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FOOTPRINT

Functional Tools for Pesticide Risk Assessment and Management

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Pesticide database holding fate and ecotoxicological values

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Foreword

The present report was prepared within the context of the work package WP5 (Development of Functional Tools) of the FOOTPRINT project (http://www.eu-footprint.org).

The preferred reference to the present document is as follows:

Lewis K., Green A. & Tzilivakis J. (2007). Pesticide database holding fate and ecotoxicological values. Report DL24 of the FP6 EU-funded FOOTPRINT project [www.eu-footprint.org], 28p.

Executive summary

The principal aim of this work was to develop a database of fate and ecotoxicological data which will be used to support the three FOOT tools. The database was made available on the internet as an online resource open and free-of-charge to all interested parties (www.eu-footprint.org).

An initial review of existing databases with regard to environmental fate and ecototoxicological properties of pesticides revealed that existing resources did not meet the expectations of the FOOTPRINT project with regard to completeness and overall quality. In addition the review identified issues associated with format, updating, maintenance and language barriers.

The objectives of the FOOTPRINT PPDB were to provide:

- a single, comprehensive resource of reliable, consistently presented pesticide data,
- simple on-line access supported by layperson interpretations and user tools,
- a portable format for direct linking to software applications.

The FOOTPRINT PPDB currently holds ~700 pesticide data records and 350 additional records for their major metabolites. The database includes general information, physico-chemical and environmental fate data, acute and chronic endpoints for a range of fauna and flora and information on human health issues. Data are maintained regularly and the range of pesticides and data held are under constant review. Data have been cross-checked against a number of other resources and agreements to share data with holders of other databases have been put in place.

An indication of data quality and 'fitness for purpose' is provided by assigning each parameter with a confidence code that reflects the data source and the confidence database administrators have in the value.

Monitoring of visits of the FOOTPRINT PPDB web page suggests that the resource is extremely useful to a large range of individuals involved in pesticide risk assessment activities throughout the globe.

1 INTRODUCTION

The demand for detailed data on the physico-chemical and toxicological parameters of pesticides has grown considerably over the last couple of decades. This is, in part, due to more stringent regulatory controls and the use by regulators, policy makers and others of data-hungry modelling and risk assessment approaches.

Although it is difficult to be precise there may be as many as 1000 pesticides available globally. Many have been withdrawn from the European market by the ongoing review process (Directive 91/414), but it is not unusual for an individual European State to have around 300 pesticides registered for use at any given time. For example, it is estimated that approximately 330 active ingredients are currently registered in the UK, 380 in France and 250 in Germany. A wide range of parameters are required depending on the type and purpose of the application being used. It would not be unreasonable to suggest that a minimum of 6 to 10 parameters are required to calculate predicted environmental concentrations. In addition, ecotoxicological threshold values are needed for mammals, birds, earthworms, honey bees and aquatic species (e.g. fish, invertebrates, lower and higher aquatic plants). Therefore one might need up to 18 parameters for each pesticide studied, 6000 for all registered pesticides within one European State and potentially 18000 to study the full range.

It would appear, at first glance, that these data are readily available via a diversity of sources including government departments, manufacturers, universities and environmental bodies. One may also assume that the Internet has made access to these data simple, fast and unproblematic. Both assumptions are incorrect. Most of the datasets currently available are extremely limited regarding the range of pesticides they cover. As may be expected, national datasets are usually constrained to those pesticides registered for use in a particular country. Table 1 summarises the main resources which have been identified as of late 2006. From the table it can be seen that most datasets have around 200-400 records. However, there is a great deal of overlap in the active substances covered and most suffer from large gaps in information and presentation inconsistencies. Consequently, other sources of information, of which there are many, are essential.

Some datasets are comprehensive regarding the types of data they contain (e.g. environmental fate, human health). However, for the majority of pesticides, different datasets must be interrogated for different data types. For example, IPCS INCHEM might be used for basic chemical information such as molecular mass and structure, the ECOTOX database might be searched for ecotoxicological information and medical databases interrogated for information on human health. There are also commercial databases that contain comprehensive datasets,

but these require annual subscriptions and are rarely available for direct linking to software applications without payment of significant licence fees.

Resource name	No.	Data	Comments
Resource name	records	type [#]	Comments
91/414 EU /	140/	A, B, C,	ec.europa.eu/food/plant/protection/evaluation/index_
EFSA Evaluation	110	D, E	en.htm.
Dossiers		,	 www3.efsa.europa.eu/DAR/displaySubstance.cfm
ACP Evaluation	170	A, B, C,	 www.pesticides.gov.uk/publications.asp?id=202
Documents UK		D, E	• Some documents are quite old & have limited data
AGRITOX,	370	A, B, C,	• www.inra.fr/internet/Produits/agritox/php/fiches.php?
France		D [*] , E	PHPSESSID=ae0e236e3de4999ae0f50e9ef45eada7
UK Pesticide	880	A, B, C,	Commercial, priced publication
Manual 14 th Ed		D [*] , E	Variable useful content. Significant data gaps.
PAN Pesticides	Large	A, B, C,	www.pesticideinfo.org/Index.html
Database, USA	dataset	D [*] , E	Not user friendly. Mainly portal links, large data gaps
EXTOXNET,	180	A, B, C,	 extoxnet.orst.edu/ghindex.html
USA		D, E, F	Poor presentation which can undermine data
			integrity
US EPA	77	A, B, C,	www.epa.gov/opprd001/factsheets
Pesticide Factsheets		D, E	Mainly new actives
US EPA	Large	E / A, B,	cfpub.epa.gov/ecotox/
ECOTOX	dataset /	C C	 cipub.epa.gov/ecolox/ cipub.epa.gov/pfate/Chem_details.cfm
Database / Fate	189	U	 Needs careful choice of data best fit for purpose
Database			• Needs caleful choice of data best in for purpose
PMRA Pesticide	70	A, B, C,	www.pmra-arla.gc.ca/english/pubs/prdd-e.html
Factsheets,		D [*] , E	Limited dataset
Canada			
PIC Decision	350	A*, B*,	www.pic.int/en/Table7.htm
Guidance (DGD)		C*, D,	DGD produced for chemicals listed in Annex III,
Documents, FAO		E*	Rotterdam Convention on Hazardous Chemicals &
			subject to a PIC.
Pandora, NL	225	A*, B,	Mainly banned or severely controlled pesticides
Pandora, NL	225	С, Е	Research report RIVM no. 679101014 (1994)
KingTai	60	A, B §	Quite old, report may not still be available www.kingtaichem.com
Chemicals	00	А, Б §	5
Datasheets			Very slow website, but does contain some useful data
ChemIDPlus,	Unknown	A§	Chem.sis.nlm.nih.gov/chemidplus
USA	Ontriown	1.3	 Need CAS number to search, Useful for basic
			information
Pesticide Data	400	A, B, C,	www.mst.dk/udgiv/publications
Tables, Danish		E†	 Good data source, but not referenced
EPA			
European	Unknown	D	http://ecb.jrc.it
Chemicals			Only EU registered pesticides available – many gaps
Bureau			in data
IPCS INCHEM	Unknown	А	www.inchem.org/

Table 1: Summary of the main pesticide data resources (2006 data)

Definition of data types: A – general data, B – physico-chemical, C – fate, D – human health, E – ecotoxicological
* Limited range of parameters held, § Very limited range of other data types held, † Aquatic ecotoxicolgical endpoints only

The format of presentation is also very variable ranging from tabular to narration. The latter are common and these are useful as they place the data in context. However, researchers needing specific parameters must search each document and collate their own datasets, especially if they wish to make the data available to software applications. This process is very slow and invites typographical errors.

The Internet has dramatically altered the way information is distributed and shared and has become an important research tool. However, due to its loose, forever changing structure, free of content management, it can be very difficult to locate information relevant to a specific topic. Unlike bibliographic databases it does not provide an index or contents page. Language barriers can also hinder the use of potentially valuable sites. Whilst many pesticide common names are similar from one language to the next, slight variations can cause search tools to fail. The Internet has no structural boundaries, no standard method of organisation and information available today may not be available tomorrow or necessarily stay at the same URL. There is also little peer review control and judging data credentials, i.e. fitness for purpose and accuracy, can be problematic. For example, most of the physico-chemical and toxicological data needed have a natural variability often dependent on the conditions under which they are measured. In some instances the natural data range can be large and the value selected may have a significant influence on the risk assessment outcome. This is not to mention the unavoidable errors that creep into datasets such as typographical mistakes or problems associated with units of measurement. There is also the question of data maintenance - some resources were collated some time ago and are not updated. An important issue is that the quality and utility of data should not be separated from its purpose and intent. Any simulation is only as good as the underlying data.

Consequently, there is a serious need for a single authoritative source to capture, archive, validate, manage, maintain and provide access to data for the majority of pesticides available world-wide for pesticide risk assessments. The FOOTPRINT Pesticide Properties Database (FOOTPRINT PPDB) recently launched solves many of the problems discussed here.

2 DATABASE PURPOSE, DESIGN AND DEVELOPMENT

The origins of the FOOTPRINT PPDB can be traced back to 1994 to the development of the award-winning Environmental Management for Agriculture (EMA) software (Lewis & Bardon, 1998). This software package included a suite of decision support tools to help UK farmers improve their environmental performance and included a pesticide risk module with an embedded pesticide database (Lewis et al., 2003). The pesticides within the database were restricted to those active substances registered for use in the UK and included both physico-chemical parameters and ecotoxicological data. The EMA software and the pesticide database have been constantly maintained and updated and are still available today. However, recent

EU funding for a new approach to pesticide risk assessment (FOOTPRINT – Functional Tools for Pesticide Risk Assessment and Management, www.eu-footprint.org) has provided the opportunity to re-assess the database in terms of i) the range of pesticides covered; ii) the data stored; and, iii) their 'fitness for purpose'.

The objectives of the new FOOTPRINT database is to provide:

- a single, comprehensive resource of reliable, consistently presented pesticide data having common syntax, units and semantics
- a portable format for direct linking to software applications such as risk assessment systems
- on-line access using a simple tabular format supported by layperson interpretations and user tools.

If the new database was to provide a solution to many of the problems experienced by users of pesticide data then it was essential that the data stored was suitable for a wide range of applications and different user types. To this end the data stored covers:

- General information. For example common and chemical names, language translations, chemical group, formula, structures, pesticide type, CAS/EC numbers and data related to country registration.
- **Physico-chemical data.** Including solubility, vapour pressure, density, dissociation constants, melting point and information on degradation products.
- Environmental fate data. For example the octanol-water partition constant (Log P), Henry's law constant, degradation rates in soil, sediments and water (DT₅₀), the Freundlich sorption coefficient (Kf) and exponent (nf) and the organic-carbon sorption constant (K_{oc}).
- Human health information. This includes World Health Organisation toxicity classifications, Acceptable Daily Intakes (ADI), Maximum reference dose (ArfD), toxicity to mammals, other exposure limits and toxicity endpoints, plus the EC risk and safety classifications, maximum concentration in drinking water (MAC).
- **Ecotoxicology**. For example, acute and chronic toxicity data for a range of fauna and flora plus information on bioaccumulation.

Two distinct user types have been identified: (i) those requiring large datasets for software applications such as risk assessments and (ii) users seeking specific data items or data on a specific chemical. Microsoft Access 2000 Database format has been selected as the primary storage method. It is probable that this format will satisfy the requirements of users needing to embed datasets into software applications. The database is then streamed through various 'data filters' for formatting into HTML pages for online access and translation from English

language into a range of EU languages. This process helps simplify the updating and maintenance process.

The online version of the database has various user tools available including a search feature that can identify a pesticide record by active substance, common name (in any of the EU languages offered), alternative names or the chemical registration number (CAS RN). There is also a full index page and direct electronic links from parent chemicals to their metabolite data pages. To enable laypersons to use the on-line resource standard interpretations of the data are offered as hazard classifications. In most cases the thresholds used are those used for regulatory purposes or are 'rules of thumb' in wide and general use such as the guidelines used by the UK pesticide industry for developing Pesticide Environmental Information Sheets. Two risk indicators have also been calculated from the available data: (i) the GUS Index for groundwater leaching potential (Gustafson, 1989) and (ii) a measure of particle bound transport which indicates the pesticides risk of being transported with runoff (Goss and Wauchope, 1990).

3 DATA COMPILATION

Probably the best sources of information currently available for pesticide properties are the monographs produced as part of the EU review process and data within these documents has been first choice for populating the database. Where EU documents are not available, alternative sources have been used including:

- Databases and documents from the EU and national government departments including the UK's PSD, Germany's Federal Environment Bureau, the Danish Environmental Protection Authority, the US EPA and the French registration authorities (Agritox)
- On-line databases e.g. ARIS, EXTOXNET, ARS/OSU, PAN, AGRITOX (see Table 1)
- Manufacturers safety datasheets and environmental fact sheets, on- and off-line
- Hardcopy, peer reviewed scientific publications and data derived from research projects.

As the primary purpose of the database is risk assessment, data have been selected for this particular use. The values quoted for physico-chemical properties are usually a mean of the various studies identified. Where a parameter is particularly sensitive, to climate or soil for example, information on the data range has been added. Where a parameter is just naturally very variable, we have attempted to select the most appropriate value for EU conditions. For ecotoxicological data, the 'worst case' value has been selected unless it appears wildly out of character with the majority of studies published. The data relate to specific species and endpoints, where possible, to ensure a harmonised and balanced dataset.

The FOOTPRINT PPDB has been extensively cross-referenced against other datasets as an evaluation exercise. This has helped to identify erroneous and inconsistent data highlighting the need for further investigation and further consultation of the original data source (rather than the dataset).

The accuracy of the data always challenges the accuracy of the model or risk assessment system. No matter how good the model is, the outcome of the modelling will only ever be as good as the input data. Due to the importance of the quality aspects, a 'code' has been attached to all data contained in the FOOTPRINT PPDB with information on the source of the data and on the confidence that should be assigned to them. Confidence values are in the range 0 (very little confidence) to 5 (reliable data) and are a function of the data source, publication date, referencing, the match to the desired parameter and fitness-for-purpose. For example, avian toxicity data taken from a recent EU dossier that exactly matches the endpoint required (e.g. acute oral LD₅₀ mallard) would be assigned A5. 'A' indicates the source as an EU dossier and '5' indicates high confidence in the data quality. However, a soil DT_{50} extracted from an ad-hoc publication which gives no details of the original data source or the conditions under which the data was collected would be assigned Q1. 'Q' being the reference code for miscellaneous documents and '1' referring to the poor level of data confidence. It should be remembered, however, that the process of confidence scoring is somewhat subjective in nature and only meant as a guide. A low score does not, necessarily, indicate inaccurate or poor data. Full details of the quality and source codes can be found on the database web site.

4 COMPARISON WITH OTHER RESOURCES

The FOOTPRINT PPDB currently holds approximately 700 pesticide data records and a further 350 records for associated metabolites (Appendix 1). Table 2 provides information on gaps for the main parameters and provides a rough comparison with sub-sets of 100 records taken from two other datasets. Records for the subsets were randomly selected and only the presence of numerical data has been counted. Qualitative statements (e.g. high, low) have been ignored as they cannot be used as data input with any accuracy.

Parameter	FOOTPRINT PPDB	AGRITOX	EXTOXNET
Number records examined/total	700/700	100/370	100/180
Presentation style	Tabular	Tabular	Narration
General description & generic name	100%	100%	100%
CAS RN Number	100%	99%	99%
Chemical formula	100%	94%	0%
Molecular mass	100%	94%	100%
Structural picture	97%	51%	0%
Relative density / bulk density	78%	0%	2%
рКа	33%	32%	0%
Aqueous solubility	97%	90%	94%
Solubility in organic solvents	75%	81%	6%
Partition Coefficient Log P	95%	77%	58%
Vapour Pressure	94%	85%	84%
Henry's constant	87%	59%	0%
Soil DT50	86%	64%	85%
Sorption Coefficient Koc	80%	44%	84%
Aqueous photolysis DT50	49%	37%	30%
Neutral hydrolysis DT50	66%	86%	34%
Water-sediment system DT50	45%	25%	0%
Bioconcentration data	45%	18%	58%
Ecotoxicity – mammals	99%	97%	97%
Ecotoxicity – birds	87%	82%	88%
Ecotoxicity – acute fish	93%	84%	92%
Ecotoxicity – acute aqueous invertebrates	89%	76%	10%
Ecotoxicity – honeybees	76%	74%	40%
Ecotoxicity – earthworms	56%	46%	9%
Ecotoxicity – algae	75%	61%	0%
Ecotoxicity – higher aquatic plants	39%	14%	0%
Toxicity – oral mammals	99%	97%	97%
Toxicity – WHO classification	100%	0%	0%
Toxicity – EC Risk & safety classifications§	58%	0%	0%
Average % across record set	78%	61%	44%

 Table 2: Comparative analysis of the FOOTPRINT PPDB and two other databases

 in terms of availability of the data

5 DATABASE ACCESS AND CURRENT USAGE

The Microsoft Access database on CD is available to all individuals subject to an administration fee and, if it is to be used with software that will be distributed for third party or commercial use, a modest licence fee. The fees include database updates for 12 months.

A prototype on-line version of the database was launched on a free-to-all basis during 2006 via the FOOTPRINT website (www.eu-footprint.org). An example of the data provided for an active ingredient is presented in Appendix 2. In early 2007 the format and content were finalised and the database was made available more widely via ADLib (www.adlib.ac.uk) and other websites (www.herts.ac.uk/aeru/footprint). Shortly after the launch, processes were put in place to monitor activity on the site and provide user statistics. The monitoring has highlighted the fact that the database is being used extensively. Figure 1 shows user statistics for the first 28 days of the official database launch. A typical weekday approximately 200 page loads of data were downloaded with around 50 unique visitors. Figure 2 shows the same statistics for the first three months and illustrates a significant increase in visitors to the online site with typically 400-500 page loads of information being downloaded.

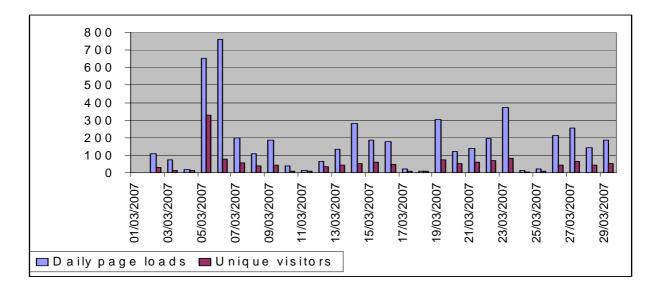


Figure 1: Database usage statistics in the first month following launch

The peak shown shortly after the launch coincides with the start of the working week and, as the statistical counters were all set to zero, shows the initial level of interest. Since this time, usage is quite steady at around 200 hits each working day. Initially, the majority of users were finding the database using Internet browsers and not via direct website links. However, current statistics indicate the site is now being bookmarked and users are returning on a frequent basis.

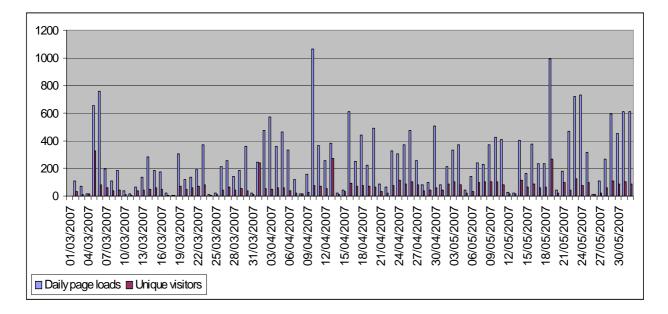


Figure 2: Database usage statistics in the first 3 months following launch

Another interesting issue is the wide range of countries being represented by users. Figure 3 shows the main areas of activity across the globe. The pink dots represent a cluster of one or more users.

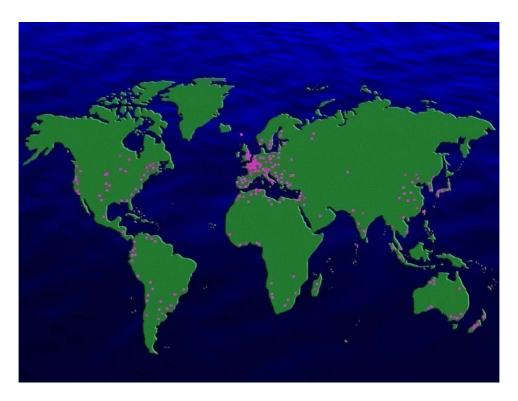


Figure 3: Geographical origin of website visitors

6 CONCLUSIONS AND PERSPECTIVES

The amount of pesticide data required for risk assessment exercises is very significant and despite the Internet and greater public availability, identifying the right data that is fit-forpurpose can be time consuming and frustrating. The Internet has often been heralded as revolutionising publishing, information sharing and research. This is undoubtedly true, but this revolution has introduced its own problems. The new FOOTPRINT PPDB does not pretend to hold full datasets for all pesticides; indeed, there are still many data-poor pesticides in use. However, basic analysis and comparison of these datasets show it to be a great improvement on existing resources bringing together the best data from the most reliable sources. Usage statistics show that the database is in global use and website activity is increasing month on month.

The MS Access database will enable external software applications to extract data directly avoiding the need for users to source and input their own data. This effectively reduces data input time and ensures that the best available data is used, helping to optimising the performance of the risk assessment process. This is the approach taken by the EU FOOTPRINT project which is currently developing a suite of harmonised pesticide risk assessment tools at national, regional and farm level. The on-line database and associated tools provide a more complete service to users. Language translations, comprehensive indices and extensive search facilities plus the layman data interpretations all contribute to a user-friendly access to the data.

7 REFERENCES

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2,4,5-trichlorophenol

Appendix 1 - List of active ingredients and metabolites listed in the FOOTPRINT PPDB in June 2006

((E,E)-methoxyimino-[2-[1-(3trifluoromethylphenyl)ethylideneaminooxymethyl] -phenyl]acetic acid) (+-)-2-[4,5-dihydro-4-methyl-4-(1-methylethyl)-5-oxo-1Himidazol-2-yl]-3,5,pyridinecarboxylic acid (1R,3R,E)-3-(4chlorobenzylidene)-5,5dimethyl-1-((1H)-1,2,4triazol-1-ylmethyl)cyclopentan-1,3-diol (4-trifluoromethoxy)phenyl urea (6-cyclopropyl-2phenylaminopyrimindin-4yl)methanol (CONH2-Fen) (D+)-2-(4-(6-chloro-2benzoxazolyloxy)phenoxy)-propionic acid (DTPU) (E)-2-(2-[6-cyanophenoxy)pyrimidin-4-yloxyl]-phenyl-3-methoxyacrylic acid (E)-2-(4-chlorobenzylidene)-5,5-dimethyl-1-((1H)-1,2,4triazol-1-ylmethyl)cyclopentan-1,3-diol (E)-methoxyamino(alpha-(otolyloxy)-o-tolyl]acetic acid (E)-methyl 5-chloro-2,3dihydro-2-hydroxy-1-[[[(methoxycarbonyl)[4trifluoromethoxy)phenyl]am ino]carbonyl]hydrazono]-1H-indene-2-carboxylate (R)-2-[4-(6-chloro-quinoxaline-2-yloxy)

2-yloxy) phenoxy]propanoic acid (TPSA) (Z)-2-chloro-3-[2-chloro-5-(((2hydroxycarbonyl)cyclohexe n-1yl)carbonylamino)phenyl]a crylic acid (Z)-2-chloro-3-[2-chloro-5-(1,3,dioxo-4,5,6,7tertahydroisoindol-2yl)phenyl]acrylic acid [3-cyano-4-methanesulfonyl-2methyl phenyl](5-hydroxy-1-methyl-1H-pyrazol-4yl)methanone [E-o-(2-hydroxycarbonyl-5methyl)phenoxymethyl]-2methoxyimino-Nmethylphenyl acetamide [E-o-(5-hydroxycarbonyl-2methyl)phenoxymethyl]-2methoxyimino-Nmethylphenyl acetamide 1-(2,4-dichlorophenyl)2imidazol-1-ylethanol 1-(3,5-dichlorophenyl)-5isopropyl biuret 1,2,4-triazole 1,3-dichloropropene 1-methylcyclopropene 1-naphthol 2-(3,5-dichlorophenyl)-4,4dimethyl-5-methyleneoxazoline 2-(3trifluoromethylphenoxy)nic otinamide 2-(3trifluoromethylphenoxy)nic otinic acid 2,2-dimethyl-1,3-benzodioxol-4ol 2,3,6-TBA

2.4-D 2,4-DB 2,4-dichloroaniline (2,4-DCA) 2,4-dichloroanisole 2,4-dichlorophenol 2,5-dichloroaniline 2,6-dichloro-1,4phenylenediamine (DCPD) 2,6-dichlorobenzamide (M02) 2,6-dichlorobenzoic acid 2,6-difluorobenzoic acid 2-[4-(2,4dichlorophenoxy)phenoxy] propanoic acid 2-[N-[3-((1Z)-2-carboxy-2chlorovinyl)-4chlorophenyl]carbamoyl]-?hydroxycyclohex-1enecarboxylic acid 2-amino-4,6dimethoxypyrimidine 2-amino-4,6-dimethylpyrimidine 2-amino-4-methoxy-6-methyl-1,3,5-triazine 2-amino-4methylsulfonylbenzoic acid (AMBA) 2-aminobenzimidazole 2-aminobutane 2-amino-N-isopropylbenzamide 2-butanesulfonic acid (BSA) 2-chloro-4-methylsulfonylbenzoic acid (CMBA) 2-dodecyl-3-hydroxy-1,4naphthoquinone 2-ethylsulfinyl ethane sulfonic acid 2-hydroxy alachlor 2-hydroxy-3-fluoro-5-chloropyridine

2-hydroxyquinoxaline 2-isopropyl-4-methyl-6hydroxypyrimidine 2-methyl-4-chlorophenol 2-pyrroline-3-carbonitrile,4bromo-2-(4-chlorophenyl)-5-(trifluoromethyl)chlorfenapyr 3-(2,2-dichlorovinyl)-2,2dimethylcyclopropanecarb oxylic acid (DCVA) 3-(3-chloro-p-tolyl)-1methylurea 3-(4,5-dihydro-isoxazol-3-yl)-4methanesulfonyl-2-methylbenzoic acid 3-(4-cyclopropyl-6methylpyrimidin-2ylamino)phenol 3-(ethylsulfonyl)-2pyridinesulfonamide 3,3-dichloro-4,4dimethylazobenzene 3,4-dichloroaniline 3,5,6-trichloro-2-pyridinol (TCP) 3,5-dichloro-2,4difluorophenylurea 3,5-di-iodo-4hydroxybenzamide 3,5-di-iodo-4-hydroxybenzoic Ν

3,6-dichlorosalicyclic acid 3-aminophenyl methylcarbamate 3-chloro-4-methylaniline 3-chloro-5-trifluoromethylpyridine-2-carboxylic acid (M03) 3-chloro-8-quinoline-carboxylic acid 3-chloroallyl alcohol 3-formamidophenyl methylcarbamate 3-hydroxycarbofuran

acid

3-hydroxyformanilide

3-hydroxymethyl sulfentrazone (N-[2,4-dichloro-5-[4-(difluoromethyl)yl]pheny]methanesulfonam ide 3-hydroxyquinoxyfen 3-ketocarbofuran 3-methyl-4-nitrophenol (NMC) 3-phenoxybenzoic acid 3-trifluoromethylbenzoic acid (TFMBA) 4-(1,1-dimethylethyl) benzene ethanol 4-(4-chlorophenyl)-2-(methyl-1H-1,2,4-triazole)-4-oxo-2phenylbutanenitrile 4,4-dibromobenzilic acid 4,5-dihydro-5-hydroxy-6methyl-4-[3pyridinylmethylene)amino]-1,2,4-triazine-3-(2H)-one 4,5-dimethyl-thiophene-3carboxylic acid allyamide 4,6-Bis(amino)-2-chloro-striazine 4,6-dimethoxypyrimidine-2-ylurea 4-amino-2-[3-(4,6dimethoxypyrimidin-2yl)ureidosulfonyl]-N, Ndimethylbenzamide 4-amino-2-chloropyridine (ACP) 4-amino-3,5-dichloro-6-fluoro-2-pyridinol 4-amino-3,5-dichloro-6-fluoromethoxypyridine 4-chloro-2-methylphenol 4-chloro-5-p-tolylimidazole-2carbonitrile (CCIM) 4-chloro-5-p-tolylimidazole-2carboxamide (CCIM-AM) 4-chloro-5-p-tolylimidazole2carboxylic acid (CTCA) 4-chlorophenylurea 4-chloroprothiofos

4-CPA 4-fluoro-3-phenoxybenzoic acid (FPBacid) 4-fluoro-3-phenoxybenzoic acid (FPBsyra) 4-hydroxy saccharin 4-hydroxy-2,5,6trichloroisophtalonitrile 4-hydroxyquinazoline 4-methoxybiphenyl 4-N-[3-chloro-5-trifluoromethylpyridin-2-yl-(hydroxyl)methyl]-2,6dichlorobenzamide (M01) 4-tert-butyl-2-6, dinitroaniline 4-trifluoromethylnicotinic acid 5-(2,4-dichlorophenoxy)-2nitrobenzoic acid 5-(4-chlorophenyl)-N-(4oxocyclohexyl)-4-methyl-2oxothiazolidine-3carboxamide 5-(aminosulfonyl)-1H-1,2,4triazole-3-carboxylic acid (ASTCA) 5-[4-(4hydroxyphenoxy)phenyl-5methyl-3-(phenylamino)-2.4-oxazolidine dione 5-amino-2,4dimethyltrifluoromethanesu Ifonanilide 5-amino-N-(2,6-dichloro-3methylphenyl)-1H-1,2,4triazole-3-sulfonamide 5-hvdroxy florasulam 5-hydroxy pyrimidine amine 5-methyl-2-(3H)-oxazolone 6-(2-ethylsulfinylpropyl)-4-oxy-2-propyl-4,5,6,7tetrahydro-1,3,benzoxazole 6-(3-trifluoromethylphenoxy)-2pyridine carboxylic acid

6-{5-hydroxy-1-methyl-1Hpyrazol-4-yl)carbonyl]-5methyl-2,3-dihydro-4H-1benzothiopyran-4-one 6-chloro-3-phenyl-pyridazin-4ol 6-chloronicotinic acid 6-ethoxy-2-ethyl-4hydroxypyrimidine abamectin acephate acequinocyl acetamiprid acetochlor acibenzolar-s-methyl acid sulphonamide acid sulphonimide acifluorfen-sodium aclonifen acrinathrin acrolein alachlor alanycarb albendazole aldicarb aldicarb sulfoxide aldoxycarb aldrin allethrin allethrolone alloxydim alpha-cypermethrin alpha-hydroxy-alpha-methyl-4phenoxybenzene acetic acid aluminium ammonium sulphate aluminium sulphate ametryn amide amidosulfuron aminomethylphosphonic acid (AMPA) aminopyralid aminopyrimidine amitraz

amitrole ammonium acetate ammonium carbonate ammonium hydroxide ammonium sulphamate ammonium sulphate ammonium thiocyanate ancymidol anilazine aniline anthracene oil anthraquinone asulam atrazine aviglycine-HCl azaconazole azadirachtin azafenidin azamethiphos azimsulfuron azinphos-ethyl azinphos-methyl aziprotryne azocyclotin azoxystrobin Bacillus sphaericus **Bacillus** subtilis **Bacillus thuringiensis** beflubutamid benalaxyl benalaxyl-M benazolin bendiocarb benfluralin benfuracarb benfuresate benodanil benomyl benoxacor bensulfuron-methyl bensulide bensultap bentazone benthiavalicarb benzaldehyde

benzfendizone benzo[1,2,3]thiadiazole-7carboxylic acid benzothiazole benzothiazolyloxyacetic acid benzoximate benzyl alcohol beta-cyfluthrin beta-cypermethrin bifenazate bifenox bifenthrin binapacryl bioallethrin bioresmethrin biphenyl bispyribac-sodium bistrifluron bitertanol bitertanol-benzoic acid bone oil Bordeaux mixture boscalid brodifacoum bromacil bromadiolone bromethalin bromocyclen bromofenoxim bromophos bromophos-ethyl bromopropylate bromoxynil bromuconazole bronopol bupirimate buprofezin butachlor butanamide butocarboxim butoxycarboxim butralin butvlate cadusafos calciferol

calcium carbonate calcium chloride calcium hydroxide calcium phosphate camphechlor captafol captan carbaryl carbendazim carbetamide carbofuran carbon dioxide carbophenothion carbosulfan carboxin carboxin sulfone carboxin sulfoxide carfentrazone-ethyl carpropamid cartap carvone cetrimide chinomethionat chitosan chlomethoxyfen chloralose chloramben chlorbromuron chlorbufam chlordane chlorethoxyfos chlorfenapyr chlorfenson chlorfenvinphos chlorfluazuron chlorflurenol chloridazon chlormephos chlormequat chloride chlorobenzilate chlorobenzoxazolone chloroneb chlorophacinone chlorophyllin chloropicrin

chloropropylate chlorothalonil chlorotoluron chloroxuron chlorpropham chlorpyrifos chlorpyrifos-methyl chlorsulfuron chlorthal-dimethyl chlorthiamid chlozolinate cholecalciferol choline chloride chrysanthemic acid cinidon ethyl cinmethylin cinosulfuron cis- 5-(4-chlorophenyl)-dihydro-3-phenyl-3-(1H-1,2,4triazole-1-ylmethyl)-2- 3Hfuranone clethodim clethodim sulfoxide clethodim sulfuron clodinafop-propargyl clofencet clofentezine clomazone clopyralid cloquintocet-mexyl clothianidin codlemone copper acetate copper carbonate copper chloride copper dimethyldithiocarbamate copper hydroxide copper oxide copper oxychloride copper sulphate coumachlor coumafuryl coumaphos coumatetralyl

crimidine

cyanamide cyanazine cyanophos cyazofamid cyclanilide cycloate cyclopropylpropane-1,3-dione cycloxydim cycloxydim sulfone (T2SO) cycloxydim sulfoxide (TSO) cycluron cyflufenamid cyfluthrin cyhalofop acid cyhalofop amide cyhalofop diacid cyhalofop-butyl cyhalothrin cyhexatin cymiazol cymoxanil cypermethrin cyproconazole cyprodinil cyromazine dalapon-sodium daminozide dazomet DCPMU DCPU DDT DE-535 phenol DE-535 pyridinol DE-535 pyridinone decamethrinic acid (Br2CA) deethyl ametryne (DEA) deltamethrin demethoxyisoxaben demeton-S-methyl desaminodiketometribuzin (DADK) desamino-metamitron desethyl azinphos-ethyl desethylatrazine

desethylsimazine desmedipham desmethyl sulfosulfuron desmethylisoproturon desmetryn di-1-p-menthene diafenthiuron di-allate diazinecarboxylic acid, 2-(4methoxy-[1,1-biphenyl]-3yl),1-methylethyl ester diazinon dicamba dichlobenil dichlofenthion dichlofluanid dichloracetic acid dichlorodiphenyldichloroethane (DDD) dichlorodiphenyldichloroethylen e (DDE) dichloroethanol dichlorophen dichlorprop dichlorprop-P dichlorvos diclofop-methyl dicloran dicofol dicrotophos dicyclanil dicyclopentadiene dieldrin dienochlor diethofencarb diethylenetriaminopentamethyl phosphonic acid (DTPP) diethylthiophosphate difenacoum difenoconazole difenoxuron difenzoquat difethialone diflovidazin diflubenzuron

diflufenican dihydroxyallethrolene diisobutylamine diketo-metribuzin (DK) dimefox dimefuron dimepiperate dimethachlor dimethenamid dimethenamid-P dimethipin dimethirimol dimethoate dimethomorph dimethyl amino oxoacetic acid (DMOA) dimethylamine dimethylaminosulfanilide (DMSA) dimoxystrobin diniconazole dinitramine dinobuton dinocap dinoseb dinoterb dioxacarb diphacinone diphenamide diquat dibromide disulfoton dithianon dithiocarbamate dithiopyr diuron DMST DM-TM DNOC dodemorph dodine endosulfan endosulfan sulfate endothal endrin epoxiconazole

EPTC

esfenvalerate ester sulphonamide ethaboxam ethalfluralin ethane sulfonic acid ethanedial ethanesulfonic acid (ESA) ethanethiol ethephon ethiofencarb ethiofencarb sulfone ethiofencarb sulfoxide ethion ethirimol ethofumesate ethoprophos ethoxyquin ethoxysulfuron ethyl 3-hydroxycarbanilate (EHPC) ethylene bisisothiocyanate pulphide (EBIS) ethylenethiourea ethylenethiourea (ETU) ethyleneurea (EU) etofenprox etoxazole etridiazole etrimfos F8426-chloropropionic acid F8426-cinnamic acid F8426-propionic acid famoxadone fatty acids fenamidone fenamiphos fenamiphos sulfone fenamiphos sulfoxide fenarimol fenazaquin fenbuconazole fenbutatin oxide fenchlorazole fenclorim

fenfuram fenhexamid fenitrothion fenoprop fenothiocarb fenoxaprop fenoxaprop-ethyl fenoxaprop-P fenoxaprop-P-ethyl fenoxycarb fenpiclonil fenpropathrin fenpropidin fenpropimorph fenpyroximate fenthion fenthion sulfone fenthion sulfoxide fentin acetate fentin hydroxide fenuron fenvalerate ferbam fipronil flamprop flamprop-M-isopropyl flazasulfuron flocoumafen flonicamid florasulam fluazifop fluazifop-butyl fluazifop-P fluazifop-P-butyl fluazinam fluazolate flubenzimine flucycloxuron flucythrinate fludioxonil flufenacet flufenoxuron flufenzin flumetsulam flumioxazine

fluometuron fluopicolide fluoroacetamide fluoroglycofen fluoxastrobin flupyrsulfuron-methyl fluquinconazole flurazole flurenol fluridone flurochloridone fluroxypyr flurprimidol flurtamone flusilazole flusulfamide flutolanil flutriafol FOE oxalate FOE sulphonic acid folpet fomesafen fonofos foramsulfuron forchlorfenuron formaldehyde formetanate formothion fosamine fosetyl-aluminium fosthiazate fuberidazole furalaxyl furathiocarb furfural gamma-cyhalothrin gamma-HCH gibberellins glufosinate-ammonium glyphosate guazatine halfenprox halofenozide haloxyfop-P HEC-5725-carboxylic acid HEC-5725-des-chlorophenyl heptachlor heptachlor epoxide heptenophos hexachlorobenzene hexachlorophene hexaconazole hexaflumuron hexazinone hexythiazox **HMCPA** hydramethylnon hydrogen peroxide hydroprene hydroxylated lambdacyhalothrin XV hydroxypropazine hydroxysimazine hymexazol icaridin imazalil imazamethabenz-methyl imazamox imazapyr imazaquin imazethapyr imazosulfuron imibenconazole imidacloprid iminoctadine indoxacarb iodofenphos iodosulfuron-methyl-sodium ioxynil iprodione iprovalicarb isazofos isofenphos isopropalin isoprothiolane isoproturon isoval isoxaben isoxaflutole isoxathion

metazachlor oxalic acid metazachlor sulfonic acid

JAU 6476-desthio JAU 6476-S-methyl kresoxim-methyl lambda-cyhalothrin laminarin lenacil limonene linuron lufenuron malathion malathion dicarboxylic acid malathion monocarboxylic acid maleic hydrazide m-aminophenol mancopper mancozeb mandipropamid maneb **MCPA** MCPB mecarbam mecoprop mecoprop-P mefenacet mefenpyr mefluidide melamine mepanipyrim mephosfolan mepiquat chloride mepronil meptyldinocap mercaptan merphos mesosulfuron acid mesosulfuron-methyl mesotrione metaflumizone metalaxyl metalaxyl-M metaldehyde metam metamitron metarhizium anisopliae metazachlor

metconazole methabenzthiazuron methamidophos methazole methfuroxam methidathion methiocarb methiocarb methoxy sulfone (M10) methiocarb sulfone phenol (M05) methiocarb sulfoxide (M01) methiocarb sulfoxide phenol (M04) methomyl methomyl oxime methoprene methoxychlor methoxyfenozide methyl bromide methyl isothiocyanate methyl-3hydroxylphenylcarbamate (MHPC) methyl-7-chloro-2,5-dihydro-2-[[[trifluoromethoxy)phenyl]a mino]carbonyl]indeno[1,3,4]oxadi azine-4a(3H)carboxylate methylcyclohexylamine methylcyclohexylurea methylisothiocyanate methylsulfonyl-2-nitrobenzoic acid (MNBA) metiram metobromuron metolachlor metosulam metoxuron metrafenone metribuzin metsulfuron-methyl mevinphos

FOOTPRINT deliverable DL24

milbemectin milbemycin A3 milbemycin A4 molinate molinate sulfoxide monalide monolinuron monuron MPA MPP muscalure myclobutanil N-(1,1-dimethylacetonyl)-3,5dichlorobenzamide N-(2,6-difluorophenyl)-5aminosulfonyl-1H-1,2,4triazole-3-carboxylic acid (DFP-ASTCA) N-(2,6-dimethylphenyl)-N-(methoxyacetyl)alanine N-(3,5-dichlorophenyl)3isopropyl-2,4dioxoimidazoline-1carboxamide N-(3-hydroxyphenol)-N-Ndimethylformamidine N-(4trifluoromethylnicotinoyl)gly cine N-(4,6-dimethoxy-2pyrimidinyl)-N-[3-(ethylsulfonyl)-2pyridinyl)urea N-[3-(ethylsulfonyl)-2-pyridinyl]-4,6-dimethyoxy-2pyrimidinamine nabam naled napropamide naptalam N-demethyl phenol N-demethyl triazine amine neburon nicosulfuron nicotine

N-methyl triazine amine N-methyl-N-formyl pirimicarb norflurazon novaluron N-phenylcarbamic acid nuarimol octhilinone O-demethyl triasulfuron O-desmethyl triasulfuron O-desmethylthifensulfuron methyl ofurace olein omethoate orbencarb oryzalin oxadiargyl oxadiazon oxadixyl oxadixyl acid oxalamide (M23) oxamyl oxamyl oxyme oxanilic acid oxasulfuron oxycarboxin oxychlordane oxydemeton-methyl oxyfluorfen oxytetracycline paclobutrazol paraguat parathion parathion-methyl p-chlorobenzylamine pebulate penconazole pencycuron pendimethalin penoxsulam pentachloroaniline pentachlorobenzene pentachlorophenol pentanochlor permethrin

pethoxamid phenmedipham phenothrin phenthoate phenyl sulfonamide phenylurea phorate phosalone phosmet phosphamidon phosphine phoxim phthalamic acid phthalic acid phthalimide picloram picolinafen picoxystrobin pinoxaden piperonyl butoxide pirimicarb pirimicarb phenol pirimiphos-ethyl pirimiphos-methyl p-methyl-phenethylamine (PMPA) polyoxin pretilachlor primisulfuron prochloraz procymidone profenofos profoxydim prohexadione-calcium promecarb prometon prometryn propachlor propamocarb hydrochloride propanil propaquizafop propargite propazine propetamphos propham

propiconazole propineb propoxur propoxycarbazone-sodium propylene urea (PU) propyzamide proquinazid prosulfocarb prosulfuron prothioconazole prothiofos prothiofos-oxon prothoate pymetrozine pyraclofos pyraclostrobin pyraflufen-ethyl pyrazophos pyrazoxyfen pyrethrins pyridaben pyridafenthion pyridate pyrifenox pyrimethanil pyrimidine amine pyriproxyfen pyrithiobac-sodium pyroquilone quinalphos quinclorac quinmerac quinoclamine quinoxyfen quintozene quizalofop-ethyl quizalofop-P-ethyl quizalofop-P-tefuryl resmethrin rimsulfuron rotenone saccharin scilliroside sethoxydim sethoxydim-sulfoxide

siduron silthiofam simazine sintofen S-metolachlor sodium carbonate sodium chloride spinosad spirodiclofen spiromesifen spiroxamine sulcotrione sulfentrazone sulfide sulfluramid sulfonamide methyl ester sulfonate (M27) sulfone sulfonmethylbenzamid sulfosulfuron sulfotep sulphanilamide sulphonamide sulphur sulphuric acid sulprofos sulprofos sulfone sulprofos sulfoxide tau-fluvalinate TCA-Sodium tebuconazole tebufenozide tebufenpyrad tebutam tebuthiuron tecnazene teflubenzuron tefluthrin temephos tepraloxydim terbacil terbufos terbumeton terbuthylazine terbutryn

tetrachlorvinphos tetraconazole tetradifon tetrahydrophthalamic acid tetrahydrophthalimide tetramethrin thiabendazole thiacloprid thiamethoxam thiazafluron thiazopyr thidiazuron thifensulfuron acid thifensulfuron-methyl thiobencarb thiodicarb thiofanox thiofanox sulfone thiofanox sulfoxide thiometon thiometon sulfone thiometon sulfoxide thiophanate-methyl thiophene sulfonamide thiourea thiram tiocarbazil TKC-94 sulfonic acid tolclofos-methyl tolylfluanid topramezone tralkoxydim tralomethrin trans-5-(4-chlorophenyl)-4methyl-2-oxothiazolidine trans-5-(4-chlorophenyl)-4methyl-2-oxothiazolidine-3carboximide trans-5-(4-chlorophenyl)dihydro-3-phenyl-3-(1H-1,2,4-triazole-1-ylmethyl)-2-3H-furanone triadimefon triadimenol tri-allate

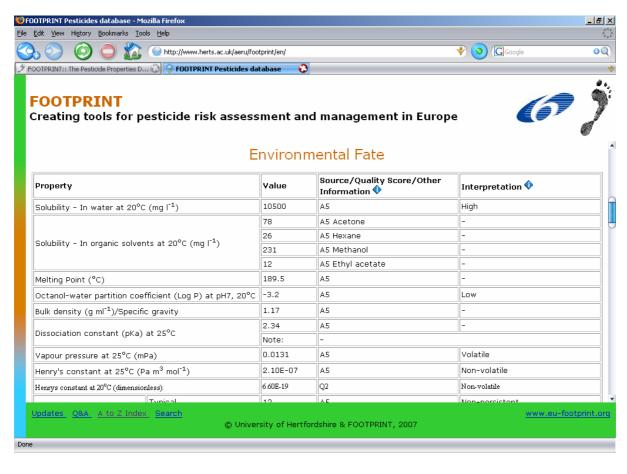
triasulfuron triazamate triazine amine triazolyacetic acid (TAA) triazophos triazoxide tribenuron-methyl tribufos trichloracetaldehyde trichloracetic acid trichlorfon trichloroacetic acid trichloronate trichloropyridinol triclopyr tricyclazole tridemorph tridiphane trietazine trifloxystrobin triflumizole triflumuron trifluoroethanoic acid trifluoromethyl benzoic acid trifluralin triflusulfuron-methyl triforine trimedlure trimethacarb trinexapac-acid trinexapac-ethyl triticonazole tritosulfuron uniconazole urea validamycin vamidothion vernolate vinclozolin warfarin zeta-cypermethrin zineb ziram zoxamide M14360-acid

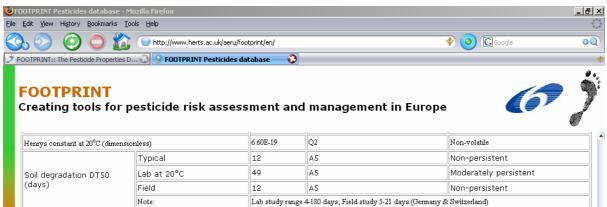
NOA 447204 NOA 407854 CL 354825 AE F161778 149-F11 M14360-alcohol BAS 500-7 RH-24549 149-F FA-1-1 BAS 500-6 IN-R9419 RPA 412708 RH-127450 RPA 413255 RH-163353 RPA 407922 RPA 412636 IN-MM671 RP 025496 CGA118245 IN-JV460 IN-KY374 IN-KV996 AE F126663 RH-5781 RP-017272 AE F136086

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Appendix 2 - Screenshots of the FOOTPRINT PPDB for glyphosate

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				_
OTPRINT:: The Pesticide Properties D 🕥 😏 FOOTPRINT Pe	esticides database 🛛 🔾	5		
OOTPRINT Treating tools for pesticide risk	assessment ar	nd management in Euro	оре 6	
General status:				
Pesticide Type	Herbicide			
Chemical Group	Glycine de	rivative		
CASS RN	1071-83-6	1		
EC Number	213-997-4			
Chemical Formula	C ₃ H ₈ NO ₅ P			
Structure diagram available?	Yes			
Molecular Mass (g mol ⁻¹)	169.1			
Generic Name	N-(phosph	onomethyl)glycine		
EC Directive 91/414 Status	Annex 1			
UK LERAP Status	LERAP Cat	egory B		
Physical State	Colourless	crystals		
	Environ	mental Fate		
Property	Value	Source/Quality Score/Other	Interpretation 🔶	
Solubility - In water at 20°C (mg I ⁻¹)	10500	A5	High	
pdates Q&A A to Z Index Search			www.eu-footp	rin

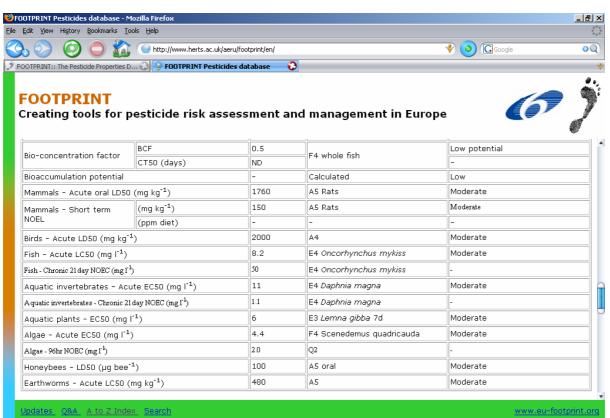




	Note:	Lab study range	Lab study range 4180 days; Field study 5-21 days (Germany & Switzerland)							
Aqueous photolysis DT50 (da	ays)	69	A5	Stable						
Neutral hydrolysis DT50 (day	/s) at 20°C	Stable	A5 Very persistent							
Water-Sediment DT50 (days	;)	37	A5 Moderately fast							
Water phase only DT50 (day	rs)	2.5	A5 Moderately fast							
GUS leaching potential index		-0.36	Calculated Low leachability							
SCI-Grow Groundwater	Value:	5.35E-03	Calculated -							
model (µg ⁻¹) for a 1 kg ha ⁻¹ or 1 ha ⁻¹ application rate	Note:	Estimated concentrations of chemicals with Koc values greater than 9995 ml g ⁻¹ are beyond the scope of the regression data used in SCI-GROW development. If there are concerns for such chemicals, a higher tier groundwater exposure assessment should be considered, regardless of the concentration returned by SCI-GROW.								
Potential for particle bound t	transport	-	Calculated	Medium						
	<i></i> 1s	21699	A5	Non-mobile						
Koc - Organic-carbon sorptic	on constant (mi g -)	Note:	-							
	Kf	46.20		-						

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		Kf	46.20		-	
	Freundlich coefficient	1/n	0.87		-	
		Note:		soils. Argaltoll OC~2%, pH=6.5, pH=6.1. Clay 17.1%, Silt 75.69	Clay 29%, Silt 61% Kf=50.3; T 6 Kf=42.1.	ypustalf
1	1etabolites					
Ē					Estimated Maximum Forma	tion
	Metabolite		Formation) Medium	Fraction	cion
	aminomethylphosphonic aci	d (AMPA)	Soil		0.290	-
			_			
			Ecoto	oxicology		0
Г				Source/Quality Score/Ot	hau	
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i i		BCF	0.5		Low potential	
	Bio-concentration factor CT50 (days)		ND	F4 whole fish	-	
Ī	Bioaccumulation potential		-	Calculated	Low	
Ī	Mammals - Acute oral LD50	(mg kg ⁻¹)	1760	A5 Rats	Moderate	
	Mammale - Chort torm	(ma ka ⁻¹)	150	A5 Rats	Moderate	
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