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Modelling-based strategy for the Prioritisation Exercise under the Water Framework Directive

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Abstract

The Water Framework Directive 2000/60/EC (WFD) aims to protect the aquatic environment at European level by achieving the good chemical and ecological status of all water bodies. In order to reach the good chemical status of their waterbodies, Member states should monitor the Priority Substances listed in Annex 10 of the WFD and they should ensure that the concentrations of these substances or groups of substances in the aquatic environment do not exceed the related Environmental Quality Standards, set to protect human health and the environment (Directive 2008/105/EC amended by Directive 2013/39/EU). Priority substances that are persistent, toxic and liable to bioaccumulate or which give rise to a similar level of concern are identified as Priority Hazardous Substances. Under Article 16 (4) of the WFD, later amended by Directive 2013/39/EU, the Commission is required to review the list of substances designated as Priority Substances and Priority Hazardous Substances every six years. The ongoing prioritisation process is coordinated by JRC in collaboration with DG ENV and the expert sub-group of the Working group chemicals. The process includes two approaches, the monitoring and modelling based exercises. The first has been developed considering the available monitoring data and criteria for selection of substances undergoing this exercise. The latter has been conceived for those substances for which either monitoring data are insufficient or completely missing. This report is focused on the modelling-based exercise to explain the screening phase process and the models used to derive the Predicted Environmental Concentration (PEC) required to determine the risk assessment based on the ratio between the PEC and Predicted No Effect Concentration (PNEC).

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1 Abbreviations

ADI	Acceptable Daily Intake
API	Active Pharmaceutical Ingredient
BCF	Bioaccumulation Factor
BMF	Biomagnification Factor
CIS	Common Implementation Strategy
CLP	Classification, Labelling and Packaging
CMR	Carcinogenic, Mutagenic, toxic for Reproduction
CoRAP	Community Rolling Action Plan
CRED	Criteria for Reporting and Evaluating Ecotoxicity Data
DB	Database
DG ENV	Directorate-General for Environment
DNEL	Derived No Effect Level
DSD	Dangerous Substance Regulation
dw	Drinking Water
ECETOC	European Centre for Ecotoxicology and Toxicology of Chemical
ECHA	European Chemical Agency
ECOSTAT	Expert group for Ecological Status of water quality
EC10	Effect Concentration for 10% of the individuals in a toxicity test
EC50	Effect Concentration for 50% of the individuals in a toxicity test
ED	Endocrine Disruptor
EFSA	European Food Safety Authority
EMA	European Medicines Agency
EMEA	Former EMA acronym
EPA	Environmental Protection Agency
ERC	Environmental Release Category
ESVAC	European Surveillance of Veterinary Antimicrobial Consumption
EQS	Environmental Quality Standard
EPA	Environmental Protection Agency
ESIS	European chemical Substances Information System
ETUC	European Trade Union Confederation
EqP	Equilibrium partitioning
FDA	Food and Drug Administration
FOCUS	FOrum for the Co-ordination of pesticide fate models and their USe
fw `	Freshwater
GDP	Gross Domestic Product
hh	Human Health
HPV	High Production Volume
Koc	Soil Organic Carbon-Water Partitioning Coefficient

70	IARC	International Agency for Research on Cancer
71	INERIS	Institut National de l'Environnement Industriel et des Risques
72	IUCLID	International Uniform Chemical Information Database
73	JDS2	Second Joint Danube Survey
74	LC50	Lethal Concentration for 50% of the individuals in a toxicity test
75	LD50	Lethal Dose for 50% of the individuals in a toxicity test
76	LOD	Limit Of Detection
77	LOQ	Limit Of Quantification
78	MACRO	Model of water flow and solute transport in field soils
79	MEC	Measured Environmental Concentration
80	MS	Member State
81	NOAEL	No-Observed Adverse Effect Level
82	NOEC	No-Observed Effect Concentration
83	OECD	Organisation for Economic Co-operation and Development
84	OSPAR	Convention for the Protection of the marine Environment of the North-East Atlantic
85	PBT	Persistent, Bioaccumulative and Toxic
86	PEC	Predicted Environmental Concentration
87	PNEC	Predicted No Effect Concentration
88	PHS	Priority Hazardous Substance
89	PPP	Plant Protection Product
90	PRZM	Pesticide Root Zone Model
91	PS	Priority Substance
92	QC	Quality Criteria
93	RBSP	River Basin Specific Pollutants
94	SPIN	Substances in Preparations in Nordic Countries
95	REACH	Registration, Authorisation and Restriction of Chemicals
96	RIWA	Association of River Water Supply Companies
97	RIVM	National Institute for Public Health and the Environment (NL)
98	RA	Risk Assessment
99	RQ	Risk Quotient (PEC/PNEC)
100	sec pois	Secondary poisoning
101	sed	Sediment
102	SG-R	Sub-group of experts
103	SIDS	Screening Information DataSet
104	SMILES	Simplified Molecular Input Line Entry System
105	spERC	specific Environmental Release Category
106	STE	Spatial, Temporal and Extent
107	STOT RE	Specific Target Organ Toxicity Repeated Exposure
108	SVHC	Substances of Very High Concern
109	SWASH	Surface WAter Scenarios Help

110	T	Toxic
111	TDI	Tolerable Daily Intake
112	TCNES	Technical Committee for New and Existing Substances
113	TG n. 27	Reference no. 18
114	TOXSWA	TOXic substances in Surface WAters
115	TRA	Targeted Risk Assessment
116	UBA	Umwelt Bundesamt (Federal Environment Agency of Germany)
117	vB	Very Bioaccumulative
118	vP	Very Persistent
119	WFD	Water Framework Directive

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2 Background

The Water Framework Directive 2000/60/EC (WFD) has established a strategy for water protection that includes specific measures for pollution control to achieve good ecological and chemical status at European level. Good chemical status has been defined in terms of compliance with European environmental quality standards (EQS) for priority substances (PS).

The PS are substances identified as posing a significant risk to or *via* the aquatic environment at EU level, according to article 16(2) of the WFD. The EQS are the environmental threshold concentrations in water, sediment or biota that should not be exceeded in order to protect human health and the environment. The PS are listed in Annex X of the WFD, which also identifies priority hazardous substances (PHS) i.e. the PS that are persistent, toxic and liable to bioaccumulate, or that give rise to an equivalent level of concern. Member States should take measures to progressively reduce the pollution from PS and to cease or phase-out of discharges, emissions and losses of PHS (Directive 2000/60/EC).

The first list of PS in the field of water policy was published in the Commission Decision 2455/2001/EC, and subsequently included in European Directive 2008/105/EC on environmental quality standards (EQS Directive). It included 33 PS and groups of PS. EQS values for annual average (AA) or maximum allowable concentrations (MAC) have been derived to protect against long-term exposure or short-term peak concentrations, respectively and are listed in Annex I of Directive 2008/105/EC.

Under Article 16 (4) of the WFD, later amended by Directive 2013/39/EU, the Commission is required to review the list of substances designated as PS and PHS every six years. Each review comprises a re-assessment of existing PS and PHS and related EQSs, and also the selection of candidate substances for consideration as new PS and derivation of their related EQSs.

3 Introduction

The scientific and technical methodology for the current review has been developed by the JRC in consultation with the Directorate-General for Environment (DG ENV) of the European Commission and the sub-group of experts for the review (or SG-R), sub-group of the Working Group Chemicals.

The identification of new priority substances is based on two parallel and interactive processes: the monitoring based exercise and the modelling based exercise [3].

In order to perform the current review, the JRC first compiled an initial list of substances which could potentially be harmful to the environment, using all available databases (DB) provided by institutions, stakeholders and peer-reviewed papers.

Substances with enough monitoring data (from at least 4 Member States (MS), more than 50 samples, more than 10 sites) were included:

1) in the monitoring exercise as the main basis for their ranking, and
2) in the screening phase of the modelling exercise to check whether the results from the modelling and the monitoring based approaches were consistent.

For substances with no monitoring data or insufficient monitoring data, the SG-R judged that the Spatial, Temporal and Extent (STE) score alone would not be reliable enough since it would be based on too few data. These substances were included in the modelling-based approach as the main basis for their ranking.

For the substances highly ranked through the modelling based exercise, when MSs had reported some data for these substances, the STE score was calculated and is provided in this report, only as an indicative value, in complement to the modelled Risk Quotient (RQ, see below for further explanation).

The modelling-based exercise described in this report relied on two successive steps: the screening phase and the risk assessment phase. The screening phase ranks the substances using both exposure and hazard scores. The exposure score is based on the use type and the tonnage of a substance, while the hazard score is based on both the environmental and human toxicity.

The screening score was then used, along with other criteria described in section 6.4 and 6.5, to select the substances that would go through the risk assessment phase, where both Predicted Environmental Concentration (PEC) and Predicted No Effect Concentration (PNEC, that is an estimate of the exposure at which ecosystems are likely not to suffer any harm) were derived, and the corresponding Risk Quotient (RQ, PEC/PNEC) was calculated. The RQ is an estimate of the risk in the environment [4].

This report focuses on the modelling-based exercise to explain the screening phase process and the models that are used to derive the PEC required for the RQ calculation.

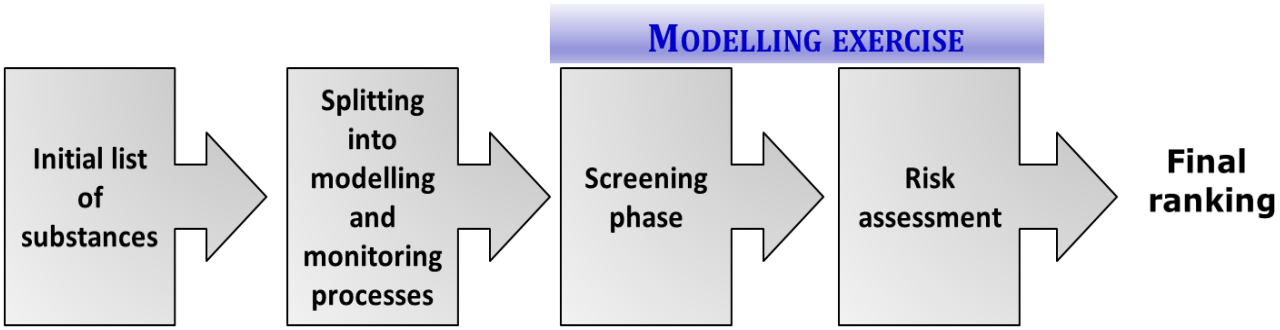

Figure 1. Outline of the modelling based exercise. The present report is focused on the modelling based exercise, which comprises a screening phase and a risk assessment phase.

3.1 Participants in the review

The technical process for the review was developed by the Joint Research Centre (JRC) in consultation with the DG Environment (DG ENV) of the European Commission and the sub-group of experts for the review of PS (SG-R). The SG-R is a sub-group of the Working Group Chemicals (formerly called Working Group E) and gathers experts nominated by Member States and relevant stakeholders (environmental NGOs and Industry associations).

At the kick-off meeting of the SG-R, the JRC firstly presented a draft methodology for the review of the PS list. Following the comments received from the experts at this meeting and in the following months, the methodology was modified and an updated version was presented at the 2nd SG-R meeting. Then, the updated methodology was additionally discussed, tested, verified and further improved at the next meetings of the SG-R.

Throughout the process, the experts have provided valuable suggestions to improve and validate the screening phase process and the modelling. Furthermore, the experts have been informed of the progress in the implementation of the methodology.

Summary of the meetings of the sub-group of experts for the review of PS (SG-R) and associated milestones in the monitoring-based exercise

Meetings of the SG-R group	Modelling-based exercise milestone
Kickoff meeting 4-5 September 2014 (Ispra, IT)	Presentation of the modelling approach (screening phase and risk assessment).
2nd Meeting 22-23 January 2015 (Ispra, IT)	Selection of substances for modelling approach and identification of the most appropriate modelling tools.
3rd Meeting 17-18 September 2015 (Ispra, IT)	Final list of substances to be screened (around 6000) for the modelling. Presentation of an automated software system for data gathering to help and speed up the screening phase procedure.
4th Meeting 25-26 January 2016 (Brussels, BE)	The screening list of the substances having enough data (around 2800) is almost completed and most of the screening risk scores are calculated. Proposal of additional criteria, to be developed, for a refined selection of the substances.
5th Meeting 9-10 June2016 (Gavirate, IT)	Presentation of additional criteria, based on hazard properties and monitoring data, for selection of the candidate substance for modelling. Review of the preliminar list of selected substances from modelling-based exercise.
6th Meeting 11-13 October 2016 (Ispra, IT)	Presentation of the proposal substances selected from modelling exercise upon SG-R comments. Agreement by the SG-R group on the selection of Deltametrin, Bifenthrin and Esfenvalerate for EQS derivation.

4 Initial list

In accordance with Art. 16 of the WFD [1], substances shall be prioritised for action on the basis of risk to or *via* the aquatic environment. For this purpose, an initial list of 11549 substances, which could potentially pose a risk to the environment, was compiled from several databases, reports and peer-reviewed papers. Inputs from stakeholders and international organizations were collated as well. Specific lists were assembled for biocides, endocrine disruptors (ED), marine pollutants, illicit drugs, pesticides, human and veterinary medicines, some cosmetic ingredients and mixtures where the composition is defined. Table 1 details the sources used and the respective number of substances.

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Source	Description	Number of substances
ECHA-SVHC [5]	List of SVHC	149
ECHA-CoRAP [6]	List of the substances included in the CoRAP 2013-2015, amended with the CoRAP list 2015-2017	260
ECHA-Biocides [7]	List of approved Biocidal active substances, updated 07/05/2015	82
EU Pesticides database [8]	List of substances approved, pending and not plant protection products	441
European Environment Agency [9]	State of the Environment reporting	630
ECOSTAT-RBSP [10]	Substances identified by MSs as River Basin Specific pollutants	377
ESIS-CLP [11]	Substances CLP classified as H400, H410, H411, H412, H413	2196
Norman List [12]	this list, identified by NORMAN, comprises the currently discussed emerging substances and emerging pollutants (latest update March 2011), such as surfactants, flame retardants, pharmaceuticals, personal care products, nanoparticles, gasoline additives and their degradation products, biocides, polar pesticides and their degradation products, and various confirmed or suspected ED compounds	913
INERIS Report from the previous review [13]	Substances of the previous Monitoring-based ranking exercise were collated as well	1014
OSPAR List of Substances of Possible Concern [14]	collection of hazardous substances which are of possible concern to the marine environment, developed by OSPAR	246
OSPAR List of Chemicals for Priority Action [15]	list of substances potentially persistent, liable to bioaccumulate and toxic	31
OECD High Production Chemicals DB [16]	list of all the HPV chemicals which have been or are being investigated in the SIDS programme	1469
Endocrine disruptor's database (EU Commission) [17]	list of substances that showed (potential) evidence for ED effects. Only chemicals that belong to Category 1 and 2 were considered	277
Substitute It Now! (SIN) List [18]	the chemicals on the SIN List have been identified by ChemSec as SVHC based on the criteria established by the EU chemicals regulation REACH	772
Second Joint Danube Survey (JDS2) [19]	list of compounds identified in the surface water of the Danube River and its tributaries during the second monitoring survey along the Danube river	271
Scoping Prioritisation Report (2014) [20]	it describes a procedure proposal for the identification and prioritisation of PS built upon the outcome of the previous review of PS. Substances from table 4.2 of the report were included. These substances ranked high in either the monitoring- or the modelling-based exercises of the last review of PS, but were not short-listed for prioritization	81
TCNES' PBT List [21]	list of substances whose PBT profile has been investigated by the TCNES group	117
First and Second Priority List of Environment Canada [22]	list of substances that should be assessed on a priority basis to determine whether they pose a significant risk to the health of Canadians or to the environment	48
European Trade Union Confederation (ETUC) List [23]	list of the most urgent SVHC for inclusion in the Candidate List and, eventually, in the Annex XIV (the Authorisation List)	711

US EPA Priority Chemicals list [24]	list of PS identified by the EPA. The American National Waste Minimization Program focuses efforts on reducing these Priority Chemicals found in their nation's products and wastes by finding ways to eliminate or substantially reduce the use of PS in production	18
Vewin-RIWA [25]	Communication from Dutch and Belgian drinking water operators on substances which breach drinking water standards or the target values for rivers in Europe.	26
Environmentally classified pharmaceuticals 2014, Stockholm County Council [26]	list of pharmaceuticals assessed by the Stockholm County Council	37
EurEau-Pharma 2014 [27]	list of pharmaceuticals of concern to drinking water	24
MistraPharma DB [28]	the MistraPharma DB, also called WikiPharma DB, contains publicly available ecotoxicity data for pharmaceutical substances, focusing on human pharmaceuticals available on the Swedish market	159
Screening program 2013 - New bisphenols, organic peroxides, fluorinated siloxanes, or-ganic UV filters and selected PBT substances [29]	the occurrence and environmental risk of a number of new bisphenols, organic peroxides, fluorinated siloxanes, organic UV filters and selected PBT substances were reported for wastewater effluents and leacha-tes, as well as sediments and biota from Oslofjord and Lake Mjøsa	38
Wikipedia Sunscreen ingredients' List [30]	list of FDA's approved active ingredients in sunscreens	28
JRC-IES marine pollutants [31]	Marine pollutants from literature collection	131
Von der Ohe et al. 2011 [32]	risk assessment of 500 organic substances based on observations in the four European river basins of the Elbe, Scheldt, Danube and Llobregat.	499
Lopez-Roldan et al. 2013 [33]	development of several indicators based on toxicity (PNEC) and on legislation levels (EQS) for river aquatic ecosystems assessment for screening potential chemical stressors.	6
Pal et al. 2013 [34]	review of the occurrence and concentration levels of illicit drugs and their metabolites in different environmental compartments (e.g. wastewater, surface waters, groundwater, drinking water, and ambient air) and their potential impact on the ecosystem.	13
Kools et al. 2008 [35]	environmental risk-based ranking of veterinary medicinal products. Only substances with risk indices higher than 5 for the compartment water and aquatic organisms have been included in the initial list	77
Grung et al. 2008 [36]	environmental risk assessment of eleven pharmaceuticals was performed following the guidelines from the EMEA.	6
Bottoni et al. 2010 [37]	review article of the relevance of pharmaceuticals, for human and veterinary use as well as of their biologically active transformation products, as environmental micropollutants.	184
Roos et al. 2012 [38]	comparison of similarities and differences in overall ranking results of 582 APIs from nine previously proposed prioritisation schemes, both risk and hazard-based.	47
Iatrou et al. 2014 [39]	estimation of the potential environmental risks associated with human consumption of antimicrobials were estimated in Greece.	8
Kostich & Lazorchak 2007 [40]	estimation of risks associated with exposure to human prescription pharmaceutical residues in wastewater from marketing and pharmacological data	4
Boxall et al. 2003 [41]	a two-stage prioritisation scheme was developed and applied to veterinary medicines in use in the UK.	52
Capleton et al. 2006 [42]	it proposes a method for prioritising veterinary medicine APIs according to estimates of their potential for indirect human exposure *via* the environment and their toxicity profile, and demonstrates its feasibility	34

	using an initial set of 83 veterinary medicine APIs approved for use in the UK.	
Zuccato et al. 2000 [43]	list of drugs thought to be putative priority pollutants according to selected criteria. Most drugs were measurable in drinking or river waters and sediments in Lombardy (Italy), suggesting that pharmaceutical products are widespread contaminants, with possible implications for human health and the environment.	16
Sarmah et al. 2006 [44]	review of the latest information available in the literature on the use, sales, exposure pathways, environmental occurrence, fate and effects of veterinary antibiotics (especially, tylosin, tetracycline, sulfonamides and, to a lesser extent, bacitracin) in animal agriculture.	14
Dong et al. 2013 [45]	paper on a prioritization approach on 200 most-prescribed drugs in the US (2009). The approach is based on the number of prescriptions and toxicity information, accounting for metabolism and wastewater treatment removal.	43

Table 1. List of data sources for compiling the initial list of substances to be reviewed in the current prioritisation exercise

Starting from the initial list of 11549 substances, and deleting duplicates and substances that are known to not pose any harm, it was possible to collect some information on hazard and/or exposure for 6523 substances. For 326 of these substances, enough monitoring data was available to apply the monitoring-based approach and to use the STE score as the main basis for their ranking. For the remaining 6197 substances, no monitoring data, or only insufficient monitoring data was available: these substances went through the modelling-based exercise.

A summary of all the sources and the related number of substances is illustrated in Figure 2.

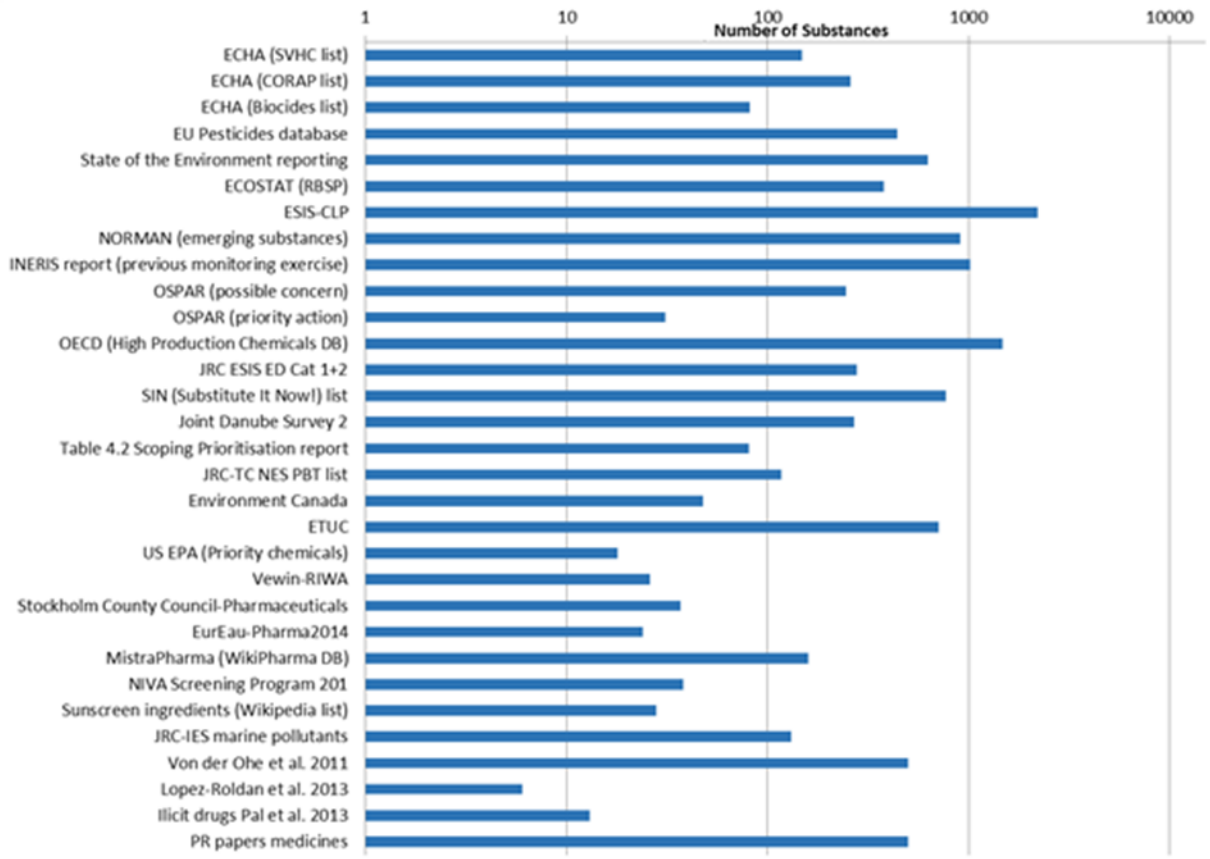


Figure 2. Summary of the sources of data used to compile the initial list of substances, with the number of substances displayed on a logarithmic scale.

5 The Modelling-based exercise

5.1 Data collection for both the screening and the risk assessment phase

The exposure and toxicological data required both for the screening phase and the risk assessment phase were retrieved from several data sources. Several web-sites and databases were consulted - European Chemical Agency (ECHA) portal, European Food Safety Authority (EFSA), National Institute for Public Health and the Environment (RIVM), EMA, International Agency for Research on Cancer (IARC), European Pesticides database, Footprint Pesticides Properties database, Environmental Protection Agency (EPA), International Uniform Chemical Information Database (IUCLID), Endocrine Disruptors Database. Generally, both the relevance and reliability of the publications retrieved from the above sources, i.e. EFSA Conclusions, Registration, Authorisation and Restriction of Chemicals (REACH) Dossiers, European Review Reports, IARC Monographs, European Risk Assessment Reports, EPA Reports, were deemed acceptable, although in some case they were not reviewed by the competent authority such as for REACH dossier[1]. The Classification, Labelling and Packaging (CLP) classification of substances, officially made by ECHA, was used for the definition of a substance as carcinogenic, mutagenic, and toxic to reproduction (Carcinogenic, Mutagenic, toxic for Reproduction; CMR scoring).

Data collected for the exposure assessment and PEC calculation comprised physical and chemical properties (molecular weight, water solubility, vapour pressure, biodegradability, sorption potential and bioaccumulation potential), tonnage (of use, manufacture and import) and Environmental Release Category (ERC) and/or specific Environmental Release Categories (spERC) codes. These codes provide indication of the usages of a substance allowing to know the percentages of dispersion in the environmental compartments for the modelling tools.

The collection of hazard data for the aquatic compartment included acute and chronic toxicity data, typically the most sensitive Lethal Concentration/ Effect Concentration for 50% of the individuals in an acute toxicity test (LC50/EC50), or No-Observed Effect Concentration / Effect Concentration for 10% of the individuals in a chronic toxicity test (NOEC/EC10) endpoints. Regarding mammalian or human toxicity effects from oral exposure, data were collected for repeated dose toxicity, carcinogenicity, mutagenicity and reproduction toxicity tests, focusing on typical endpoints such as No-Observed Adverse Effect Level (NOAEL), Derived No Effect Level (DNEL), Acceptable Daily Intake (ADI) and Tolerable Daily Intake (TDI) values. In all those cases, when new literature was considered in addition to the sources listed above, reliability assessment

[1] Even though REACH dossiers may not be reviewed by national competent authorities, the screening of thousands of substances is not compatible with a thorough investigation of each individual hazard property for each substance. More in-depths analysis was performed later for the highest ranked substances.

of the ecotoxicological data was done based on the Criteria for Reporting and Evaluating ecotoxicity Data (CRED) check list [46].

5.2 The screening phase

As explained in paragraph 4, 6197 substances were listed for the modelling exercise. These substances needed to be ranked to select the ones of most concern. To reach this goal, every substance was categorised according to its dangerousness (hazard score) and the quantity that is expected to be found in the environment (exposure score). These scores were used as the indexes of a matrix that combine the hazard with the exposure scores. Such matrix gave the final risk score for each substance that allowed to rank the substances (details will be provided in the following paragraphs of this report).

The exposure and hazard information searched for all the substances are shown in Table 2.

Exposure	Amount produced (tonnage)
	Use pattern
Hazard	Persistency
	Bioaccumulation
	Toxicity
	Carcinogenicity
	Mutagenicity
	Reproduction toxicity
	Endocrine disruption potential

Table 2. Exposure and hazard properties collected for the screening phase. Exposure was defined by the tonnage of the substance and its use pattern (that is the degree of dispersion). Hazard was defined by the ecotoxicity of a substance (persistency, bioaccumulation and toxicity) and its toxicity (carcinogenicity, mutagenicity, reproduction toxicity and endocrine disruption potential).

5.2.1 Exposure score

To determine the exposure score, both the use pattern and the total tonnage of a substance are needed (the approach is the same as one used in the previous prioritisation exercise) [47].

The use pattern corresponds to the degree of dispersion of a substance in the environment. This use pattern is associated to a numerical value as indicated in Table 3.

Use pattern	Use index
Used in the environment	1
Wide dispersive use (diffuse sources and substances in wastewater)	0.75
Non-dispersive use (industrial, controlled point sources)	0.5
Not known	0.25
Controlled system (isolated intermediate)	0.1

Table 3. Use pattern and use index association. The use pattern corresponds to the degree of dispersion of a substance that is here associated to a numerical value (use index).

Where available, the use pattern of the substances was taken from the worst case Environmental Release Category (ERC) code associated with the substance, otherwise the use pattern was assessed from any additional available sources (e.g. from literature), while in other case was straightforward (e.g. Plant Protection Products, PPPs, are always expected to be used in the environment).

To calculate the expected tonnage of a substance released to the environment, the total tonnage of the substance was multiplied by its use index. We called this "the use assessment" (in tons). This use assessment was then split (distributed) in five value ranges, as shown on Table 4. Each exposure score was associated to the corresponding range of use assessment.

Use assessment (tons)	Exposure score
0–0.1	0
0.1–10	1
10–100	2
100–1'000	3
>1'000	4

Table 4. Use assessment (the tonnage of the substance expected to be released to the environment) and corresponding exposure score.

Tonnage values for Europe were collected from several sources. Under a confidentiality agreement with the European Chemicals Agency, the JRC retrieved the information from the submitted dossiers under the REACH regulation. Additionally, the Substances in Products Preparations in the Nordic Countries (SPIN) database (countries are: Norway, Sweden, Denmark and Finland) were examined. To extrapolate a European tonnage value, the population statistics were used.

Data on pharmaceuticals consumption were available from six MSs: France [48], Greece [39], Germany [49], Portugal, Denmark and Latvia (the agency of PT, DK and LV provided directly to JRC a list of pharmaceuticals sales/consumption). These data were then used to extrapolate the total tonnage for Europe, based on population number (for human pharmaceuticals) or animal production (for veterinary pharmaceuticals).

For Plant Protection Products, tonnages were available from the Czech Republic and used for extrapolation to the whole Europe.

In all other cases, if it was not possible to extrapolate the tonnage due to the lack of data, the substance did not get a final exposure score.

5.2.2 Hazard score

A substance was evaluated considering 7 different properties of hazard: its persistence, bioaccumulation and toxicity (clustered as PBT), its carcinogenicity, mutagenicity and reproductive toxicity (clustered as CMR), and its endocrine disruptor potential (called ED). For more details about the latter classification, please refer to section 5.2.2, "Assessment of the ED properties".

All these properties were scored separately (i.e. P, B, T, C, M, R, ED), and the scores were then summed up to obtain the final hazard score, according the formula:

Hazard score = PBT score(0-3) + CMR score(0-3) + ED score (0-1)

The hazard score can range from 0 to 7.

The sources of hazard data are listed in section 5.1. The main sources of information were ECHA (for industrial and inorganic chemicals) and EFSA (for plant protection products).

In general, for each substance, more than one value/evaluation could be found for every property of the hazard assessment. Please refer to section 6.2 for more details about the assessment of hazard properties when multiple assessments were available.

Assessment of the PBT properties

The criteria used to decide whether a substance had to be regarded as PBT or very Persistent very Bioaccumulative (vPvB) were provided in the ECHA guidance for the PBT assessment, Chapter R.11 [50]. For the purposes of hazard assessment in the screening phase, whenever the respective P, or B, or T criteria were fulfilled, a score of 1 was assigned to each component, respectively. If no data was available, a default score of 0.1 was assigned as done by NORMAN [51]. The PBT scoring system is summarized in Table 5.

P score	B score	T score	Meaning
1	1	1	yes
0	0	0	no
0.1	0.1	0.1	no data available

Table 5. P, B and T scoring system adopted. Persistence (P), bioaccumulation (B) and toxicity (T) in the environment are criteria that in this exercise were either fulfilled (yes, score 1) or not (no, score 0). When no data was available, a score of 0.1 was assigned as default. Individual scores for P, B and T were summed to obtain the PBT score (0-3). [51]

Following the aforementioned table, a substance classified as PBT has score of 3. Also substances that were very persistent and very bioaccumulative in the food chain (vPvB) scored 3, in order to account for the higher hazard they likely pose. The PBT and vPvB criteria do not apply to inorganic substances, but shall apply to organo-metals.

If a dossier (e.g. from ECHA) reported a PBT assessment, its conclusions were used directly, otherwise, the PBT and vPvB properties were assessed as shown in the Figures 3-5.

In order to determine the persistence of a substance, the ECHA guidance [50] was followed. The PBT and vPvB properties were assessed according to section 1 of Annex XIII to REACH. If none of these criteria were met because of a lack of data, the instructions from section 3.1 of the same Annex XIII were applied and the conclusion was reported as “indicative” (the score for the P, B, T, anyway, did not change, but “indicative” was reported for clarity).

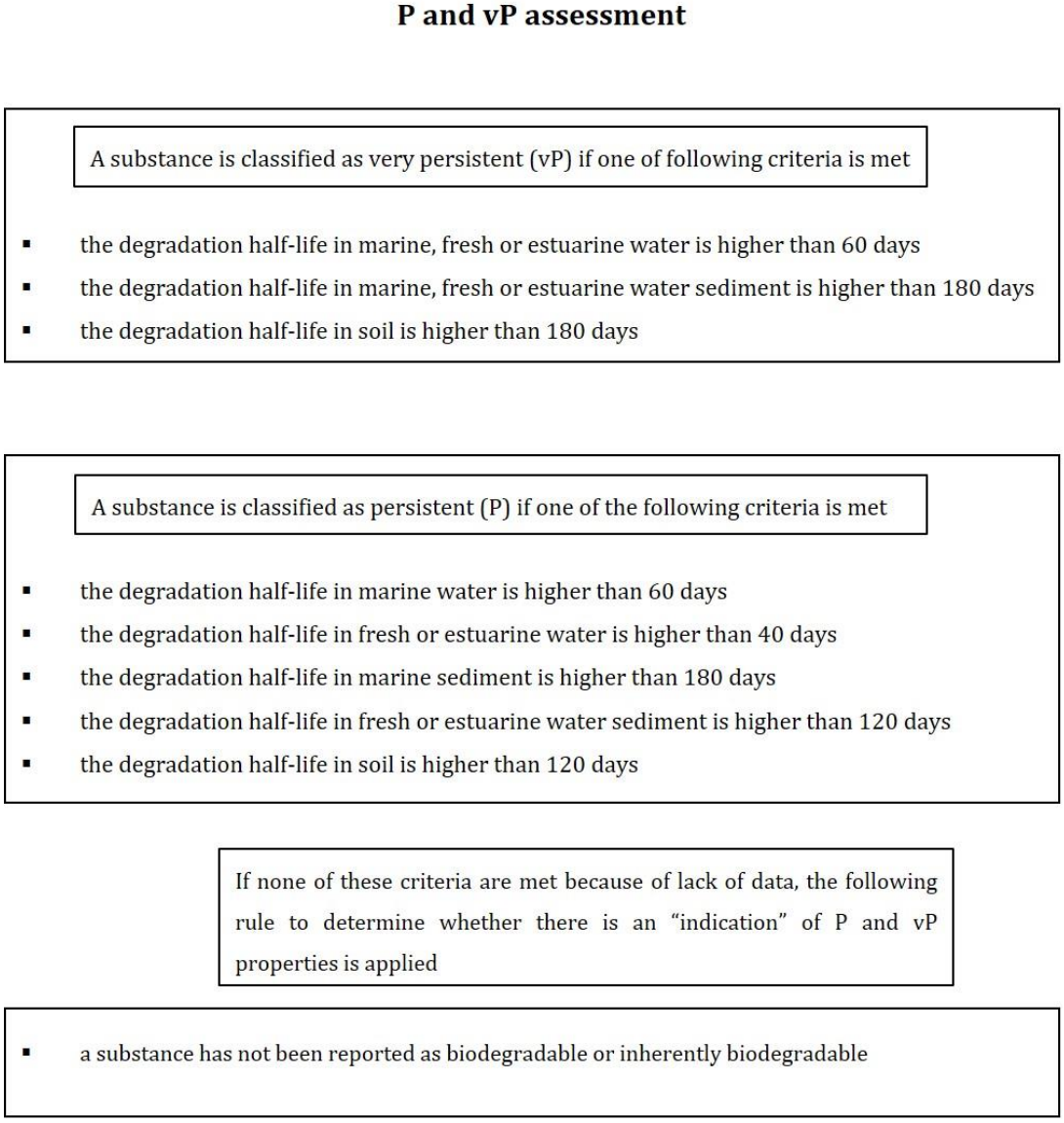


Figure 3. Rules for assessing whether a substance is Persistent (P) or very Persistent (vP). First, the rules for determining if a substance is vP or P are followed. If none of the aforementioned rules can be met, an "indication" for the P property is evaluated.

These rules were extracted from the ECHA guidance for PBT assessment [50].

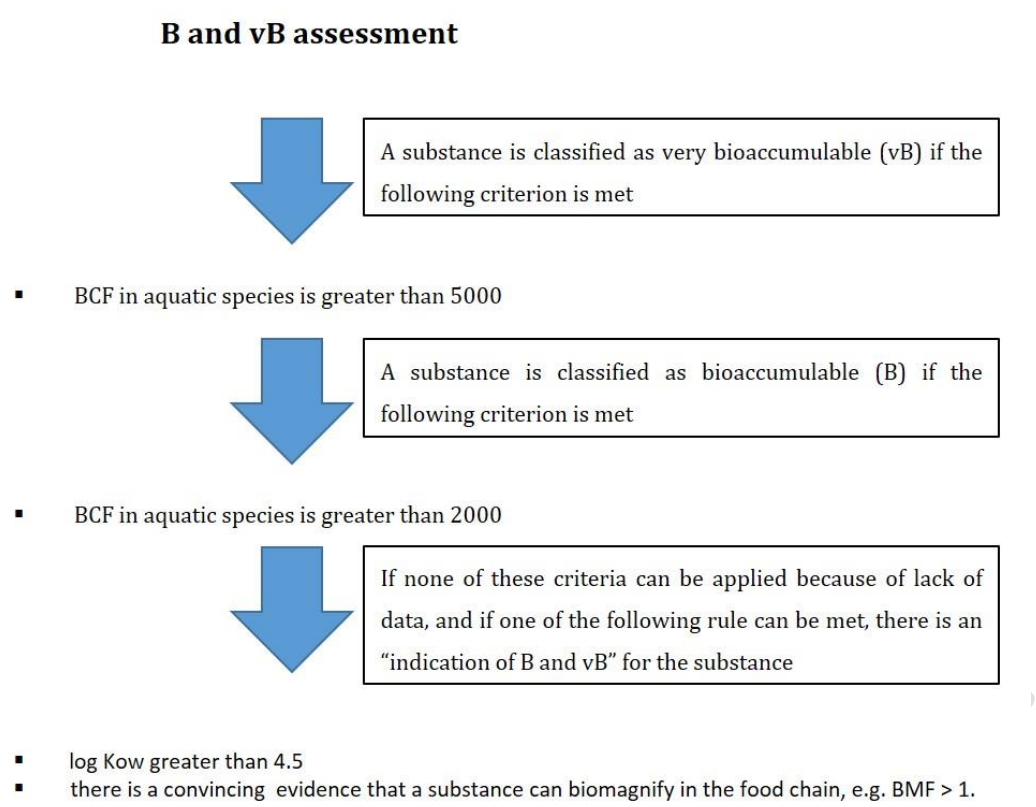


Figure 4. Rules for assessing whether a substance is Bioaccumulative (B) or very bioaccumulative (vB). First, the rules for determining if a substance is vB or B are followed. If none of the aforementioned rules can be met, an "indication" for the B property is evaluated.

These rules were extracted from the ECHA guidance for PBT assessment [50].

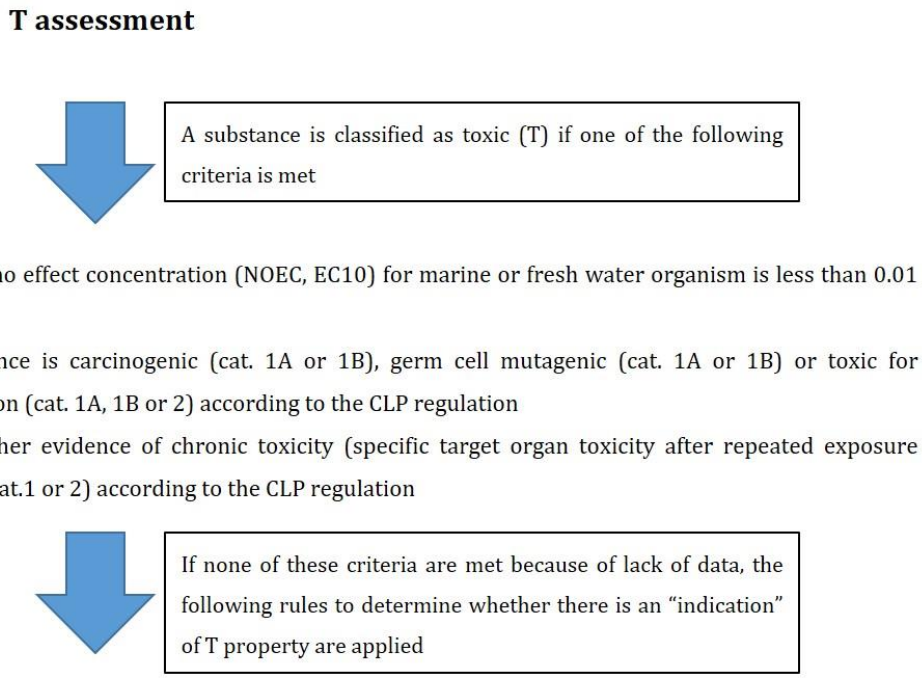


Figure 5. Rules for assessing whether a substance is Toxic (T). First, the rules for determining if a substance is T are checked, then if not fulfilled, an "indication" for the T property is evaluated.

These rules were extracted from the ECHA guidance for PBT assessment [50].

Assessment of the CMR properties

Regarding the scoring system assigned to the CMR (Carcinogenicity, Mutagenicity, and Reproduction Toxicity) properties, the IARC classification for carcinogenicity (http://monographs.iarc.fr/ENG/Classification/), the older Dangerous Substance Directive (DSD) classification system, and the Classification, Labelling and Packaging (CLP) Regulation (http://echa.europa.eu/en/regulations/clp) were followed to classify the substance. The categories among these 3 different classifications were harmonised as shown in Table 6, and the categories 1 to 3 (as in DSD classification) were used in the present assessment. Table 7 summarises the scores for each property.

Directive/Regulation	DSD	CLP	IARC
Category	1	1a	1
	2	1b	2a
	3	2	2b

Table 6. Equivalence among classification systems of the different Regulations/directives, i.e. DSD, CLP, IARC. Cat. 1 – known human carcinogen/mutagen/reproductive toxicant; Cat. 2 – presumed human carcinogen/mutagen/reproductive toxicant; Cat. 3 – suspected human carcinogen/mutagen/reproductive toxicant.

C score	C MEANING	M score	M MEANING	R score	R MEANING
1	1:CAT. 1	1	1:CAT. 1	1	1:CAT. 1
0.75	0.75: CAT.2	0.75	0.75: CAT.2	0.75	0.75: CAT.2
0.5	0.5:CAT. 3	0.5	0.5:CAT. 3	0.5	0.5:CAT. 3
0.25	0.25: UNDER EXAMINATION/EXAMINED AND INSUFF INFO/NOT EXAMINED	0.25	0.25: UNDER EXAMINATION/EXAMINED AND INSUFF INFO/NOT EXAMINED	0.25	0.25: UNDER EXAMINATION/EXAMINED AND INSUFF INFO/NOT EXAMINED
0	0: EXAMINED AND NOT CLASSIFIED	0	0: EXAMINED AND NOT CLASSIFIED	0	0: EXAMINED AND NOT CLASSIFIED

Table 7. Scoring system used for the classification of substances according to the CMR properties (C means carcinogenic, M means mutagenic, and R means toxic for reproduction). For each property, scores: 0.5, 0.75 and 1 were associated to a DSD category (see Table 6 for more details). The remaining scores were 0, when the property was not fulfilled, or 0.25 (default value), when the substance was under study or not sufficient data was available to assess the property. Modified from [51]

Assessment of the ED properties

Finally, endocrine disrupting (ED) properties were investigated as well, although information on these was often missing. The corresponding scoring system is shown in Table 8. It is here recalled that the European Commission had not yet made its proposal on how to define the term "endocrine disruptor" when the scores were applied using Table 8. Although a proposal has now

been made (Commission Communication of 15 June 2016[2], with two draft Commission acts setting out scientific criteria for the determination of such endocrine disruptors in the context of the EU legislation on plant protection products and biocidal products[3]), the criteria have not been yet formally agreed by the European Union, and the prioritisation will therefore continue to use the existing information on endocrine disruptors for the time being, including the EU database on endocrine disruptors.

(The proposed Commission regulation on plant protection product is for adoption *via* the regulatory procedure with scrutiny, while the proposed Commission delegated regulation on biocidal product is for adoption as a delegated act. The Commission will present both texts simultaneously to the EU co-legislators for them to exercise their control function.)

ED	ED MEANING
1	1: PROVEN ED EFFECTS
0.5	0.5: SUSPECT ED EFFECTS
0.25	0.25: NOT EXAMINED
0	0: EXAMINED AND NOT CLASSIFIED AS ED

Table 8. Scoring system used for the classification of possible endocrine disruptor substances. [51]

Data on ED were mainly retrieved from the EDS database[4] and other sources, e.g. available literature. The information retrieved was evaluated on a case-by-case basis, and a score was given according to the Table 8.

[2] COMMUNICATION FROM THE COMMISSION TO THE EUROPEAN PARLIAMENT AND THE COUNCIL on endocrine disruptors and the draft Commission acts setting out scientific criteria for their determination in the context of the EU legislation on plant protection products and biocidal products : http://ec.europa.eu/health/endocrine_disruptors/docs/com_2016_350_en.pdf

[3] DRAFT COMMISSION REGULATION (EU) …/…of XXX setting out scientific criteria for the determination of endocrine disrupting properties and amending Annex II to Regulation (EC) 1107/2009 : http://ec.europa.eu/health/endocrine_disruptors/docs/2016_pppcriteria_en.pdf

And : DRAFT COMMISSION DELEGATED REGULATION (EU) …/...of XXX setting out scientific criteria for the determination of endocrine-disrupting properties pursuant to Regulation (EU) No 528/2012 : http://ec.europa.eu/health/endocrine_disruptors/docs/2016_bpcriteria_en.pdf

[4] European Commission EDS database: http://ec.europa.eu/environment/chemicals/endocrine/strategy/substances_en.htm

5.2.3 The scoring system

In the previous prioritisation exercise [47], the matrix reported in Table 9 was used to determine the risk score, based on both the hazard score and the exposure score.

Hazard Assessment score \ Exposure assessment score	4	3	2	1	0
4	1	1	2	3	5
3	1	2	2	3	5
2	2	2	3	4	5
1	3	3	4	4	5
0	5	5	5	5	5

Table 9. Screening risk scores matrix used in the previous prioritization exercise [47].

This matrix was used in the present exercise as well; however, it was chosen to use "screening risk score" instead of "risk score" term, for more clarity at a later stage (when the "STE risk rank" term is introduced), According to the matrix, the lower the screening risk score, the higher the concern about the substance. The screening risk score is related to risk classification as follows:

- Screening risk score 1 – Risk very high
- Screening risk score 2 – Risk high
- Screening risk score 3 – Risk intermediate
- Screening risk score 4 – Risk low
- Screening risk score 5 – Risk very low

Because the hazard score in the present exercise spans from 0 to 7, it needed to be rescaled (to span from 0 to 4 as indicated by the matrix in Table 9). This way, 5 classes of hazard score range were generated in the present exercise, as shown in the Table 10.

		Exposure assessment score				
		4	**3**	**2**	**1**	**0**
Hazard score	**Class 4 (5.6 to <= 7.0)**	1	1	2	3	5
	Class 3 (4.2 to < 5.6)	1	2	2	3	5
	Class 2 (2.8 to < 4.2)	2	2	3	4	5
	Class 1 (1.4 to < 2.8)	3	3	4	4	5
	Class 0 (0.0 to < 1.4)	5	5	5	5	5

Table 10. Screening risk scores matrix using rescaled ranges of hazard scores. Red numbers indicate the highest risk/concern.

The screening risk score was one of the criteria applied to select the substances for the risk assessment phase, as described in section 6.4.

5.3 The Risk Assessment Phase

5.3.1 Introduction

Modelling tools were used to calculate the predicted environmental concentrations (PEC). In a broad sense, they are based on mathematical methodologies which simulate the environmental scenario where a substance is supposed to be applied. In these approaches, different classes of substances are usually simulated by different tools because they are differently expected to be released into environment. For example, a pesticide requires a scenario which is different compared to a human pharmaceutical, since the first one is directly applied to the environment, while the second one is expected to be released in the sewage system.

For substances that were expected to be released directly in the environment (plant protection products and veterinary pharmaceuticals in the present exercise), the FOrum for the Co-ordination of pesticide fate models and their USe (FOCUS) surface water scenario tools were chosen. Basically, these tools simulate the fate of substances upon virtual scenarios based on real data.

The FOCUS tools allowed calculations for four levels of a tiered approach, spanning from level 1 (the simplest one that required minimum input data, giving the highest PECs because it was set as the worst case scenario, e.g. worst case loading, no specific climate etc.), to level 4, which was the most refined one. In this exercise, level 3 was selected as the best compromise between required input data and accuracy of the prediction. Ten representative EU scenarios, with their related hydrology, soil type and weather conditions, were simulated. For the chosen scenario(s), the crop type, and the pattern of application of a substance were crucial, because they both impact the substance's fate. FOCUS steps do not require the tonnage of the applied substance. This tool

was chosen instead of European Centre for Ecotoxicology and Toxicology of Chemical (ECETOC) for PPP because discussions in the 4th SG-R meeting concluded that for these substances, the result given by the FOCUS model were more reliable than the estimate of the ECETOC model. It is here also recalled that the model of water flow and solute transport in field soils (MACRO) tool, part of the FOCUS Step 3, takes into account drainage of the chemical through the soil up to the water bodies. In addition to this, it was not possible to retrieve the adequate information on the tonnage for all the pesticides considered here. The tonnages extrapolated (see section 5.2.1 on Exposure assessment) were not deemed precise enough for the purpose of RQ derivation.

Due to the likely entry route of veterinary pharmaceuticals into environment, i.e. by direct release to the soil, or as manure application, it was possible to estimate the application rate of these substances, and therefore to carry out PEC calculations with the FOCUS tools - Step 3. The FOCUS tool is deemed more appropriate than the VetCalc tool because the FOCUS models have been the subject of much investment and testing and are recognised by regulatory authorities; they also are continually re-evaluated and updated (for more details see EMEA/CVMP/ERA/172074/2008 Rev. 5 [5]).

For the inorganic compounds, industrial substances and biocides, the ECETOC Targeted Risk Assessment (TRA) tool, developed by the ECETOC organisation, was chosen for PEC calculations. The simulated scenarios are based on default environmental release codes (ERC), which were developed by ECHA. The ERCs are industrial and consumers use descriptors which set specific substance release percentages into the environmental compartments (air, water and soil). However, in the present exercise, specific Environmental Release Category (spERC) codes were used as a refinement of the ERC-based emission estimation. This way, more realistic default values of the fractions released to water, air, and soil were considered. The main issue with using ECETOC was the need of tonnages as input data.

The last class of substances considered were human pharmaceuticals. In this case, the related exposure scenario consisted of substances that were released in the sewage, and thus ending in the wastewater treatment plant. The PEC calculation of human pharmaceuticals is done using a formula from Besse et al. [48]. This formula was chosen because it takes into account the excretion factors which are pivotal for pharmaceuticals, while ECETOC (used for industrial chemicals) does not.

The following Table 11 details the tools used in this exercise for the aforementioned class of substances.

[5] http://www.ema.europa.eu/docs/en_GB/document_library/Other/2009/10/WC500004391.pdf

Class of substances	PEC calculation method	Compartment involved
Plant Protection Products (PPPs)	FOCUS Step 3	Water, Sediment
Biocides	ECETOC – Tier 2	Water, Sediment
Generic industrial uses	ECETOC – Tier 2	Water, Sediment
Inorganic compounds	ECETOC – Tier 2	Water, Sediment
Veterinary pharmaceuticals	FOCUS Step 3	Water, Sediment
Human pharmaceuticals	Besse et al. [48]	Water

Table 11. Methods used for calculating PEC values of the different classes of substances. FOCUS is a set of tools and scenarios that simulates the fate of substances released in the environment (FOCUS is tailored for plant protection products, but can also be adapted for veterinary pharmaceuticals). ECETOC Tier 2, available as a set of Excel files, is a set of models that simulate the fate of substances and is tailored for industrial/indoor use of substances.

5.3.2 PEC for freshwater

5.3.2.1 Plant protection products

FOCUS Step 3 was selected for the PEC calculation of plant protection products (PPP).

The exposure assessment of PPPs was performed according to the Generic guidance for FOCUS surface water Scenarios - Version 1.4 [52]. A tiered approach was used to assess the exposure assessment of PPPs in surface water, and the guidance document [52] details how to choose the appropriate application windows, crop interception factors, degradation rates and coefficient of distribution Soil Organic Carbon-Water Partitioning Coefficient (Koc) of the substance. The FOCUS Surface WAter Scenarios Help (SWASH) shell (Step 3), which handles the input data and the requested tools, was adopted for estimating concentrations of PPPs in ditches, ponds and streams based on ten different European scenarios. The SWASH shell coordinates models which simulate runoff and erosion (corresponding tool: PRZM, corresponding scenarios are called R), leaching to field drains (corresponding tool: MACRO, corresponding scenarios are called D), spray drift (internal in SWASH) and finally aquatic fate in ditches, ponds and streams (corresponding tool: TOXSWA, that gathers the output of all the aforementioned tools to calculate the final concentration of the chemical in the water bodies). These simulations provided detailed assessments of potential aquatic concentrations in a range of water body types for up to ten separate geographic and climatic scenarios.

Once physical-chemical parameters of the substances to be assessed were provided to SWASH, 10 EU representative soil-climate scenarios were available for simulations and, for each scenario, a set of representative crops was available. Location of scenarios are showed in Figure 6.

For every PPP under evaluation, different scenarios for different crops in FOCUS were used for PEC calculation. This was accomplished first by choosing the type of crops. When possible, depending on the available information, in this exercise all representative types of crops for the PPP were chosen. Choosing a list of representative crops usually allows to cover a broad range of cases. After this step, it was possible to choose the water body types (ditch, pond, stream) and then the association with the scenario (runoff or drainage).

The next step was to build a table that defined the applications of the PPP. Concerning the timing of application, we relied on FOCUS tools calculations, while the amount of PPP applied (usually reported as kg/ha) was collected from GAP (Good Agricultural Practices, sources include: EFSA dossiers, FAO, agricultural books, etc.). If recommended quantities were reported as ranges and/or multiple applications, the highest values were taken as a worst case scenario.

Once the scenario, the crops and the application rates of PPP were set, the simulation programs were executed to obtain the PEC for every scenario. First MACRO and PRZM were run, then their output was used as input into TOXWA for final PEC calculation in water bodies.

After running all simulations, all values for PEC for fresh water were collected and the maximum value was recorded for subsequent RQ calculations.

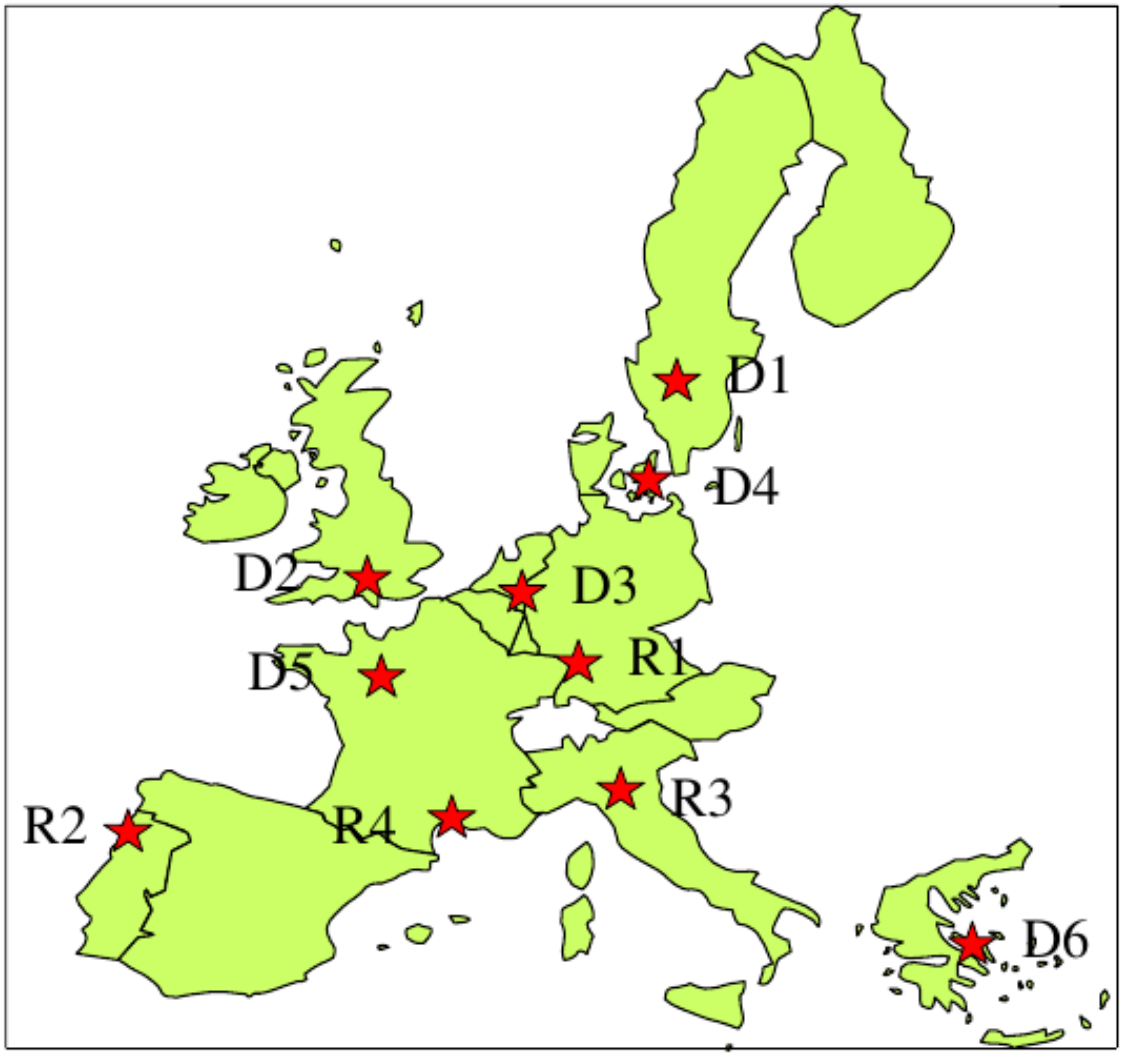


Figure 6. FOCUS EU scenario locations for surface water PEC calculations (D = drainage, R = runoff). Details and representativeness of the scenarios can be found in the generic guidance for FOCUS surface water scenario [52].

5.3.2.2 Biocides, metals and generic industrial uses compounds

The ECETOC Targeted Risk Assessment (TRA) tool was selected for the PEC calculation for biocides, inorganics and generic industrial uses compounds. This tool handles scenarios that correspond to the different ERC/spERC codes which were based on substance's usage. Tonnages and usage information were retrieved from IUCLID and the SPIN databases. This type of information was crucial for the outcome of the present exercise, since ECETOC needs tonnage values. For inorganic compounds, modelled/measured K_p water-soil or water-sediment was used, along with biotic and abiotic degradation rates set to 0.

For every substance more than one ERC/spERC code might be available, as illustrated in Figure 7. For each of the ERC/spERC codes, the PEC was calculated and the worst-case value was selected for the calculation of the final RQ.

ECETOC allowed to calculate PECs according to the pertinent tonnage for every type of usage of a substance (i.e. whether it is an intermediate or is a cleaning product, for example), but since the relative percentages of the usages were usually missing, in these cases the worst case assumption was made applying the whole tonnage in all simulated scenario.

Life cycle stage	Annual EU Tonnage (tonnes/year)	Fraction of tonnage to region	Use ERC or spERC as release estimation approach	ERC
Manufacturing	1.00E+03	1	ERC	ERC1
Formulation	3.00E+02	1	ERC	ERC2
Formulation	3.00E+02	1	spERC	ERC2
Formulation	3.00E+02	1	spERC	ERC2
Processing	3.00E+02	1	ERC	ERC4
Processing	3.00E+02	0.1	spERC	ERC8a
Processing	3.00E+02	1	spERC	ERC6c

Figure 7. Example of part of ECETOC input about tonnages and ERC/spERC codes.

5.3.2.3 Veterinary pharmaceuticals

As outlined in the EMA guidance [53], VetCalc model and the suite of models developed by the FOCUS were the two main available options for refined freshwater PEC (PEC_{fw}) calculations. In the current prioritisation exercise, FOCUS models were selected as the tool of choice for the exposure assessment of veterinary pharmaceuticals. In fact, although being specifically developed for plant protection products (PPPs), FOCUS models' predictions could also be used for veterinary pharmaceuticals, with appropriate precautions and model settings (see Table 12). This is due to the similarities between the field application of PPPs and the spreading of veterinary pharmaceuticals (by means of manure or grazing animals) to the soil. The preferred scenario recommended by the EMA guidance (the "pure grassland" scenario) is not available in FOCUS, therefore the "winter cereals" scenario was used to calculate the PECs. This scenario is the best option identified by the EMA guidance, because the application of manure to arable and grass land is considered to coincide with the drilling of cereals in autumn.

The key point was the calculation of the application rate (kg/ha) of the pharmaceutical. The formula for this calculation required a PEC for soil. This PEC for soil was calculated using both default values (that depends on how the animals are supposed to be reared), and values which were calculated on the basis of the available data, such as the quantity of manure containing the active residue, the daily dose of the active ingredient used, the number of days of treatment, the animal body weight.

After the PEC for soil was obtained, the application rate (kg/ha) that was necessary for using FOCUS as a modelling tool, could be calculated. All scenarios that used the winter cereals (crop suggested by the EMA document) were then calculated, and the highest PEC was selected.

Parameter	Input values considered
Crop	Winter cereals
Application timing	Pre-emergence application dates
Application rate (AR)	Calculated from $PEC_{soil,initial}$ (in general, use of PEC_{soil} calculated for intensively reared animals, or pasture animals) by using EMA equation.
DT_{50} of substance	Experimental value, if available. Otherwise, set to zero.
Crop uptake	None
Application method	Soil or granular incorporation
Wash-off factor	Wash-off factor (m^{-1}): ≥ 10^{-6}, even if there is no wash-off.
Depth (m)	Soil depth used to calculate PEC_{soil}

Table 12. FOCUS model settings for exposure assessment of veterinary pharmaceuticals. [53]

5.3.2.4 Human pharmaceuticals

For human pharmaceuticals, PEC values were calculated using the following equation [48]

$$PEC_{fw} = (consumption \times F_{excreta} \times Fstp_{water}) / (WWinhab \times hab \times dilution \times 365)$$

where *WWinhab* is the volume of wastewater per person per day (default value of 200 [L/(hab*day]), *hab* is the number of inhabitants, $F_{excreta}$ is the excretion factor of the active substance, $Fstp_{water}$ fraction of emission from wastewater treatment plants to surface water (set to 1 as worst case assumption), *dilution* is the dilution factor (default value of 10), *consumption* is the quantity (mg/year) of active ingredient consumed by the population during 1 year.

This simplified approach was chosen because of the relatively simple scenario when modelling human pharmaceutical fate (because of the excretion of these substances, wastewater is the most common fate). Consumption was the most difficult value to be found because data was available only for few MSs (as detailed in section 6.1.1.1) and often only for a limited number of substances. As a consequence, in the present modelling based exercise, the tonnage for the Europe was extrapolated for the EU total population.

5.4 Hazard assessment – estimation of PNEC values

5.4.1 PNEC derivation

A Substance risk assessment in the water compartment is relevant for the protection of organisms inhabiting the water column. Therefore, the protection threshold concentrations $PNEC_{fw}$ was estimated for the substances that were selected from the screening phase.

Here, the PNEC value is the concentration of a substance for which no harm is expected to or *via* the aquatic environment (in the present exercise only long-term PNEC values, i.e. those for chronic effect, were considered).

Whenever sufficient data were available, the probabilistic approach was carried out for the derivation of the PNEC. An adequate AF was then applied to the derived HC5 (Hazardous Concentration to 5 % of species) [55].

When there was not enough data available, the deterministic approach was used. For the calculation of the PNEC, representative trophic levels have to be considered - algae, crustaceans and fishes, which mimic a typical hypothetical food chain of a fresh water body. For each trophic level, the highest toxicity level of a representative species was considered.

6 Screening Phase – Data collection and selection of substances

6.1 *Data collection for exposure score*

The exposure determination consists of two parts, the tonnage of the substance (in Europe) and the use index. The use index has been already explained in Table 3 and is linked to the use pattern of the substance, which shows basically how much the substance is expected to be dispersed in the environment. This information is available in substance dossier(s) or other online sources, and in case of multiple uses of a substance, the worst case scenario is taken.

It is more complicated to access the European tonnage data of the substances released; this tonnage can be reported in public or confidential sources (see further explanations about confidentiality on section 6.1.2). In the present exercise, tonnages were also provided by some MSs (for details see section 5.2.1).

6.1.1 Public data

Tonnages are sometimes publicly available as for example tonnage bands from ECHA or national tonnage data information, e.g. for plant protection products from the Czech Republic. Apart from information about tonnage bands from ECHA, usually tonnages are available for one or more countries but never for the whole EU. In these cases, extrapolations were necessary as explained below.

6.1.1.1 Tonnage extrapolation

ECHA (industrial substances)

In order to reduce the number of requests for confidential tonnages from ECHA, the available public tonnage bands were used as a first choice. Since the substance screening risk score depends on both exposure and hazard scores, the hazard score was first calculated as a reference point, and then the minimum and maximum values of tonnage bands were applied. If the screening risk score did not differ by applying either the minimum or maximum tonnage, the tonnage band was used; otherwise a request to ECHA was done.

Tonnages from SPIN database

The SPIN database collects the tonnages of chemicals used in Denmark, Finland, Sweden and Norway. Since the total use of a substance depends on the peculiarities of the MS, the extrapolation cannot just be based on population only; therefore, the Gross Domestic Product (GDP) from Eurostat 2014 was used in addition, i.e. extrapolating tonnages to the whole EU (28 MSs) was done accordingly to the ratio of the GDP of the whole EU divided by the GDP of every MS.

So, when for example the tonnage from one MS was available, tonnage extrapolation for the whole EU was calculated as:

EU tonnage extrapolation = (MS tonnage / MS GDP) x EU GDP

If more than one MS provided the information about the tonnage, then the average of the corresponding EU extrapolations was used.

Human pharmaceuticals

Tonnage data were taken from medicinal sales in Portugal for the year 2013 (last available data), and extrapolated to the whole European Union (28 MSs) according to the ratio of the Portuguese population (10.46 million) to the whole EU population. From Portuguese data, the active substance quantity for the whole EU was relatively easy to determine, even though a custom software procedure had to be developed because of the very different forms of every medicine available on the market, including combined pharmaceuticals. A more refined EU-wide approach was not possible because the percentage of usage of the active substances for every MS was not available for the extrapolations. (It is expected that the usage of certain medicines is usually different among the MSs).

733

734 Veterinary pharmaceuticals

735 To extrapolate the tonnage of the veterinary pharmaceuticals for the whole Europe (28 MSs), the
736 meat production was considered since it is supposed that the veterinary pharmaceutical usage is
737 proportional to the animal meat produced [55]. Tonnages for veterinary pharmaceuticals were
738 available from sales in Latvia (year 2013, last available data). Meat production in the EU can be
739 found in Eurostat, and data is reported by type of animals. For Latvia, Eurostat recorded the
740 production of bovine animals, pigs and poultry meat.
741 In order to extrapolate the tonnage for EU the first step was to determine, for every type of animal,
742 the ratio between the total production of meat in EU and the meat produced in Latvia, as

743

744 Eurostat ratio of meat production for *animal type*

745 $$= \frac{\text{tonnes of } animal\ type \text{ meat produced in EU}}{\text{tonnes of } animal\ type \text{ meat produced in Latvia}}$$

746

747 Then the EU extrapolated tonnage of substance used for each *animal type* has been calculated as

748

749 EU tonnage extrapolation for *animal type*

750 $$= \text{tonnes of pharmaceutical used for } animal\ type$$

751 $$\times \text{ Eurostat ratio of meat production for } animal\ type$$

752

753 The total EU extrapolation is given summing all animal types EU extrapolations.

754

755 Pharmaceutical used both for human and veterinary use

756 For all pharmaceuticals that are used both in veterinary and human products, the relative
757 tonnages calculated as explained in the previous two sections, were added.

758

759 Plant protection products (PPPs)

760 Tonnage data of active substances were kindly provided by the Czech Republic (CZ) and available
761 for few MSs in the SPIN database, in both cases for the year 2013. To extrapolate the values for
762 the other MSs, Eurostat was used as an additional source of information (even though in Eurostat
763 the available tonnages are reported only by classes of pesticides, i.e. “insecticide and acaricide”,
764 “herbicide”, “fungicide and bactericide”, “plant growth regulator” and “other PPP”).
765 From the tonnage of the active substance used in a MS (e.g. the Czech Republic), and having the
766 list of MSs where the substance is approved, it was possible to extrapolate the tonnage for every
767 MS using the following two formulas:

$$\text{Eurostat Ratio of } \textit{the class} \text{ of PPP} = \frac{\begin{array}{c}\text{Eurostat tonnage of } \textit{the class} \text{ of PPP for the MS for} \\ \text{which the tonnage} \\ \text{of the active substance should be estimated}\end{array}}{\begin{array}{c}\text{Eurostat tonnage of } \textit{the class} \text{ of PPP of the MS} \\ \text{providing the tonnage of the same active substance}\end{array}}$$

Extrapolated tonnage of the active substance for a MS

$$= \text{tonnage of the active substance used in the MS providing this information} \times \text{Eurostat Ratio of } \textit{the class} \text{ of PPP}$$

These two formulas were repeated for all countries where the PPP(active substance) was approved and the results were summed, thus providing a final total tonnage as an EU extrapolation.

In order to verify the approach, since we received additional data from France (kindly provided by Institut National de l'Environnement Industriel et des Risques, INERIS), the extrapolated data for France was compared to the tonnage bands provided by them. From 135 substances for which tonnage band was available (i.e. having a minimum and a maximum value), the comparison resulted in 72 of the extrapolated tonnages that were within the tonnage band, 38 that were above a maximum, and 25 that were below a minimum tonnage value.

If more than one MS provided a source of tonnage for a substance, e.g. the Czech Republic and other MSs from the SPIN database, the whole procedure was repeated for every "source" MS, then the average of the extrapolations for the whole EU was taken.

6.1.2 Confidential data

JRC is linked by a confidentiality agreement to the ECHA, in order to protect intellectual property rights of the companies providing data to the ECHA. This means that sometimes tonnages from ECHA (e.g. for intermediates) were available only under confidentiality commitment and this information cannot be made public. As a consequence, only the final screening risk score can be shared; neither exposure nor hazard scores can be provided in order to avoid guessing (by back calculations) the possible tonnage band of the substance.

6.2 Data collection for hazard score

To deal with many data in this exercise, whenever possible, tasks were automated by software.

The first step was to build a dataset of ordered data, allowing the easier/faster selection of the most suitable information on PBT, CMR, and ED properties of the chemicals. Therefore, all possible data of interest (chemical properties, PBT, CMR and ED) were collected, put in a dataset,

and software procedures were written to read these data (following the instructions already explained in this document to calculate the score).

Not all data sources available were appropriate for an automated data-mining procedure, in this case hazard data were introduced manually in the final table for the screening phase. The most important data sources used for this task are listed here:

- ECHA website (data downloaded in July 2015)
- ECHA CL inventory data from ECHA website (data downloaded in August 2015).
- SPIN database, last version available in 2016
- ChemIDPlus database (data downloaded in June 2015)
- IARC Monographs
- European Comissiom EDS database

Moreover, additional sources of information (either websites or documents) were searched manually.

An automated procedure was developed to screen the substances of interest from websites, as ECHA and ChemIDPlus, and download all the pertinent dossiers/data. Other sources which were already available as off-line resources (once downloaded), were used directly to write tables that could be read by the same automated procedure. The aim was to harmonize the different sources in a dataset which could then be treated efficiently. Off-line data were quickly explored by software, which in this case was written for the purpose of choosing the most relevant data for the hazard properties of a substance.

Rules for the selection of the most relevant data were as follow:

i) ECHA dossiers: multiple values were usually available for the same data classified also by reliability. In this case, first the most reliable data were collected, from which the most conservative value was chosen;

ii) CL Inventory: sets of data were available but entries were not flagged by reliability. In these cases, the most represented data (the ones that had the highest number of entries) was taken instead of the most conservative.

ECHA website provided most of the data because the dossiers are often very comprehensive. Moreover, the studies included in the dossiers not classified as reliable were excluded. Data from ECHA, however, was available only for a number of substances of the screening list, i.e. 2215 substances at the time the database was built. Therefore, the second choice was to obtain the physical-chemical properties data from ChemIDplus (5411 substances available at the time), while the CMR properties were evaluated using the CL Inventory (5468 available at the time).

Other than the automated procedure, alternative sources were available online and served to complement the data mentioned above (e.g. the missing data for the PPP was taken mainly from the EFSA dossiers). In addition the environmentally classified pharmaceuticals from the Stockholm County Council of the years 2014-2015 were used [26].

A very useful online information source was the eChemPortal which links to all the relevant sources. In addition, TOXNET (whose subsections HSDB and ChemIDPlus were the most common choice) and INERIS databases were used.

6.3 Results

The following substances were included in the screening phase:

1. Substances collected from several databases (see Table 1)
2. Substances, for which enough monitoring data was available. These substances went through the monitoring-based exercise.
3. Priority Substances (total number 84). All congeners and isomers were considered separately, which explains why we have 84 substances while in the Directive 2013/39/EU only 45 are reported.

The aim of including the substances analysed in the monitoring exercise and the PS was to check the level of accuracy of the screening procedure. It has yet not been possible to fully analyse the results of the screening phase concerning the PS.
Some information could be retrieved only for 6523 substances out of the 11549 included in the initial list. Only for 2790 of them was possible to find all needed data for deriving the screening risk score (hazard properties and use assessment to derive the hazard score and the exposure score, respectively), while for 3733 substances we retrieved only partial information (no tonnage was available so only hazard properties were considered in the analysis).
Annex I shows the data set for the 2790 substances and the source of hazard properties is reported for all of them.

In case of PS, the screening risk score was derived for 31 substances.

6.3.1. Validation and statistical analysis

6.3.1.1 Validation of the screening risk scores

To validate the screening phase procedure, the STE scores (converted to as STE risk rank, see Table 13) of 203 substances from the monitoring based exercise were compared to the modelling screening risk scores. For the reasonability of this comparison, it is here also recalled that even though the hazard properties are not included in the calculations of the STE approach, these properties are intrinsically included in the PNEC calculation.

The first step was to convert the "STE scores" that span from 0 (very low risk) to 3 (very high risk) (Ref.: *Report on the monitoring based exercise, 2016*) into STE risk rank, spanning from 1 (very high risk) to 5 (very low risk) (Table13).

STE score	STE risk rank	Risk classification
2.4 - 3	1	Very high
1.8 - 2.4	2	High
1.2 - 1.8	3	Intermediate
0.6 - 1.2	4	Low
0 - 0.6	5	Very low

Table 13: Conversion of the STE scores into STE risk rank, which has the same scale as the screening risk score. The aim of introducing the STE risk rank is to make STE results comparable to the screening risk scores.

The STE risk ranks were used for a direct comparison with the screening risk scores. For an analysis of the correspondence between them, the following assumption were made:

- Good correspondence: when the STE risk rank and the screening risk score is the same or differ by 1
- Acceptable correspondence: when the STE risk rank and the screening risk score differ by 2
- No correspondence: when the STE risk rank and the screening risk score differ by 3 or 4.

The results of the comparison are summarized in Figure 8 and Figure 9. For 84% of the substances, the correspondence between the screening risk score and the STE risk rank was assumed to be good or acceptable, which reinforces the validity of the screening phase process.

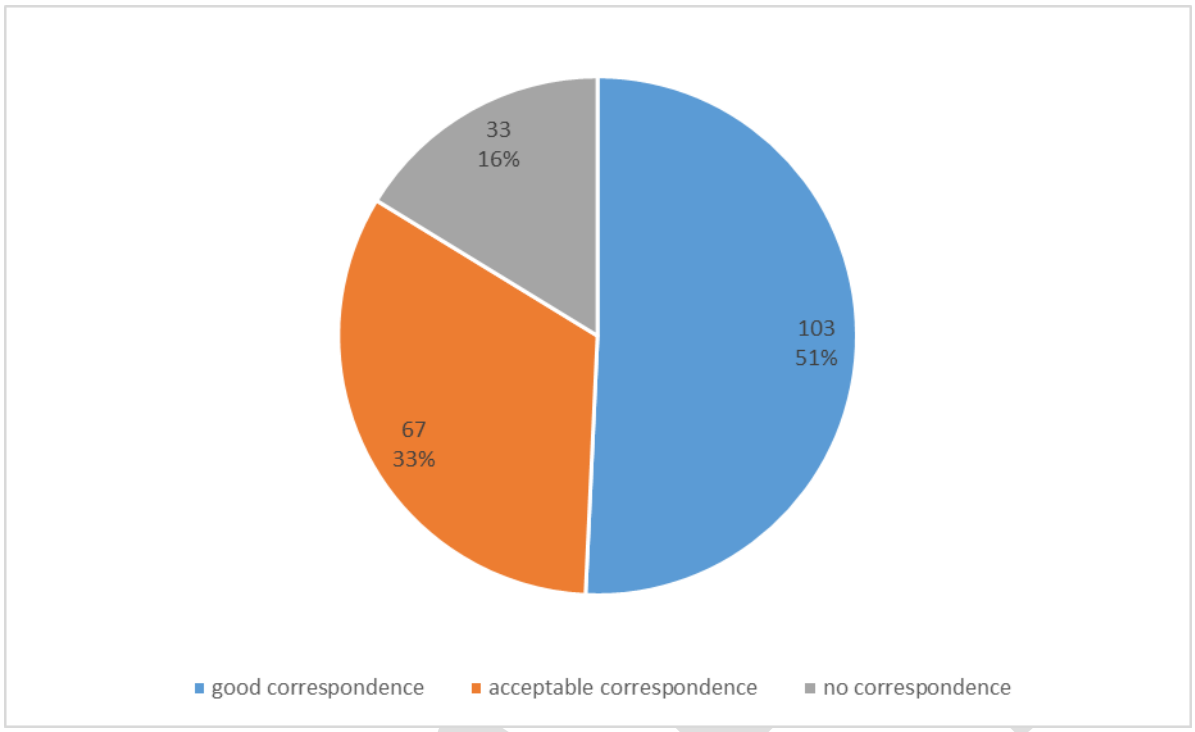


Figure 8. Correspondence between the screening risk scores and the STE risk ranks, indicating the number and the percentage of the substances (203 in total). Good correspondence - if the screening risk score and STE risk rank were equal or the difference between these two values was 1; acceptable correspondence - if the difference between screening risk score and STE risk rank was 2; no correspondence - if the difference between screening risk score and STE risk rank was greater than 2.

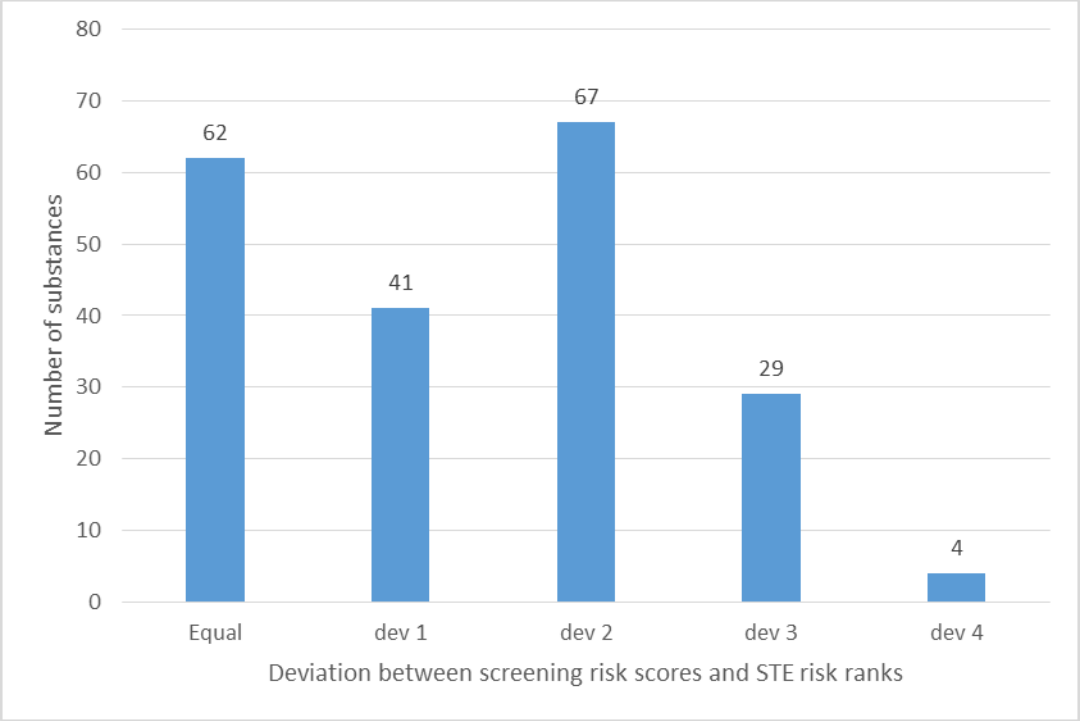


Figure 9. Deviation between the screening risk scores and the STE risk ranks (comparison made for 203 substances in total). The x-axis values refer to equal (no difference between the screening risk score and STE risk rank); deviation 1 (difference of 1 between the screening risk score and STE risk rank); deviation 2 (difference of 2 between the screening risk score and STE risk rank); deviation 3 (difference of 3 between the screening risk score and STE risk rank); deviation 4 (difference of 4 between the screening risk score and STE risk rank).

6.3.1.2 Statistical analysis of the screening phase scores

The screening risk scores were obtained from the screening phase procedure for 2759 substances. This number includes the 203 substances from the monitoring exercise, but excludes 31 PS that were only used to verify how they ranked (see Annex I), ranged from 1 to 5 (for details please see the Risk Scores Matrix; paragraph 5.2.3). A screening risk score of 1 corresponds to a very high risk, while a screening risk score of 5 corresponds to a very low risk. As expected, the very high risk and high risk were identified only for a small number of the substances (score 1 and 2, respectively, see Figure 10).

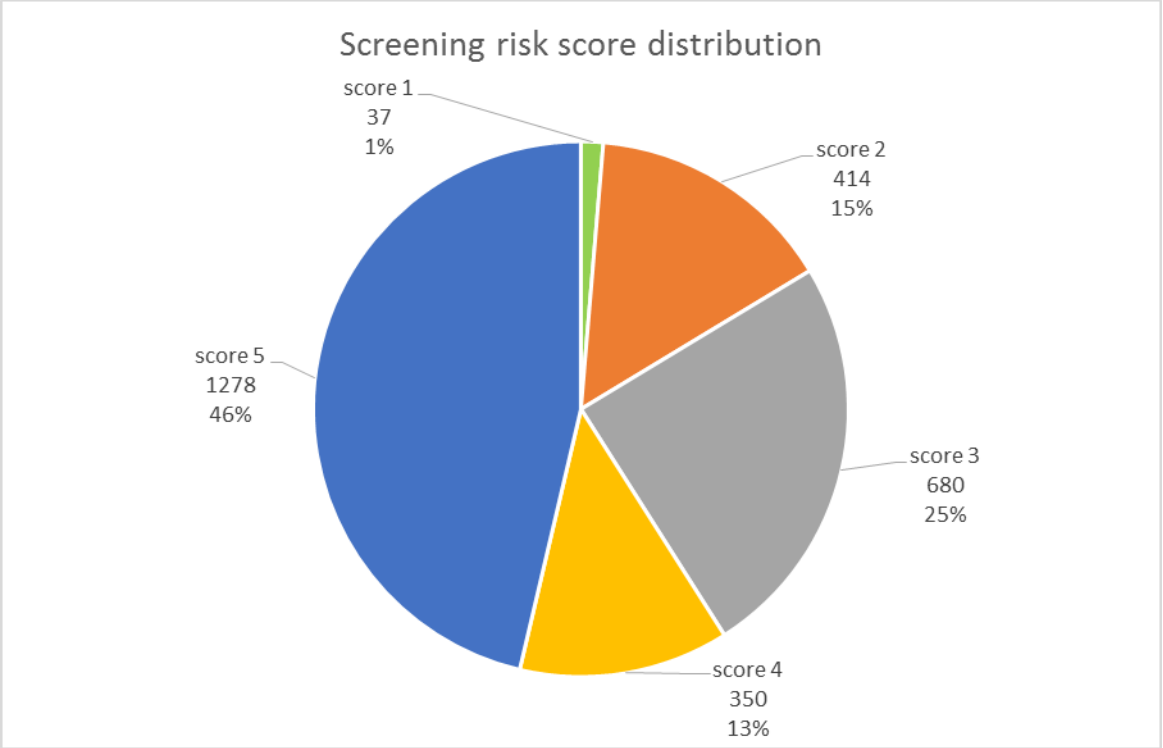
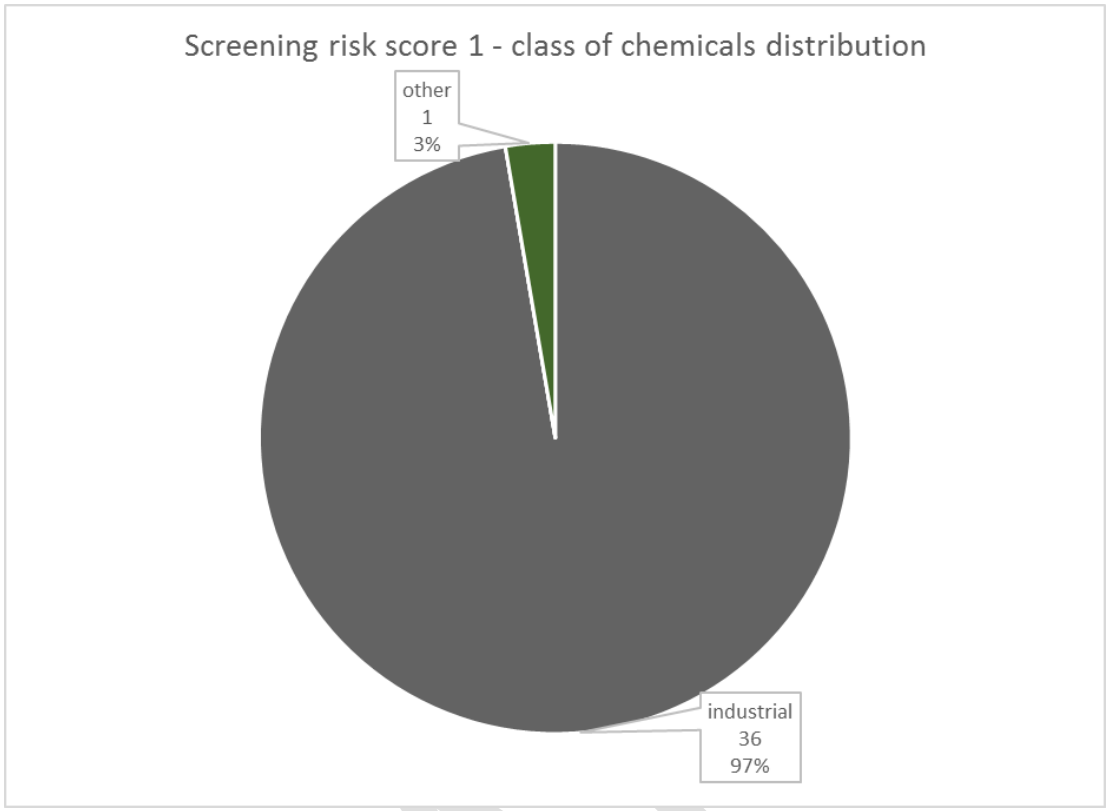
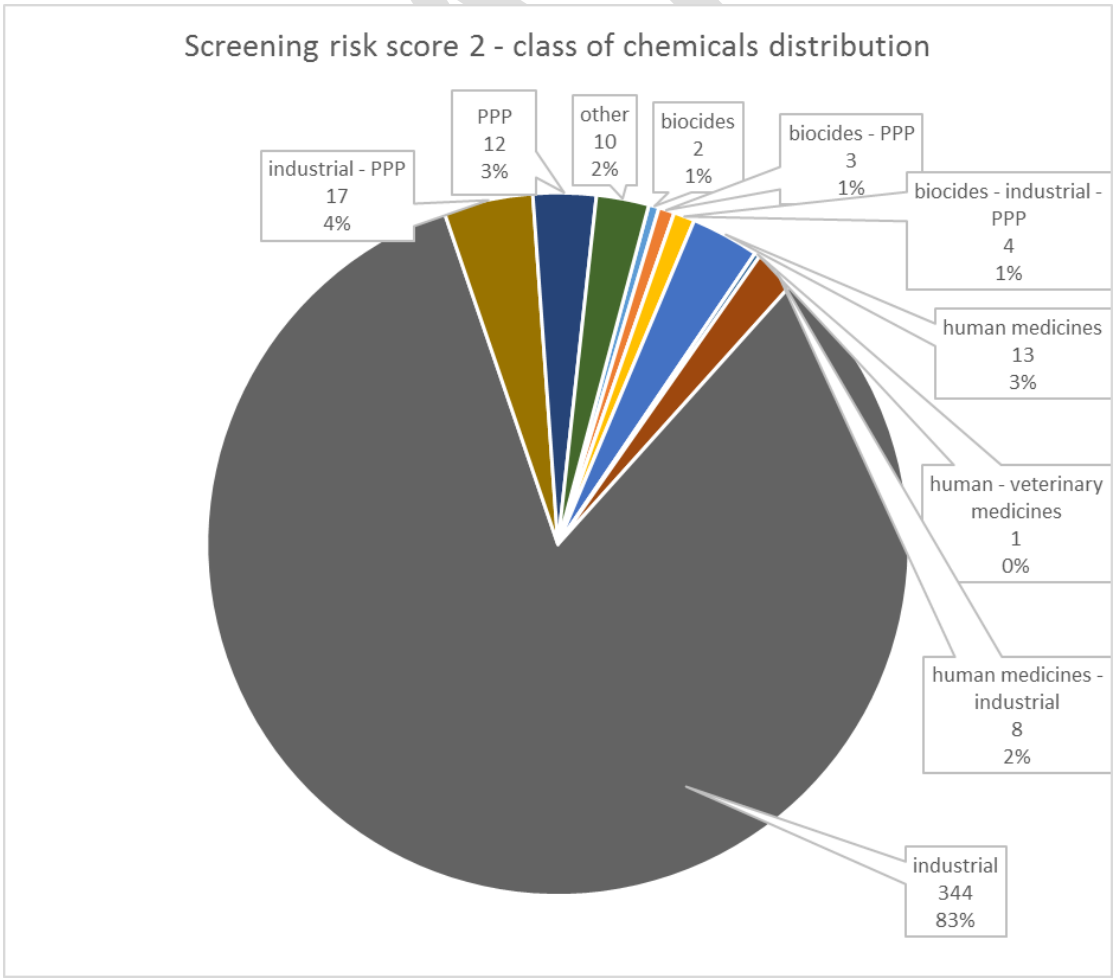


Figure 10. Distribution of the screening risk scores obtained during the screening phase (2759 substances in total), indicating the number and percentage of the substances.

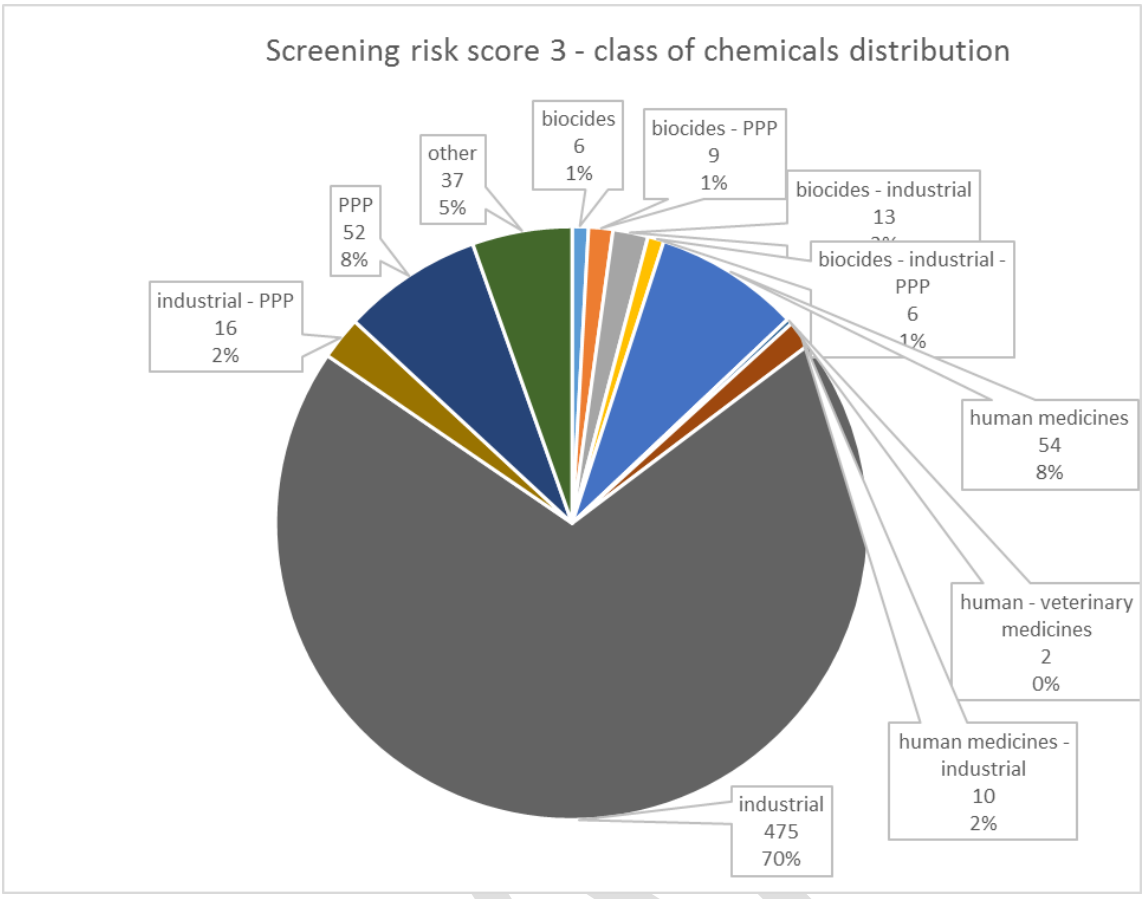
The distribution of the different classes of chemicals for each screening risk score is summarized in Figure 11. The score 1 and 2 comprise mainly substances for industrial usage. Detailed distribution of screening risk scores within the different classes of substances, obtained during the screening phase, is summarized in Figure 12.


Screening risk score 1 - class of chemicals distribution
other
1
3%
industrial
36
97%

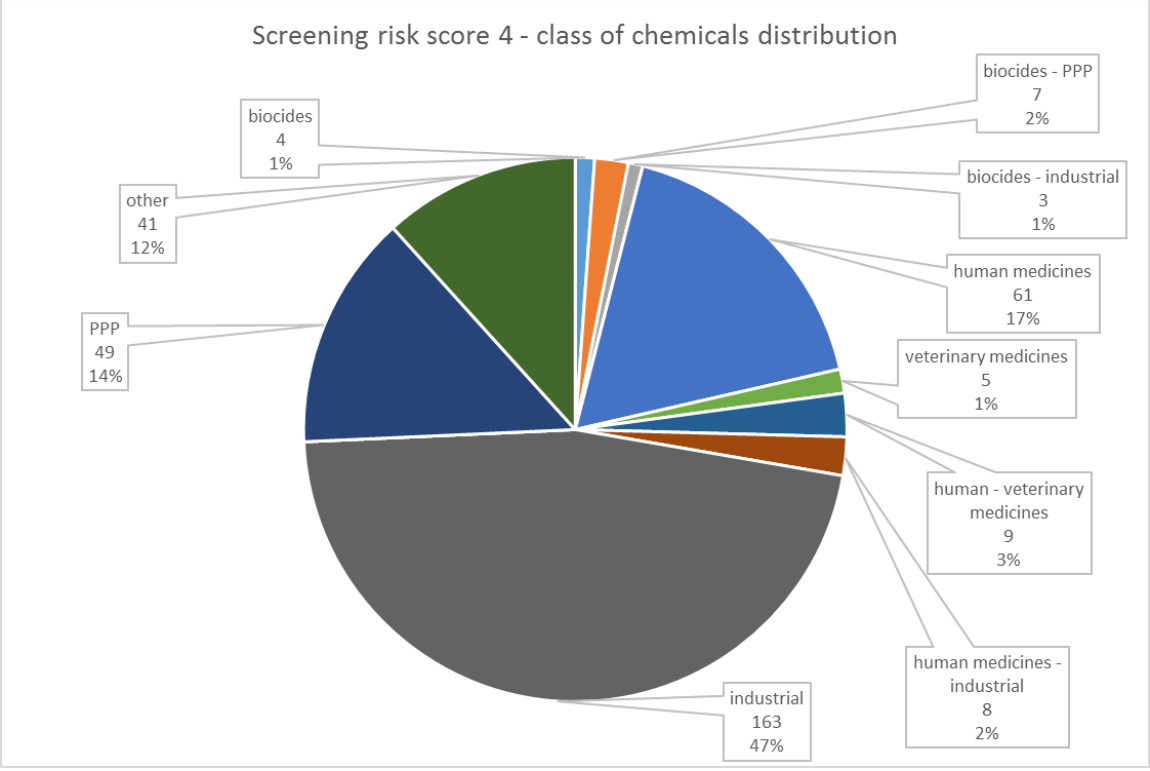
938


Screening risk score 2 - class of chemicals distribution
PPP
12
3%
other
10
2%
biocides
2
1%
biocides - PPP
3
1%
industrial - PPP
17
4%
biocides - industrial - PPP
4
1%
human medicines
13
3%
human - veterinary medicines
1
0%
human medicines - industrial
8
2%
industrial
344
83%

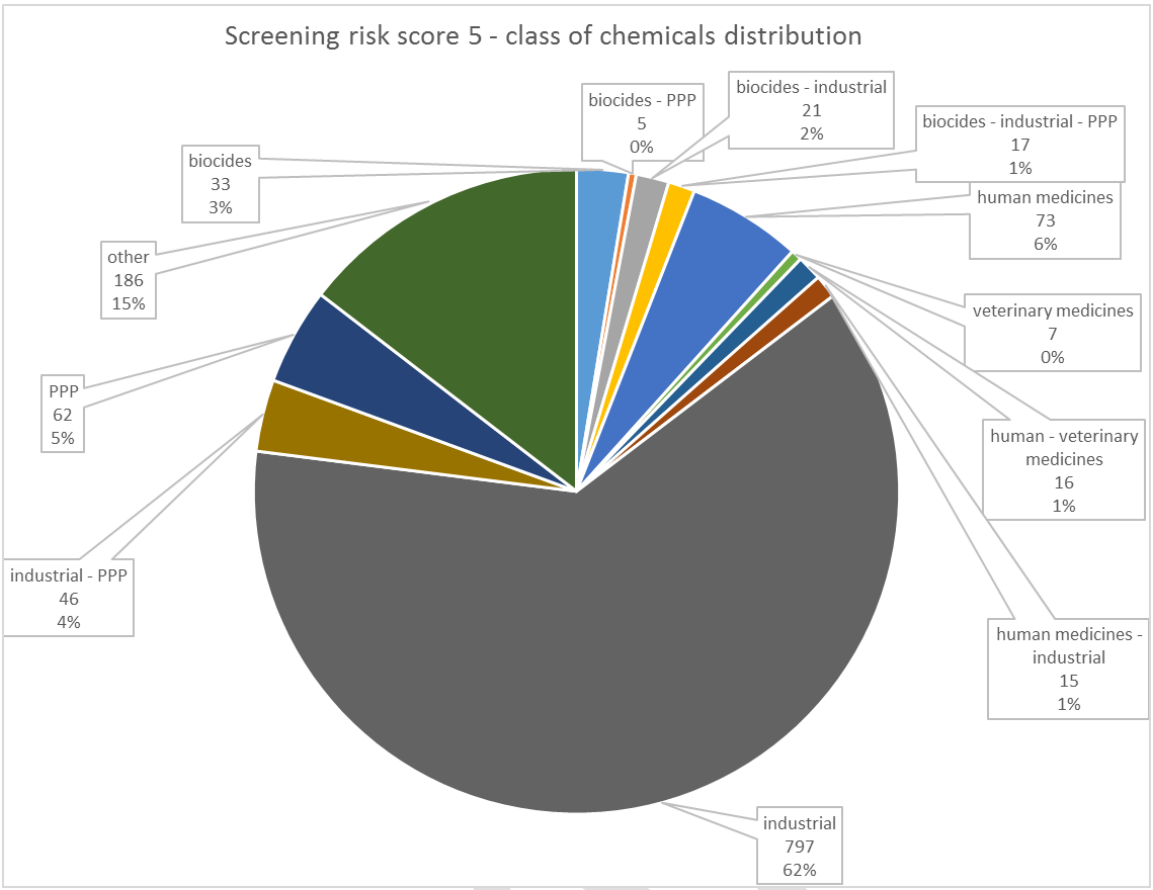
939


Screening risk score 3 - class of chemicals distribution
biocides
6
1%
biocides - PPP
9
1%
biocides - industrial
13
biocides - industrial - PPP
6
1%
human medicines
54
8%
human - veterinary medicines
2
0%
human medicines - industrial
10
2%
industrial
475
70%
industrial - PPP
16
2%
PPP
52
8%
other
37
5%

940


Screening risk score 4 - class of chemicals distribution
biocides - PPP
7
2%
biocides - industrial
3
1%
human medicines
61
17%
veterinary medicines
5
1%
human - veterinary medicines
9
3%
human medicines - industrial
8
2%
industrial
163
47%
PPP
49
14%
other
41
12%
biocides
4
1%

941



942

943 **Figure 11**. Distribution of the different classes of chemicals for each of the screening risk score, obtained

944 during the screening phase, indicating the number and percentage of the substances.

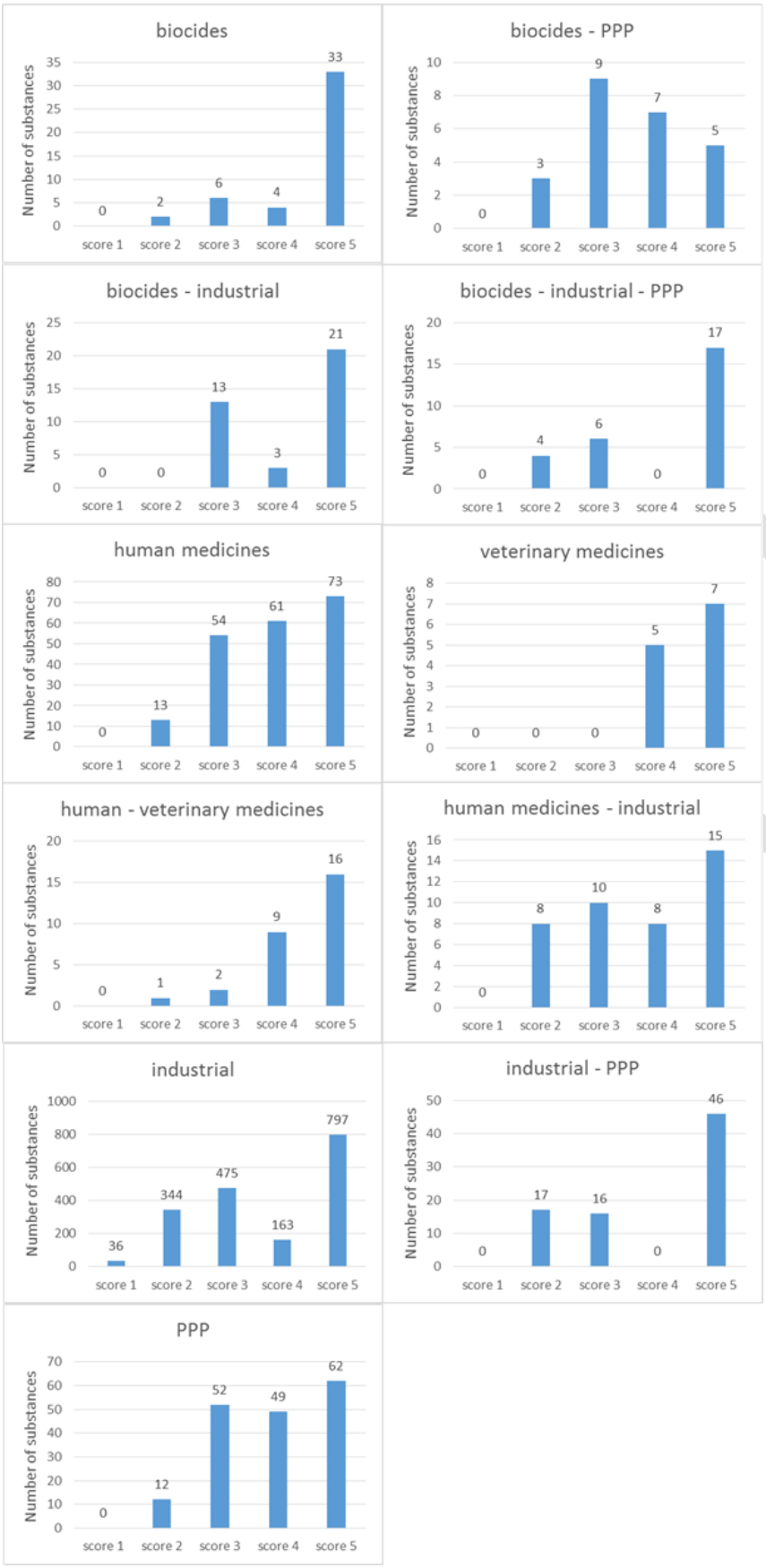


Figure 12. Number of substances distributed by type of use within screening risk scores.

6.4 Criteria for selection of substances for modelling

The selection of 53 substances, starting from the list of the 2556 having a screening risk score (i.e. 2790 substances from the whole list, excluding the 31 PS and the 203 substances from the monitoring exercise, as explained in 6.3.1.2), and from the list of remaining 3733 substances lacking the exposure score (but with available hazard properties, as explained in the section 6.3), has been done in three steps:

Step 1. 415 substances were preselected according to the criteria detailed in Figure 13.

Step 2. From these 415 substances and 29 substances added from the monitoring exercise (listed in Table 14), 131 substances were selected according to the criteria detailed in Figure 14.

Step 3. A further set of criteria, described in section 6.4, was applied, and resulted in a list of 53 substances.

Figure 13 shows the criteria applied in Step 1. All these criteria were applied independently from the screening risk score and independently from each other: all substances that matched at least one the criteria 1a-4a, were preselected for the Step 2.

The Criterion 1a was based on the number of MSs (≥3) having available monitoring data about the substances. This was done to ensure selection of substances for which measured environmental concentrations were available as supportive information, to be able to compare with the predicted environmental concentrations (PEC).

Criteria 2a-4a were driven by the hazard properties, independently from the exposure. The Criterion 2a was driven by the PBT or vPvB properties. The Criterion 3a was driven by properties such as PB or BT or PT, in combination with at least one of the following: C, M, R or ED (i.e. known/proven PB or BT or PT properties, and at least one of C, M, R, ED property is at least suspected). The criterion 4a was based on the substance having ED properties (proven or suspected ED), and at least one additional suspected/known hazard property: P, B or T, or C, M or R.

Criterion 2a, 3a and 4a were included to ensure selection of substances having hazard properties of concern (such as ED or suspected ED properties) even if the information about their exposure is lacking or the exposure score is low.

The Annex II reports the list of the 415 substances obtained after Step 1.

In the Step 2, the number of 415 substances was further refined. First, substances excluded from the monitoring exercise after applying the PNECQC criteria (Sc2_PNEC QC; for details see: *Carvalho et. al, Monitoring based exercise report, 2016*), were added to the list of 415 substances obtained in the Step 1. These substances are shown in Table 14.

As shown in the Figure 14, first all substances from STE exercise with STE risk rank equal to 1-3 (16 substances), were included directly in the final list of 131 substances (criterion 0b). For all other substances, including those from the monitoring exercise with STE risk rank equal to 4 or 5 (13 substances), 3 different criteria (1b-3b) were applied. These criteria were applied independently of each other because they were deemed having the same weight for the decision, and are explained in Figure 14. All substances that matched at least one of these criteria, were selected to the Step 3.

The Annex III reports the list of 131 substances obtained after Step 2.

In the Step 3 the 131 substances were finally further scrutinised (see Section 6.5 for the details) to get out the proposal list of 53 potential candidate substances, which includes only approved substances. The Table 16 shows the proposed list.

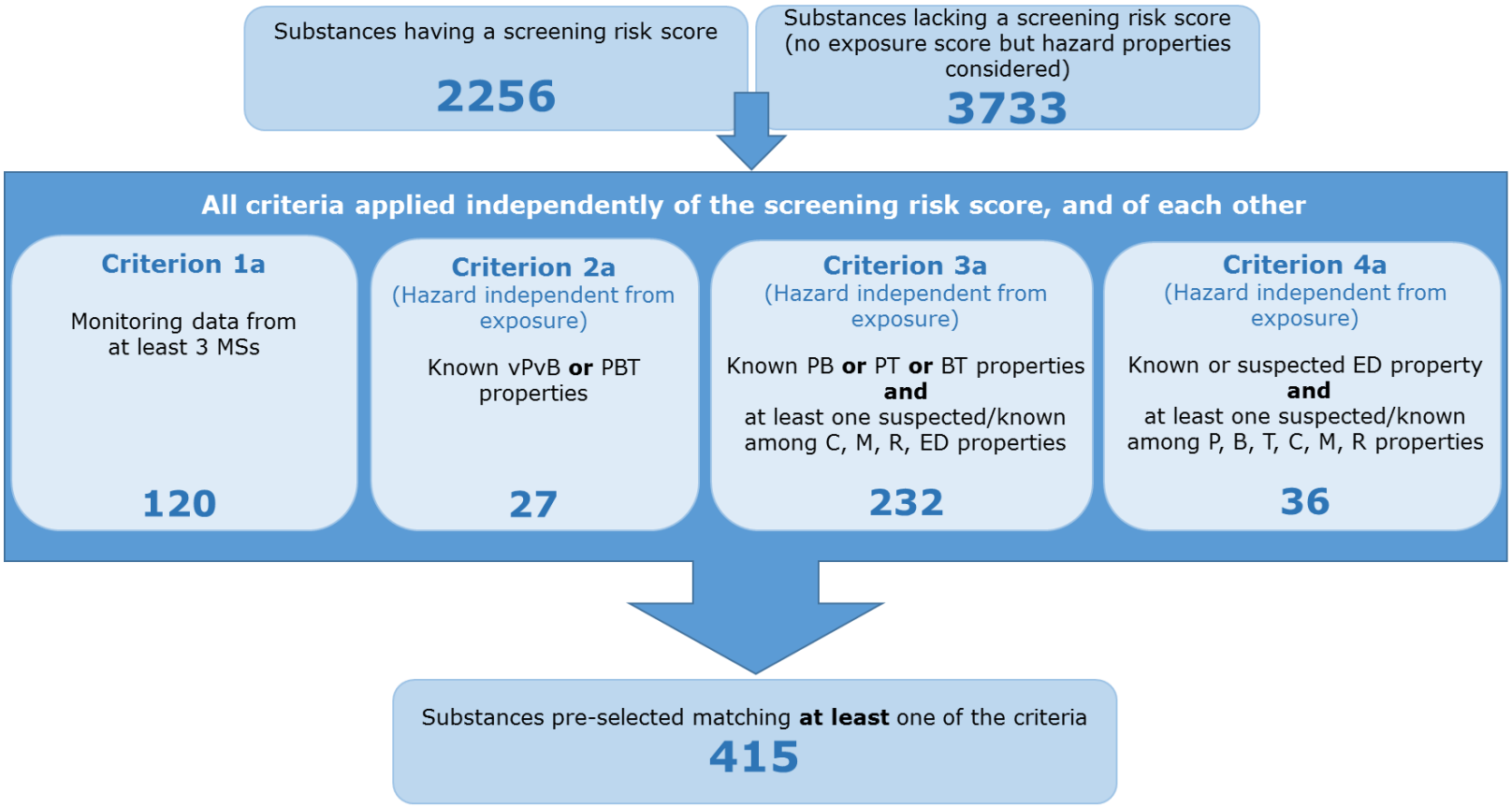


Figure 13: **Criteria for the pre-selection of 415 substances (Step 1)**

Starting from a list including 6289 substances, 120 of them were identified as monitored in at least 3 MSs (Criterion 1a). The remaining substances were assessed for their hazard properties of being PBT or vPvB (Criterion 2a, 27 substances were selected). If this criterion was not fulfilled, substances were evaluated to be characterised by having at least one of the properties such as PB or BT or PT, in combination with at least one of the following: C, M, R or ED (Criterion 3a, 232 substances were selected). Finally, if substances didn't match any of the criteria 1a-3a, their ED property and one of the other properties (P, B, T, C, M, R) were checked (Criterion 4a, 36 substances were selected). All the criteria were analysed independently of each other.

Abbreviations: MS (Member State), **PBT** (Persistent, Bioaccumulative, Toxic), **vPvB** (very Persistent, very Bioaccumulative), **P** (Persistent), **B** (Bioaccumulative), **T** (Toxic), **C** (Cancerogenic), **M** (Mutagenic), **R** (Reprotoxic), **ED** (Endocrine Disruptor)

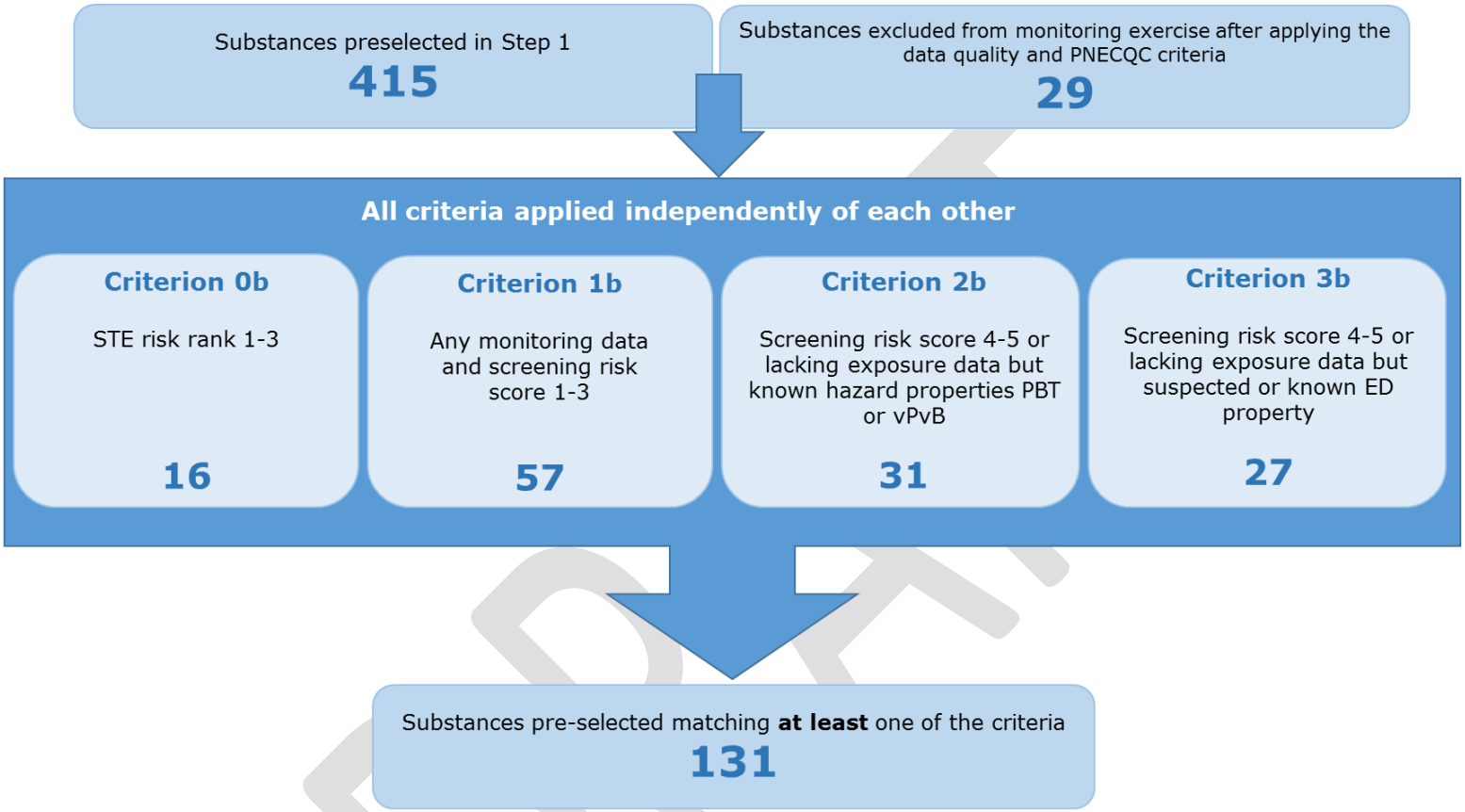


Figure 14: Criteria for the selection of the 131 substances (Step 2)

First, all substances from STE exercise with STE risk rank equal to 1-3 (16 substances), were included in the final list of 131 substances (criterion 0b). For all other substances, including those from STE exercise with STE risk rank equal to 4 or 5 (13 substances), 3 different criteria (1b-3b) were applied. The substances were analysed to check if the monitoring data were available and if they had a screening risk score between 1-3 (Criterion 1b, 57 substances were selected). Substances characterised by having a screening risk score higher than 3 or lacking exposure data, but proven hazard properties PTB or vPvB (corresponding to a hazard score ≥2), were also scrutinised (Criterion 2b, 31 substances were selected). If substances had a screening risk score higher than 3 or lacking exposure data and did not show PTB/vPvB characteristics, they were evaluated for having a suspected/known ED property (corresponding to a hazard score ≥1) (Criterion 3b, 27 substances were selected). All the criteria have been analysed independently of each other.

Abbreviations: PBT (Persistent, Bioaccumulative, Toxic), **vPvB** (very Persistent, very Bioaccumulative), **ED** (Endocrine Disruptor), **STE** (Spatial Temporal Extent)

Table 14: Substances which have been excluded from monitoring exercise after the data quality and PNECQC criteria were applied, and which have been included in the Step 2 of selection. The substances in red text were directly included in the final list of 131 substances based on their STE risk rank equal to 1-3 (criterion 0b). The other substances were scrutinized according to the criteria 1b-3b (Figure 14) and put in the final list of 131 substances only if at least one of the criteria was fulfilled.

CAS	Substance	Type	STE	STE Risk Rank	PNEC	Count MSs	Count sites	Count samples	Status
52918-63-5	Deltamethrin	PPP; veterinary medicine	3.00	1	3.10E-06	3	91	173	Approved
57-74-9	Chlordane	PPP	3.00	1	5.00E-05	3	20	37	Not approved in EU
60168-88-9	Fenarimol	PPP	3.00	1	2.00E-05	3	16	40	Banned
106-93-4	1,2-Dibromoethane	Industrial; solvent	3.00	1	0.002	5	10	18	Banned
950-37-8	Methidathion	PPP	2.75	1	0.0022	3	8	9	Banned
66230-04-4	Esfenvalerate	PPP	2.52	1	1.00E-04	2	26	87	Approved
563-12-2	Ethion	PPP	2.41	1	0.00056	3	44	105	Banned
83121-18-0	Teflubenzuron	PPP	2.28	2	0.0012	1	1	9	Approved
56-72-4	Coumaphos	PPP	2.18	2	7.00E-04	2	16	30	Approved for veterinary use
24017-47-8	Triazophos	PPP	2.17	2	0.001	2	67	157	Banned

82097-50-5	Triasulfuron	PPP	2.11	2	0.0032	2	2	3	Approval expired on 31 June 2016. The substance could be used until 30 September 2017
52-68-6	Trichlorfon	PPP	2.00	2	0.00057	3	28	56	Banned
150-68-5	Monuron	PPP	1.67	3	0.0065	3	25	95	Banned
90-13-1	1-Chloronaphthalene	Industrial; solvent	1.55	3	0.01	3	180	627	Banned
2385-85-5	Mirex	PPP	1.33	3	0.001	2	39	654	It is not possible to export this chemical; regulated under the Stockholm convention
35367-38-5	Diflubenzuron	PPP; Biocide	1.22	3	0.004	2	13	218	Approved
68359-37-5	Cyfluthrin	PPP	1.17	4	0.001	3	163	897	Banned
298-04-4	Disulfoton	PPP	1.14	4	0.004	3	90	741	Not approved in EU
57-63-6	17-alpha-Ethinylestradiol	Human medicine	1.12	4	3.50E-05	2	39	146	Approved
14816-18-3	Phoxim	PPP	0.93	4	0.008	3	1333	13983	Not approved in EU
1163-19-5	BDE-209 (Decabromodiphenyl ether)	Flame retardant	0.51	5	0.046	2	2278	31479	Approved; SVHC substance
3397-62-4	Desisopropyldesethylatrazine	PPP metabolite	0.43	5	0.01	3	143	941	n. a.

102851-06-9	Tau-fluvalinate	PPP	0.40	5	0.0021	2	6	61	Approved
301-12-2	Oxydemeton-methyl	PPP	0.25	5	0.035	3	602	3316	Banned
79-11-8	Chloroacetic acid	Industrial	0.25	5	0.6	3	462	2514	Approved
67306-00-7	Fenpropidin	PPP	0.12	5	0.0032	3	69	796	Approved
145701-23-1	Florasulam	PPP	0.06	5	0.0126	3	123	1039	Approved
173159-57-4	Foramsulfuron	PPP	0.04	5	0.036	3	42	1577	Approved
98-87-3	Dichlorotoluene (alpha, alpha)	Industrial	0.00	5	0.034	2	144	1336	Approved

1029
1030

6.5 Draft list of substances for PEC derivation

To draft the list of substances for which a PEC could be derived and to calculate the Risk Quotient (PEC/PNEC), the 131 substances were then further scrutinised.

The further selection aimed to reach a reasonable number of substances for PEC derivation; during the 5th SG-R meeting, it was agreed to focus only on 10 or less substances. As also agreed at the meeting, the substances that were not approved/banned, were excluded from the final list. Therefore, from 16 substances with an STE risk rank 1-3 (Table 14), only 6 were directly included in the final list as shown in the Table 15. These substances were excluded from the STE exercise after the application of data quality and PNEC quality criteria (Sc2_PNEC QC).

For all other substances from the list (Annex III) their approval status was checked, and in case of not approval/ban, they were excluded from the further evaluation.

The remaining substances were further scrutinised (Table 15), assessed one by one, and the hazard properties were the main driver for the further selection of the substances. The substances were thus selected for PEC derivation if at least one the following criteria, as also shown in Figure 15, was met:

0c - STE risk rank from 1 to 3

1c - proven ED

2c - at least two of the following hazard properties: P, vP, B, vB, T

3c - substance of high concern

4c - substance of very high concern

5c - at least one proven hazard property among C, M or R and one suspected property among C, M or R.

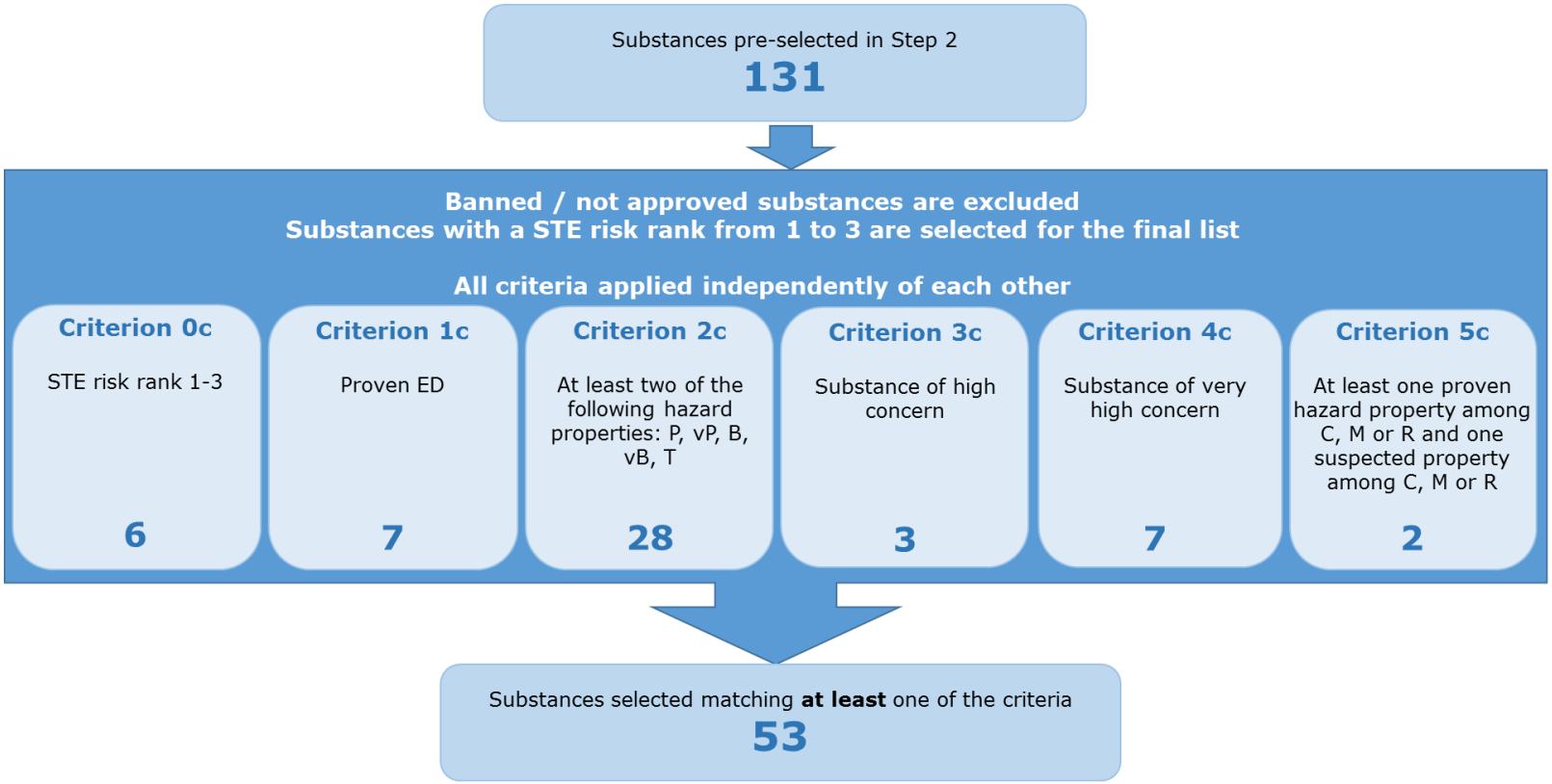


Figure 15: Criteria for the selection of the 53 substances (Step 3)

Starting from the list of 131 substances, those which are banned / not approved were excluded, and those with and STE risk rank between 1 and 3 (criterion 0c, 6 substances) were directly selected for the final list. Then criteria 1c-5c were applied, independently, to complete the final list. Substances reported as proven endocrine disruptors (criterion 1c) were selected (7 substances). Substances were also selected if at least two of the following hazard properties (criterion 2c) were fulfilled: P, vP, B, vB, T (28 substances were selected). Substance were also selected if classified as of high concern (criterion 3c, 3 substances were selected) or of very high concern (criterion 4c, 7 substances were selected). If none of the aforementioned criteria were fulfilled, substances were finally checked and selected if at least one proven hazard property as C, M or R and one suspected property among C, M, R were fulfilled (criterion 5c, 2 substances were selected).

Abbreviations: PBT (Persistent, Bioaccumulative, Toxic), **vPvB** (very Persistent, very Bioaccumulative), **CMR** (Carcinogenicity, Mutagenicity, Reprotoxic), **STE** (Spatial Temporal Extent)

These criteria are identified in the Table 16.

This final list includes a total number of 53 substances (Table 16).

Concerning the distribution per classes (classes are counted separately for substances having multiple class), the PPP represents roughly 34% of the selected substances, human medicine 29%; industrial 16 %, biocides 11% and veterinary medicine 10%.

Table 15. The table summarises the number of substances selected for PEC derivation

Criterion used in selection in Step 2	No. of substances selected in Step 2	No. of substances selected for possible PEC in Step 3
0b	16	6
1b	57	28
2b	31	13
3b	27	6

Table 16. The table shows the 53 substances selected in Step 3 as potential substances to derive the PEC. The last column on the right summarizes if the PEC was derived and if PNEC was available to calculate the RQ (ratio PEC/PNEC). Substances that were excluded from the monitoring exercise which used PNEC QC methodology, are reported here with monitoring data taken from scenario 2. This allowed to have STE scores that could be used as supporting information during the final selection of the substances from the modelling exercise. Additional monitoring data were added for some substances (Deltamethrin, Triclosan, Gemfibrozil, Triallate and Mestranol), found after 5th meeting of SG-R.

CAS	Substance name	Monitored No. MSs	Monitored No. Sites	Monitored No. Samples	Class	SCREENING SCORE	Concern	Exposure SCORE	Class of Hazard SCORE	Status	P	B	T	vP	vB	C	M	R	ED	Criteria used in Step 3	Modelling	Drinking water
#52918-63-5	Deltamethrin	7	2766	28842	Human medicine Veterinary medicine Biocide (ECHA) Plant protection product	2		3	2	Approved	0.1	1	0.1	0	0	0.25	0.25	0.25	1	0c	Derived PEC / PNEC available	
#66230-04-4	Esfenvalerate	4	1152	8661	Biocide (ECHA) Plant protection product	4		1	2	Approved	0	1	1	0	0	0.5	0	0.25	0.25	0c	Derived PEC / PNEC available	
#83121-18-0	Teflubenzuron	4	822	6970	Veterinary medicine Plant protection product	No exposure	high concern		2	Approved	1	1	1	0	0	0.25	0	0	0.25	0c	Derived PEC / PNEC available	
#56-72-4	Coumaphos	6	1329	15312	Plant protection product Veterinary medicine	No exposure			0	Approved for veterinary use	0.1	0	0.1	0	0	0.25	0.25	0.25	0.25	0c	Derived PEC / PNEC available	
#82097-50-5	Triasulfuron	4	831	6580	Plant protection product				1	Approval expired on 31 June	0	0	1	0	0	0	0.25	0.25	0.25	0c	Derived PEC / PNEC available	

										2016. The substance could be used until 30 September 2017												
#35367-38-5	Diflubenzuron	4	415	4725	Veterinary medicine Biocide (ECHA) Plant protection product	5		1	0	Approved	0	0	1	0	0	0	0	0	0.25	0c	Derived PEC / PNEC available	
#54-31-9	Furosemide	4	72	864	Human medicine	2		3	2	not regulated except for Doping (veterinary and human)	0.1	0	1	0	0	0.5	0.5	1	0.25	5c	Derived PEC / no PNEC available	
#3930-20-9	Sotalol	10	342	4743	Human medicine	3		2	2	not applicable	1	0	1	0	0	0.25	0.25	0.25	0.25	2c	PNEC not available	Drinking water relevant
#120-47-8	Ethyl 4-hydroxybenzoate	1	147	664	Industrial (ECHA)	3	very high concern	conf	conf		conf	conf	conf	conf	conf	conf	conf	conf	conf	4c	PNEC not available	
#125116-23-6	Metconazole	3	702	5742	Plant protection product	2		3	2	Approved	1	0	1	1	0	0.25	0.25	0.5	0.25	2c	Derived PEC / PNEC available	
#131807-57-3	Famoxadone	3	623	5528	Plant protection product	3		3	1	Approved	0	1	1	0	0	0	0	0.25	0.25	2c	Derived PEC / PNEC available	

#137-26-8	Thiram	3	217	3546	Industrial (ECHA) Biocide (ECHA) Plant protection product	2		4	2	approved	0.1	0	1	0	0	0.25	0.25	0.25	1	1c	Derived PEC / PNEC available	
#189278-12-4	Proquinazid	1	31	1285	Plant protection product	3		2	2	Approved	1	1	1	1	0	0.5	0	0.25	0.25	2c	Derived PEC / PNEC available	
#1918-02-1	Picloram	3	418	2740	Plant protection product	3		2	2	Approved	1	0	1	1	0	0.75	0	0.25	1	2c	Derived PEC / PNEC available	
#220899-03-6	Metrafenone	3	75	1852	Plant protection product	3		3	1	Approved	1	0	0	1	0	0.25	0	0.25	0.25	2c	Derived PEC / PNEC available	
#25812-30-0	Gemfibrozil	12	364	2632	Human medicine	2		2	3	not applicable	1	1	1	0	0	0.5	0.25	0.5	0.25	2c	Derived PEC / PNEC available	
#50-18-0	Cyclopho-sphamide	3	153	764	Human medicine	2		2	3	not applicable	0.1	0	1	0	0	1	0.75	1	1	5c	Derived PEC / PNEC available	
#64902-72-3	Chlorsulfuron	3	1239	15973	Plant protection product	3		2	2	Approved	1	0	1	0	0	0.5	0	0.25	0.25	2c	Derived PEC / PNEC available	
#657-24-9	Metformin	2	103	2090	Human medicine	2		4	2	not applicable	1	0	1	0	0	0.25	0.25	0.25	1	1c	Derived PEC / PNEC available	Drinking water relevant
#67-43-6	Diethylene-triaminepen-taacetic acid	2	533	7130	Industrial (ECHA)	2	high concern	conf	conf	not regulated	conf	conf	conf	conf	conf	conf	conf	conf	conf	3c	PNEC not available	Drinking water relevant

#80844-07-1	Etofenprox	3	91	1116	Biocide (ECHA) Plant protection product	3		3	1	Approved	0	1	1	0	0	0	0	0.5	0.25	2c	Derived PEC / PNEC available	
#84-61-7	Dicyclohexyl phthalate (DCHP)	1	47	358	Industrial (ECHA)	2	very high concern	conf	conf	not regulated	conf	conf	conf	conf	conf	conf	conf	conf	conf	4c	PNEC not available	
#99-99-0	4-Nitrotoluene	3	148	1112	Industrial (ECHA)	2	very high concern	conf	conf	not regulated	conf	conf	conf	conf	conf	conf	conf	conf	conf	4c	PNEC not available	
#96-45-7	Ethylene Thiourea (ETU)	1	1	9	Industrial (ECHA)	2		3	3	Not regulated	1	0	1	0	0	0.5	0.25	0.75	1	1c	PNEC not available	
#137-58-6	Lidocaine	2	27	471	Human medicine	2		3	2	not applicable	1	0	1	0	0	0.25	0.25	0.5	0.25	2c	PNEC not available	
#79902-63-9	Simvastatin	1	16	98	Human medicine	2		3	3	not applicable	1	1	1	0	0	0.5	0.25	0.5	0.25	2c	PNEC not available	
#149961-52-4	Dimoxystrobin	1	720	6078	Plant protection product	2		3	2	Approved	1	0	1	0	0	0.5	0	0.5	0.25	2c	Derived PEC/ PNEC available	
#116539-59-4	Duloxetine	1	60	983	Human medicine	3		2	2	not applicable	1	0	1	0	0	0.25	0.25	0.5	0.25	2c	PNEC not available	
#443-48-1	Metronidazole	1	4	86	Human medicine	3		2	2	not applicable	1	0	1	0	0	0.75	0.5	0.5	0.25	2c	PNEC not available	
#112281-77-3	Tetraconazole	2	1132	11075	Plant protection product	3		3	1	Approved	1	0	1	1	0	0	0	0.5	0.25	2c	Derived PEC/ PNEC available	
#134098-61	Fenpyroximate	1	35	1506	Plant protection product	3		2	2	Approved	1	1	1	0	0	0	0	0	0.25	2c	Derived PEC/ PNEC available	
#79538-32-2	Tefluthrin	1	441	2879	Plant protection product	3		2	2	Approved	1	1	1	0	0	0.25	0.25	0.25	0.25	2c	Derived PEC/ PNEC available	

#75-56-9	Methyloxirane (Propylene oxide)				Industrial (ECHA)	1	very high concern	conf	conf	regulated	conf	conf	conf	conf	conf	conf	conf	conf	conf	4c	PNEC not available	
#57-63-6	17-alpha-Ethinylestra-diol	4	48	180	Human medicine Veterinary medicine	4		1	2	not applicable	0.1	0	1	0	0	0.5	0.25	1	1	1c	Derived PEC/ PNEC available	Drinking water relevant
#81103-11-9	Clarithromycin	3	415	4997	Human medicine	2		3	2	not applicable	1	0	1	0	0	0.25	0.25	0.25	0.25	2c	PEC available (watch list) / PNEC available	Drinking water relevant
#3380-34-5	Triclosan	10	686	5430	Industrial (ECHA) Human medicine Biocide (ECHA)	2	high concern	conf	conf	Restricted	conf	conf	conf	conf	conf	conf	conf	conf	conf	3c	Derived PEC/ PNEC available	
#2303-17-5	Triallate	3	1915	18559	Plant protection product	No exposure	high concern		2	Approved	1	1	1	0	0	0	0	0.25	0.25	3c	PEC available / PNEC available	
#131-18-0	Di-n-pentylphtha-late (DPP) = Dipentyl-phthalate	1	73	463	Industrial	5		0	3	Included in the candidate list of very high concern substances	0.1	1	1	0	0	0.25	0.25	0.75	1	1c	PNEC not available	
#136426-54-5	Fluquinconazole	3	1188	16051	Plant protection product	4		1	2	Approved	1	0	1	1	0	0.5	0	0.25	0.25	2c	Derived PEC/ PNEC available	

#139968-49-3	Metaflumizone				Plant protection product	No exposure			2	Approved	1	1	1	1	1	0	0.25	0.5	0.25	2c	Derived PEC/ PNEC available	
#68-22-4	Norethisterone	1	19	20	Industrial (ECHA) Human medicine	No exposure	very high concern	conf	conf	not applicable	conf	conf	conf	conf	conf	conf	conf	conf	conf	4c	Derived PEC / PNEC available	
#72-33-3	Mestranol	2	172	731	Human medicine	No exposure			3	not applicable	0.1	1	1	0	0	0.5	0.5	1	1	1c	PNEC not available	
#77-09-8	3,3'-Bis(4-hydroxyphenyl)phthalid | Phenolphthaleine				Industrial (ECHA) human medicine	4	very high concern	conf	conf	not regulated	conf	conf	conf	conf	conf	conf	conf	conf	conf	4c	PNEC not available	
#82657-04-3	Bifenthrin (@Talstar)	3	1132	7572	Biocide (ECHA) Plant protection product	No exposure			3	Approved	1	1	1	0	0	0.5	0	0.25	1	1c	Derived PEC/ PNEC available	
#93413-69-5	Venlafaxine	1	93	1395	Industrial (ECHA) update Human medicine	No exposure	very high concern	conf	conf	not applicable	conf	conf	conf	conf	conf	conf	conf	conf	conf	4c	Derived PEC / PNEC available	
#95233-18-4	Atovaquone				Human medicine	4		1	2	not applicable	1	1	1	0	0	0.25	0.25	0.25	0.25	2c	PNEC not available	
#71125-38-7	Meloxicam				Human medicine Veterinary medicine	4		1	2	not applicable	1	0	1	0	0	0.25	0.25	1	0.25	2c	PNEC not available	
#210631-68-8	Topramezone				Plant protection product	4		1	2	pending	1	0	1	1	0	0.5	0	0.75	0.25	2c	Derived PEC/ PNEC available	

#96489-71-3	Pyridaben	2	785	5395	Plant protection product	4		1	2	approved	1	1	1	0	0	0	0	0.25	0.25	2c	Derived PEC/ PNEC available	
#113-15-5	Ergotamine				Human medicine	5		0	3	not applicable	1	1	1	0	0	0.25	0.25	0.5	0.25	2c	PNEC not available	
#437-38-7	Fentanyl				Human medicine	5		0	2	not applicable	1	0	1	0	0	0.25	0.25	0.5	0.25	2c	PNEC not available	
#28772-56-7	Bromadiolone	2	793	5368	Biocide (ECHA) Plant protection product	5		0	2	not applicable	0	1	1	0	0	0.25	0	1	0.25	2c	Derived PEC/ PNEC available	
#51630-58-1	Fenvalerate	1	9	70	Veterinary medicine	No exposure			2	not applicable	0.1	1	1	0	0	0.25	0.25	0.25	0.5	2c	PNEC not available	

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Substances with screening score of 1

The substances ranked high (obtained screening risk score of 1) were mainly petroleum products (PP) with high tonnage. They were excluded for two reasons.

1. PPs are combusted and most of the reported tonnage is turned into $C0_2$ and water[6].

The residual non-combusted PPs (non or partially burned hydrocarbons such as volatile organic compounds, VOCs) are released almost exclusively into the atmosphere (93% in the case of Benzene, the most abundant VOC from vehicle exhausts [56], and are degraded quickly (Chemical degradation reactions, primarily reaction with hydroxyl radicals, limit the atmospheric residence time of benzene to only a few days, and possibly to only a few hours (http://www.atsdr.cdc.gov/toxprofiles/tp3-c6.pdf.)

2. The risk from surface/groundwater contamination from small amount of the various non combusted PPs on our initial screening list is already sufficiently addressed [7] through a series of substances that are subject to the existing WFD monitoring (Directive 2008/105/EC), and which are part/indicators for those PP fractions, i.e benzene, fluoranthene, pyrene, benzo[b]fluoranthene and benzo[a]pyrene.

7 Risk assessment phase - PEC and RQ derivation

From the substances listed in Table 16, only those having available PNEC (or EQS) value (or available data for derivation of PNEC value by JRC), i.e. 33 substances (Table 17) were selected for the modelling exercise to derive the PEC and then the Risk Quotient (RQ, PEC / PNEC) calculation.

Whenever monitoring data for these substances were available, even if they failed to pass the minimum representativeness criteria in the parallel monitoring-based prioritisation exercise (i.e. the number of monitoring MSs, and usually also number of samples and sites), the measured

[6] The International Energy Agency (IEA) published the sectorial use of petroleum consumption in 2011 as 61.5 % transportation, 20, 9% industrial (e.g. as fuel) and 12.4% heating and electricity generation and agriculture, all of which is combusted. The remaining 17.1% is used as a raw material for chemicals and pharmaceuticals, etc., and is transformed into other chemical classes or inert products such as polymers (http://worldoceanreview.com/en/wor-3-overview/oil-and-gas/sating-our-energy-hunger?)

[7] For information: The predominant PAH from in the exhaust from various biomass fuels are fluoranthene, pyrene, benzo[a]anthracene, chrysene, benzo[b]fluoranthene and benzo[a]pyrene. The most abundant VOCs from vehicle exhausts and biomass combustion (in the order of their abundance) are benzene, toluene, ethyl benzene and xylene followed by 1,2,4- and 1,3,5- trimethylbenzene, styrene and 1,4-dichlorobenzene. (Gadi et al 2010)[56]

environmental concentration (MEC, the 95th percentile of the monitoring data) and MEC Risk Quotient (RQ MEC, MEC / PNEC ratio) were calculated.

Then the substances were ranked by the obtained value of RQ PEC, and compared with RQ MEC. For these substances, a comparison between the modelled risk and available monitoring data and is given in Table 17.

The list of top 10 substances was circulated to the SG-R for comments. Meanwhile, four substances listed below, having a high modelled risk quotient (RQ PEC), and monitoring data from at least 3 MSs (Sc2) and high STE score, were selected to collect additional data from literature and the preparation of factsheets (including statistical analysis of the monitoring data, see Annex IV).

1) Deltamethrin shows very high risk quotient using both PEC and MEC (Table 17), and a STE score of 3. Almost 29000 monitoring data in 7 MSs are available with almost all of them below Limit of Quantification (LOQ, range 0.00006-0.1) or Limit of Detection (LOD; range 0.00002-0.01). 206 quantified samples are available from 3 MSs; the data quality of these quantified samples was checked and was very good for 128 samples of one country, but worse for the other two countries because many identical values were reported which could possibly be false positive non-quantified measurements. After suggestion from stakeholders, the PEC value was refined to a lower value of 0.03 μg/L. PNEC value has been also refined to a value of 0.00007 μg/L proposed tentative EQS_{fw} in the draft dossier prepared by JRC. The derived Risk Quotient (RQ, PEC/PNEC), using the lower values (PEC =0.03 μg/L and PNEC= 0.00007 μg/L) is still very high (RQ PEC = 429), see Table 18.
2) Bifenthrin (@Talstar) has high RQ PEC, corresponding to 2705. The RQ MEC of Sc2 is 1250, but should be carefully considered, because only 2 quantified records are available in Sc2-PNECQC, and in Sc2 7040 records are marked as < LOQ and 530 records as < LOD. Refined PEC values from FOCUS step 4 (EFSA conclusion, 2011 [57]) has been used, leading to RQ PEC values ranging from 245 to 25, corresponding to the maximum and minimum PEC values respectively (see Table 18).
3) Esfenvalerate has high and similar values of RQ PEC and RQ MEC (i.e. 634 and 500, respectively, see Table 17), and a STE score of 2.56 (Sc2). The number of monitoring samples, from 4 MSs, is around 8600 with most of them below LOQ (range 0.003-0.1) but above LOD (range 0.0002-0.001). Most of the records were classified as "< LOQ" (between LOD and LOQ), which means that they were positively detected above the EQS (even though not quantified; the countries also gave "< LOD" values so that we concluded that the "< LOQ" records are not false positives). The stakeholders proposed a PNEC value of 0.0005 μg/L (based on inclusion of a mesocosm study, EFSA conclusion, 2014 [58]), which

is still under the SG-R experts' evaluation. By using the value of 0.0005 μg/L, the STE score would be still high (1.73). Applying refined PEC values from FOCUS Step 4 (EFSA conclusion, 2014 [58]),, the RQ PEC ranged from 54 to 8, corresponding to the maximum and minimum PEC values respectively (see Table 18), suggesting that the risk could be realistic (even applying a higher PNEC value of 0.0005 μg/L, the RQ PEC ranged from 11 to 1.5, see Table 18).

4) Teflubenzuron has a high RQ from modelling estimation and a much lower RQ from the monitoring exercise (i.e. 3847 and 21 respectively, see Table 17). The STE score of Sc2 is 2.28. The number of monitoring samples, from 4 MSs, is almost 7000 with almost all of them below LOQ (range 0.005-0.05) and none below LOD. Only 9 quantified samples from 1 MS are available. This substance was not put forward for EQS derivation, after SG-R comments, because the monitoring data were considered to be not sufficient, and therefore as EU-wide concern for freshwater is not proven.

Table 17: Summary table comparing the modelling and monitoring results. The PECs were chosen as the highest values among the different modelled scenarios for every substance. For monitored substances, the risk quotient was calculated using the measured concentration (MEC) of the 95th percentile of the monitored data. Caution should be taken when directly comparing the two risk quotients as the number of sample, sites and/or countries was not considered sufficient for proper statistical analysis of the monitoring data. Given that the tonnage for Triclosan is confidential, the highest value of the corresponding band was used for the calculation of the risk quotient and the STE score shown in the table is only referred to the 3 countries. For Thiram, since the PEC obtained using the tonnage band seemed not to be realistic, the PEC derived from FOCUS Step 3 has was considered for RQ PEC. All PECs from FOCUS Step 3, reported as grey cells, were taken from EFSA dossiers FOCUS Step 3 calculations (http://www.efsa.europa.eu). (*) Coumaphos is approved for veterinary use only.

CAS	SUBSTANCE	PEC µg/L FOCUS Step 3	PEC µg/L ECETOC	PEC µg/L Human pharma formula	PNEC µg/L	PNEC source	RQ PEC	RQ MEC p95	RQ PEC / RQ MEC p95	Monitoring No. MSs	Monitoring No. Sites	Monitoring No. Samples	No. Samples < LOD	No. Samples < LOQ	No. Quantified samples	Percentage of quantified samples	STE score
#52918-63-5	Deltamethrin	0.36	0.001		0.0000031	RBSP (NL)	116097	16129	7.2	7	2766	28842	2077	26559	206	0.71	3
#96489-71-3	Pyridaben	10.40			0.00047	JRC derivation	22132	53	416	2	785	5395	0	5395	0	0.00	2.41
#149961-52-4	Dimoxystrobin	16.42			0.0032	JRC derivation	5196	8	657	1	720	6078	0	5910	168	2.76	2.13
#83121-18-0	Teflubenzuron	4.62			0.0012	NL Specific Pollutants (RBSP)	3847	21	185	4	822	6970	0	6961	9	0.13	2.28
#35367-38-5	Diflubenzuron	13.62			0.0040	EU Report 2012	3406	6.25	545	4	415	4725	116	4607	2	0.04	2.09
#82657-04-3	Bifenthrin (@Talstar)	0.05			0.00002	INERIS 2014	2705	1250	2.2	3	1132	7572	530	7040	2	0.03	3
#80844-07-1	Etofenprox	8.3			0.0054	JRC derivation	1531	1.85	827	3	91	1116	119	987	10	0.90	1.52
#66230-04-4	Esfenvalerate	0.06			0.0001	NL Specific Pollutants (RBSP)	634	500	1.27	4	1152	8661	1460	7155	46	0.53	2.56
#82097-50-5	Triasulfuron	1.5			0.0032	EU Report 2012	484	15.6	31	4	831	6580	0	6577	3	0.05	2.18
#134098-61-6	Fenpyroximate	4.4			0.010	JRC derivation	440										

#137-26-8	Thiram	61.0	306		0.200	Value provided by Marion Junghans (Oekotoxzentrum; CH)	305	0.25	1219	3	217	3546	156	3378	12	0.34	0
#64902-72-3	Chlorsulfuron	2.9			0.024	Value provided by Marion Junghans (Oekotoxzentrum; CH)	119	1.04	114	3	1239	15973	143	15781	49	0.31	0.84
#2303-17-5	Triallate	41.9			0.410	Substance factsheet (2015)	102	0.06	1675	3	1915	18559	997	17491	71	0.38	0
#125116-23-6	Metconazole	5.9			0.0582	JRC derivation	101	0.43	235	3	702	5742	0	5739	3	0.05	0
#210631-68-8	Topramezone	3.7			0.100	JRC derivation	36.6										
#57-63-6	17-alpha-Ethinylestradiol			0.001	0.00004	Substance factsheet (2015)	28.0	15.7	1.78	4	48	180	7	169	4	2.22	1.44
#139968-49-3	Metaflumizone	0.3			0.01308	JRC derivation	22.8										
#3380-34-5	Triclosan		0.42		0.02	Substance factsheet (2015)	20.9	2.33	9.00	10	686	5430	88	3044	2298	42.32	0.98
#81103-11-9	Clarithromycin			1.76	0.13	Substance factsheet (2015)	13.6	1.38	9.79	3	415	4652	28	2681	1943	41.77	0.50
#131807-57-3	Famoxadone	1.8			0.14	JRC derivation	12.6	0.18	70	3	623	5528	0	5528	0	0.00	0
#189278-12-4	Proquinazid	1.3			0.18	Value provided by Marion Junghans (Oekotoxzentrum; CH)	7.28	0.06	131	1	31	1285	0	1285	0	0.00	0
#93413-69-5	Venlafaxine			0.20	0.038	JRC derivation	5.21	4.95	1.05	1	93	1395	0	324	1071	76.77	1.36

#112281-77-3	Tetraconazole	5.9			1.9	JRC derivation	3.10	0.03	118	2	1132	11075	0	11060	15	0.14	0
#136426-54-5	Fluquinconazole	2.5			1.54	JRC derivation	1.62	0.03	50	3	1188	16051	0	15996	55	0.34	0
#220899-03-6	Metrafenone	3.3			2.25	JRC derivation	1.47	0.02	66	3	75	1852	84	1583	185	9.99	0
#68-22-4	Norethisterone			0.01	0.0354	JRC derivation	0.31	0.10	3.19	1	19	20	0	0	20	100.00	0
#657-24-9	Metformin			267.60	1000	Swiss ecotox centre	0.27	0.00	56	2	103	2090	0	51	2039	97.56	0
#28772-56-7	Bromadiolone	0.00328			0.017	Value provided by Marion Junghans (Oekotoxzentrum; CH)	0.19	2.94	0.07	2	793	5368	76	5292	0	0.00	2.07
#25812-30-0	Gemfibrozil			0.16	0.8519	JRC derivation	0.19	0.01	13	12	364	2632	70	2438	124	4.71	0
#56-72-4	Coumaphos (*)	0.00007			0.0007	RBSP (DK) - ECOSTAT, UBA (2014)	0.10	35.7	0.00	6	1329	15312	237	15045	30	0.20	2.28
#50-18-0	Cyclophosphamide			0.20	2.5133	JRC derivation	0.08	0.0020	39	3	153	764	27	728	9	1.18	0
#79538-32-2	Tefluthrin	0.00001			0.00016	Value provided by Marion Junghans (Oekotoxzentrum; CH)	0.06	156	0.00	1	441	2879	0	2873	6	0.21	2.56
#1918-02-1	Picloram	3.0			55	Value provided by Marion Junghans (Oekotoxzentrum; CH)	0.06	0.0005	121	3	418	2740	0	2740	0	0.00	0

Table 18: Table of Risk Quotients for Predicted Environmental Concentration (RQ PEC). The first two columns are CAS and substances name. The third column is referring to how the PEC was derived. The fourth column reports the calculated PEC. Values are reported in black if they are derived from a worst case assumption (values from FOCUS Step 3, using the highest PEC), and in red if a refined approach is used (values from FOCUS Step 4 or a different proposal). The fifth column reports the PNEC values, in black the lowest available values (i.e. the most conservatives) while in red the refined ones (if available). The sixth column reports the RQ PEC: in black the ones derived from the worst case assumptions of PEC and PNEC, while in red those which are based on the refined values. Concerning the use of FOCUS Step 4, the maximum and the minimum values are reported as overall picture of the RQ PEC range. For Deltamethrin the refined PNEC value is a tentative EQS derived by JRC while for Esfenvalerate is the value proposed by the stakeholder. PEC values for Bifenthrin and Esfenvalerate are from EFSA conclusions, 2011 [57] and 2014 [58] respectively.

CAS	SUBSTANCE	PEC derivation	PEC µg/L	PNEC µg/L	RQ PEC
#52918-63-5	Deltamethrin	FOCUS Step 3	0.3599	0.0000031	116097
#52918-63-5	Deltamethrin	BAYER proposal	0.03	0.00007	429

CAS	SUBSTANCE	PEC derivation	PEC µg/L	PNEC µg/L	RQ PEC
#82657-04-3	Bifenthrin	FOCUS Step 3	0.0541	0.00002	2705
#82657-04-3	Bifenthrin	FOCUS Step 4 max	0.0049	0.00002	245
#82657-04-3	Bifenthrin	FOCUS Step 4 min	0.0005	0.00002	25

CAS	SUBSTANCE	PEC derivation	PEC µg/L	PNEC µg/L	RQ PEC
#66230-04-4	Esfenvalerate	FOCUS Step 3	0.0634	0.0001	634
#66230-04-4	Esfenvalerate	FOCUS Step 4 max	0.00539	0.0001	54
#66230-04-4	Esfenvalerate	FOCUS Step 4 min	0.000774	0.0001	8
#66230-04-4	Esfenvalerate	FOCUS Step 4 max	0.00539	0.0005	11
#66230-04-4	Esfenvalerate	FOCUS Step 4 min	0.000774	0.0005	1.5

8 Final Ranking

Risk quotients (RQ_{fw}) for the respective group of substances considered, i.e. human pharmaceuticals, veterinary pharmaceuticals, biocides, inorganic compounds, generic industrial uses and PPPs were established. Measured Environmental Concentrations (MEC), whenever available, were used as a decision-supporting information for the identification of substances of high concern.

9 Conclusion

The PEC has been derived and RQ has been proposed for 33 substances. Factsheets were prepared for four substances: Deltamethrin, Bifenthrin (@Talstar), Esfenvalerate and Teflubenzuron.

Factsheets gather detailed information on the chemical identity of each substance, existing evaluations and regulatory (use) status, proposed environmental quality standards, major use, environmental behaviour and effects (toxicity), modelled concentrations, measured environmental concentrations, detailed STE results analysis/data statistics, monitoring data from the literature when available, and analytical methods in order to support decision on a possible prioritisation.

The four substances were selected because of the high PEC Risk Quotient (RQ, PEC / PNEC), the availability of monitoring data from at least 3 MSs, the high STE score and the similarity between the Risk Quotients of PEC and Measured Environmental Concentration (MEC), this similarity supports the RQ PEC.

Teflubenzuron was finally excluded for EQS derivation after feedback received from the SG-R group.

In the final 6th meeting, the SG-R group agreed on the selection of Deltamethrin, Bifenthrin and Esfenvalerate for EQS derivation.

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12 Annexes

ANNEX I: **Substances with the screening risk score.**

This annex contains a list with details of 2790 substances for which enough information was found for the calculation of both the exposure and the hazard score, thus the screening risk score could be calculated. This list includes 31 Priority Substances (PS) and 203 substances from the monitoring exercise for validation purpose of the screening phase procedure.

ANNEX II: Pre-selected substances for the modelling exercise – Step 1

This annex contains a pre-selection of 415 substances using criteria 1a-4a (see Figure 13 for more details). Substances selected by these criteria are from annex I (excluding PS and the 203 substances of the monitoring exercise) and the remaining substances, from the initial list (which lack the exposure score).

ANNEX III: Pre-selected substance for the modelling exercise – Step 2

This annex contains the selection of 131 substances using criteria 0b-3b (see Figure 14 for more details) for the modelling exercise. Substances selected by these criteria are from annex II and from the monitoring STE exercise.

ANNEX IV: factsheets for substances selected by the modelling exercise

This annex contains the factsheets of Esfenvalerate, Deltamethrin, Bifenthrin and Teflubenzuron.