortality endpoints depending on availability (incl. LR_{50}, EC_{50}, % mortality, qualitative)
Beneficial insects (Predatory mites)	Various mortality endpoints depending on availability (incl. LR_{50}, ED_{50}, % mortality, qualitative)
Fish	Acute 96-hr LC_{50} and 21day NOEC as mg l^{-1}
Aquatic invertebrates	Acute 48-hr EC_{50} and 21day NOEC as mg l^{-1}
Aquatic crustaceans	Acute 96hr LC_{50} as mg l^{-1}
Sediment dwelling organisms	96-hr LC_{50} and chronic 28-day NOEC static water only and sediment as mg l^{-1}

Higher aquatic plants	14-day EC_{50} as mg l^{-1}
Algae	Acute 72-96-hr EC_{50} and 72-96-hr NOEC biomass / growth as mg l^{-1}

7.0. For further details

Contact us at:

PPDB Management Team
Agriculture & Environment Research Unit
School of Life & Medical Sciences
University of Hertfordshire
College Lane
Hatfield
Hertfordshire
AL10 9AB
United Kingdom

Telephone: +44 (0)1707 284548
Email: aeru@herts.ac.uk