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Monitoring-based Exercise: Second Review of the Priority Substances List under the Water Framework Directive

Monitoring-based exercise

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Abstract

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1. Introduction

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 is defined in terms of compliance with European environmental quality standards (EQS) for priority substances (PS).

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 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), and included 33 PS or 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 an assessment of existing PS and PHS, and also a review of candidate substances for consideration as new PS.

The first review process was done between 2007 and 2011, resulting in 12 new PS or PS groups being added to the list, 6 of which are identified as PHS, as published in Directive 2013/39/EU amending Directive 2008/105/EC. During that review, the information (and EQS) on existing PS was also updated and the results of the hazard assessment led to the reclassification of 2 PS as PHS.

As it stands, the list of PS in Annex I of Directive 2013/39/EU (replacing former Annex 10 of the WFD) contains a total of 45 PS or PS groups, with 21 classified as PHS.

The next Commission proposal for the review of the PS list will have to be completed by the beginning of 2018 (6 years after the 2012 proposal).

As the basis for the development of the approach for the review of the PS list, the Joint Research Centre (JRC) used the documents summarising the procedures followed in the first review of PS, namely the output of the monitoring-based exercise (James, 2009) and the final report on the modelling-based exercise (Daginnus et al. 2010), as well as the proposals for the 2nd review process described in the scoping report which was presented at the 2nd Meeting of WFD CIS Working Group Chemicals (17-18 March 2014).

1.1. 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 (see Table 1).

Throughout the process, the experts have provided valuable information for the risk-based analysis of the substances under consideration. Furthermore, the experts have been informed of the progress in the implementation of the methodology.

Table 1. 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	Monitoring-based exercise milestone
Kickoff meeting 4-5 September 2014 (Ispra, IT)	Presentation of the STE approach for the risk-based ranking of substances and selection of potential candidate substances in the monitoring-based prioritisation exercise.
2nd Meeting 22-23 January 2015 (Ispra, IT)	Case study of the application of the STE approach to selected substances from the previous prioritisation exercise. Proposal for testing the robustness of the STE approach using different scenarios of data quality, in particular to verify the independence of the STE factors.
3rd Meeting 17-18 September 2015 (Ispra, IT)	List of substances included in the monitoring-based exercise presented, as well as a draft list of EQS/PNEC to be used in the STE JRC proposed a set of criteria for the verification of monitoring data: a procedure for the treatment of outliers; combining data for polar substances from whole water and dissolved fraction; the use of 95 percentile instead of max concentrations in STE runs. Presentation of results regarding the application of the STE approach to the assessment of risk for the existing priority substances for the period 2006-2015.
4th Meeting 25-26 January 2016 (Brussels, BE)	Taken a decision to evaluate substances by Scenario2 after treatment with PNEC quality criterion (Scenario2 PNEC QC) and to evaluate substances highly ranked in last prioritisation exercise together with "new" substances.
5th Meeting 9-10 June2016 (Gavirate, IT)	Methodology for monitoring-based exercise was verified considering the robustness, independence and sensitivity of STE factors. Review of the preliminary list of short-listed substances from monitoring-based exercise and selection of compounds for preparation of factsheets.
6th Meeting 11-13 October 2016 (Ispra, IT)	The uncertainties in the monitoring exercise were discussed. The factsheets and draft dossiers for the top-ranked susbstances from monitoring- and modelling-based exercises were presented. A table supporting the final selection of substances proposed as potential candidates for a new list of PS was discussed.

1.2. Approach to the review of the PS list

The approach to the review of the PS list was based on two main processes.

The first process involved the identification of new potential PS after an evaluation of the risk posed by substances of emerging concern to or via the aquatic environment in either a monitoring- or a modelling-based exercise. For this purpose, the following substances were initially considered:

(a) Substances ranked highly in the monitoring and modelling-based ranking exercises in the last PS review, but not taken forward. These substances were included in the short list of potential PS but not finally proposed for inclusion in the PS list during the last review. They were listed under Table 4.1 of the scoping report presented at the WG Chemicals meeting in March 2014. The existing factsheets for these substances have been firstly updated regarding new information on exposure and hazard. Whenever disagreements were apparent among the SG-R experts, working groups have been created to agree on updated PNEC values.

(b) Substances that were initially considered in the last review but which were *not* ranked highly, for which new information has become available since the last review that could increase the ranking, and

(c) Other substances ("new substances") selected on the basis of, e.g. information from other legislation, recent monitoring data submitted to the JRC or the European Environment Agency (EEA), information on 'river basin specific pollutants' (RBSPs), or literature reports regarding risks from emerging pollutants.

The substances identified above were then evaluated according to the available environmental exposure data. Monitoring data-rich substances were evaluated in the monitoring-based exercise, by a new approach that considers the spatial, temporal and extent of PNEC exceedances (STE) in the monitoring data, as described in section 2. The methodology for the monitoring-based exercise and its outcome are presented in the current report. The remaining substances with insufficient or low-quality monitoring data were evaluated in the modelling-based exercise, where the existing monitoring data was nevertheless used as supporting evidence for the risk estimation. The methodology and results of the modelling-based exercise are presented in an accompanying report (Lettieri et al., 2016).

Both the monitoring- and modelling-based exercises provide a rank of the substances based on their estimated risk at EU level, by comparing environmental concentrations (measured or estimated, respectively) with the substance's PNEC (predicted no-effect concentration).

Detailed factsheets were then developed for the highest ranked substances, identified through these two processes, to select the candidate priority substances for which an EQS would be derived.

The second process in the review of the PS list consisted in the re-evaluation of the existing PS and PHS dossiers whenever there was new evidence supporting the revision of the existing EQS and an analysis of the up-to-date estimated risk at EU level by considering new data on uses and available monitoring data across Europe.

2. Methodology for the monitoring-based prioritisation

The collection of monitoring data is an essential part of the prioritisation process because it provides direct evidence of the presence of substances in the environment. However, any ranking procedure which is designed to rank substances based on their detection in water bodies will be heavily influenced by the substances that each Member State chooses to measure and to report. This is a clear limitation inherent in any monitoring-based approach to the identification of candidate PS.

The previous monitoring-based prioritisation exercise was performed by INERIS (France) during the years 2008-2009 (James et al., 2009). There was a tremendous qualitative and quantitative jump from the COMMPS (Combined Monitoring-based and Modelling-based Priority Setting Scheme) monitoring database (ca. 700.000 analyses of 314 substances from 15 countries) (Fraunhofer-Institute, 1999) to the INERIS monitoring database, which was by far the best and most extensive ever compiled at European level. This process was based on 14.6 million analyses from 19.900 stations across 27 Member States. All four WFD surface water categories (rivers, lakes, transitional and coastal waters) were represented. A total of 1151 different substances were initially considered during the ranking, but this was subsequently refined to only include substances that were monitored in at least four countries, i.e. 316 substances in water, sediment or biota. In the 2009 monitoring-based prioritisation, these 316 substances monitored by 4 countries and more were chosen to constitute the manageable list of substances submitted to the prioritisation. The number of countries monitoring the substance was the only criteria used in the selection of the manageable list (James et al., 2009).

The monitoring-based prioritisation approach under the 2nd review of the PS list presented here in general follows the approach used under the 1st review process by distinguishing monitoring data-rich substances going through the monitoring-based prioritisation from monitoring data-poor substances going through the modelling-based prioritisation exercise. However, a new methodology was developed for the monitoring-based exercise, which exploits the inherent variability of measurements in the monitoring dataset, and evaluates the Spatial, Temporal and Extent of PNEC exceedances (STE approach), in order to rank and classify the substances for the risk they pose to European surface waters.

2.1. STE approach

The STE method is built on the scheme developed by von der Ohe et al. (2011) where substances were ranked for the selection of 'river basin specific pollutants' based on two indicators: the Spatial distribution of exceedance (Spatial factor), considering the variability in different monitoring sites, and the Extent of the PNEC exceedance (Extent factor). This scheme has been later tested at the level of a single Member State (Slobodnik et al. 2012). However, the STE improves the Spatial and the Extent factors described in the Von der Ohe et al. (2011) scheme and extends further this original method by including an additional temporal factor (Temporal frequency of exceedance or Temporal factor).

The monitoring-based prioritisation approach specifies how to select data for water (inland and coastal/transitional), sediment and biota compartments, respecting relevant data-quality criteria. Then, the STE method estimates for each substance whether or not the measured concentrations exceed the toxicological threshold of concern (EQS or PNEC) in a given environmental matrix for each sampling station and time the substance is measured. Finally, the STE method calculates the Spatial, Temporal and Extent factors of PNEC exceedances per substance and combines these factors in a single and representative ranking score.

The STE method is described below in further detail.

2.1.1. Spatial distribution of PNEC exceedance

To determine the risk posed by chemicals in Europe, the spatial characterisation of monitoring samples can be performed at several levels: country, region, river basin, water body, sampling station, etc. During the 1st monitoring-based prioritisation, only one statistical measure of the environmental concentrations per substance, calculated for all EU Member States, was used for the risk calculation and ranking of substances.

The subsequent study by von der Ohe et al. (2011) relied on a spatial factor calculated on the basis of the PNEC exceedances per sites. This spatial factor provided a good estimate for the spatial distribution of exceedances within a country or river basin.

In the STE method, the spatial frequency of exceedance for a given substance is quantified as a product of two proportions – one related to sampling sites (similar to that described by von der Ohe et al. (2011) and the other which specifies a correction by the number of affected countries. This additional country factor is particularly relevant since prioritised substances under the WFD should be selected amongst those that pose the highest risk at the European level, while substances whose risk may be limited to defined countries or water bodies may be regulated by other means, such as under 'river-basin specific pollutants' (RBSPs). The spatial factor in the STE approach is described in the following equation:

$$F_{spatial} = \frac{EXC_{95th\_perc,site}}{\#Site} \cdot \frac{EXC_{95th\_perc,country}}{\#Country}$$

where $EXC_{95th\_perc,site}$ corresponds to the number of monitoring sites in which the 95th percentile (P95) of the measured concentrations exceeded the PNEC; *#Site* is the number of sampling stations in which the substance was measured; $EXC_{95th\_perc,country}$ gives the number of countries in which the 95th percentile of the measured concentrations exceeded the PNEC; *#Country* is the number of countries in which the substance was measured.

Other metrics (for example the max concentrations) have been considered for the calculation of $F_{spatial}$ (as proposed by von der Ohe et al., 2011) but the 95th percentile has the advantage to avoid an accounting of erroneous records in the measurements or samples that include high background concentrations (metals for example).

The range of $F_{spatial}$ spans from 0 - meaning that a substance never exceeded the PNEC, up to 1 – when a substance exceeded the PNEC in all stations and countries in which it was measured.

2.1.2. Temporal frequency of PNEC exceedance

Substances can have extremely different temporal concentration patterns. Some substances could present sudden peak concentrations or are affected by clear seasonality (e.g. pesticides, biocides, emissions from discontinuous point sources). Such substances can represent a risk that is limited to a given time period. Therefore, the temporal frequency of PNEC exceedances is an important factor to be accounted for in the risk assessment and accordingly, a temporal component has been included in the STE approach.

The temporal frequency index considers for each sampling station the ratio between the number of measurements exceeding the PNEC and the total number of analyses for that site. Then, the sum of the ratios in all sampling stations is normalised by the total number of sites in which the concentrations exceeded the PNEC at least once. The mathematical expression of this formulation is written in the following equation,

$$F_{temporal} = \frac{\sum_{SiteECX} \frac{EXC_{sample}}{\#Analysis}}{\#SiteECX}$$

where for a given substance EXC_{sample} represents the number of samples in a given monitoring site which exceeded the PNEC, *#Analysis* is the total number of analyses in this site, and *#SiteECX* gives the total number of sampling stations in which the measured concentrations exceeded the PNEC at least once. If *#SiteECX* is zero (no stations with exceedances) then $F_{temporal}$ is automatically set to zero.

Similarly to the spatial factor, $F_{temporal}$ ranges from from zero to one: 0 - substance concentrations never exceeded the PNEC; 1 - substance concentrations exceeded the PNEC every time it was measured.

However, for a proper calculation of the temporal factor it is important that a sufficient number of samples are available for each sampling station. Therefore, an additional verification and correcting step was introduced to make sure that stations with a single measurement exceeding the PNEC for a certain substance are not over-represented in the temporal assessment. Accordingly, a two-step procedure was introduced (see Table 2), first finding two approximations for the temporal factor - $F_{temporal}$ calculated with all observation sites (f1), and $F_{temporal}$ calculated by excluding stations with less than 2 measurements when PNEC is exceeded (f2). Then at the second step, depending on how different the two estimates are, a decision is made for the final calculation of $F_{temporal}$. Thus, the final value of $F_{temporal}$ equals to f1 if the difference between both estimates is below 10% and equals to f2 in the opposite case.

Table 2. A two-step procedure for calculation of $F_{temporal}$

1st estimation f1	calculated considering all observation sites where PNEC is exceeded
2nd estimation f2	calculated excluding stations with less than 2 samples when PNEC is exceeded
Ftemporal	If | (f1-f2)/f1 | <= 0.1 then *Ftemporal* = f1 If | (f1-f2)/f1 | > 0.1 then *Ftemporal* = f2

2.1.3. Extent of PNEC exceedance

Generally, the toxicity follows a dose-response relationship, thus, the magnitude of any adverse effect is proportional to the magnitude of the exceedance of the threshold of toxicological concern or the PNEC.

Considering that the exposure may significantly vary with time and space, the use of an estimation of the central tendency (e.g the mean or median) is not appropriate to quantify the extent of exceedances. The most protective way to evaluate this would be to use the maximum of the site-specific Risk Quotients (RQ) (calculated for sites with exceedances) (von der Ohe et al. 2011). However, similarly to the spatial factor, caution needs to be taken in relying in possible erroneous max concentration values for the risk calculation in the E factor. For this reason, the 95th percentile was the preferred metric for the calculation of the risk quotient per site.

The F_{extent} has been calculated following a three-step procedure.

Firstly, the ratio between the 95th percentile of the measured concentrations in a given station and the PNEC value was calculated ($RQ_{95th\_perc,site}$) ;

Secondly, the $RQ_{95th\_perc,site}$ for all sites were used to calculate the extents of exceedances (EXC_{extent}) – by either calculating the 95th percentile or the maximum of $RQ_{95th\_perc,site}$, depending on the number of samples for a given substance in order to ensure sufficiently good spatial coverage. This decision step is displayed below.

$$EXC_{extent} = 95^{th}\ percentile\left(RQ_{95th\_perc,site}\right)\ \ if\ \ \#sites \geq 20$$

$$EXC_{extent} = \max\left(RQ_{95th\_perc,site}\right)\ \ if\ \ \#sites < 20$$

Finally, the F_{extent} was quantified by performing a normalisation of the EXC_{extent} values according to Table 3.

Table 3. Lookup table for quantification of F_{extent} factor based on values of extent of exceedances EXC_{extent}.

EXC_{extent}	F_{extent}
<1	0
1-2	0.04
2-5	0.07
5-10	0.11
10-20	0.18
20-50	0.28
50-100	0.41
100-500	0.56
500-1000	0.75
>1000	1

The above procedure separates the range of EXC_{extent} values into a higher number of categories for normalisation than the originally proposed by von der Ohe et al. (2011). It has the advantage to allow a bigger differentiation between substances in the low spectrum of its EXC_{extent} values, where the majority of the extents of PNEC exceedances occur (EXC_{extent} between 1 and 100; for details see Section 3.3.3).

The normalisation step allows the F_{extent} to adopt a range between 0 and 1, alike the $F_{spatial}$ and $F_{temporal}$ factors. The value 0 corresponds to a situation where the 95 percentile of the concentrations at each site never exceeds the PNEC, which is translated into a RQ < 1 while 1 corresponds to the highest magnitude of PNEC exceedances (RQ > 1000).

2.1.4. Calculation of STE scores for each compartment - receptor at risk

In order to assess substances in the monitoring-based exercise, the STE method finally calculates assessment scores for each compartment and receptor at risk by summing the corresponding Spatial, Temporal and Extent exceedance factors (for a given chemical):

$$Score = F_{spatial} + F_{temporal} + F_{extent}$$

The range of the STE scores is between 0 and 3 (since the individual factors vary from 0 to 1), with a score of 0 indicating no concern, while a score of 3 showing a very high concern. Five risk classes (very high, high, intermediate, low and very low) were adopted to rank the substances according to the obtained STE scores as specified in Table 4. Finally, for convenience the STE scores are converted to risk scores, when needed, according to the risk classification in Table 4.

Table 4. Risk classification based on STE score.

STE score	Risk classification	Risk score
≥ 2.4 and ≤3	Very high	1
≥ 1.8 and < 2.4	High	2
≥ 1.2 and < 1.8	Intermediate	3
≥ 0.6 and < 1.2	Low	4
< 0.6	Very low	5

The risk scores allow an easy comparison of the STE scores obtained in the different scenarios considered. These risk scores also allow a comparison of the results from the monitoring-based prioritisation exercise with those from the modelling-based exercise (Lettieri et al., 2016).

2.2. Environmental exposure information

Substances have been initially considered for the monitoring-based exercise if monitoring data were available for the period 2006-2015. An initial request for monitoring data was made by DG ENV to the EU Water Directors (on 21 March 2014). Additionally, the JRC has contacted different Stakeholders asking for available monitoring data that could be useful for the current exercise, both coming from official sources or European projects.

2.2.1. Sources of monitoring data

For this second prioritisation exercise performed during 2014-2016, the sources of the monitoring data were the following:

- **SoE**: database containing monitoring data reported by European countries under the State of the Environment (SoE) WISE (Water Information System for Europe) reporting managed by the European Environment Agency (EEA). In the framework of this SoE reporting, European countries granted the JRC permission to access disaggregated data for this second prioritisation exercise, which the JRC downloaded from the EEA WEB site (http://www.eea.europa.eu/data-and-maps/data/).
- **MSDAT**: contains data which were directly submitted to the JRC by EU member states following a request of DG ENV to the EU Water Directors (on 21 March 2014). In addition, some monitoring data have been submitted on behalf of the European drinking water companies. Monitoring data were generally submitted to the JRC either by using a simplified *Microsoft excel* sheet developed by the JRC, or by using the so-called "*end-user tool*", a *Microsoft access* database worksheet developed under the first prioritisation exercise by INERIS (http://www.oieau.fr/WISE-end-user-tool/). In addition, some Member States sent their (partly incomplete) data in different *excel* formats, which made the formatting of the data very work intensive.
- **EMPODAT**: is a database of geo-referenced monitoring and bio-monitoring data managed by NORMAN (Network of reference laboratories, research centres and related organisations for monitoring of emerging environmental substances) (http://www.norman-network.net/empodat/). The EMPODAT data were provided to the JRC on 18 March 2015.
- **JDS**: monitoring data from the third Joint Danube Survey (JDS) from the year 2013. JDS3 was the world's biggest river research expedition of its kind**,** with altogether more than 800 individual parameters and 650 target organic pollutants investigated (Liška et al., 2015; http://www.danubesurvey.org/).
- **IPCheM**: the Information Platform for Chemical Monitoring data, managed by the JRC was downloaded in January 2015 (https://ipchem.jrc.ec.europa.eu).

Most of the collected monitoring data comes from inland surface waters: 18.909.791 records were collected for inland "whole" water, and 1.436.022 records for inland water dissolved fraction (the fractions were combined later for polar water-soluble organic compounds and other compounds with log $K_{OW} \leq 5$).

Table 5 shows the distribution of the monitoring data for inland "whole" surface waters between the 5 data sources. The time-frame considered for the current monitoring-based exercise was 2006-2015.

Table 5. Number of records (as a percentage) in the initial inland "whole" surface water dataset for the 5 data sources (total number: 18.909.791)

	SoE	MSDAT	EMPODAT	JDS	IPCheM
Number of records (%)	40.1	14.0	15.3	0.03	30.6

In addition, Table 6 shows the number of records and substances for the different matrices and fractions. Most of the records and monitored substances came for inland whole water. As a comparison, transitional, coastal and marine waters (whole water) accounted for only 1% of the number of records from inland whole water. The number of records for sediment and biota were also less, and despite the significant number of substances monitored in

these two fractions, only a few were monitored in at least 4 MS, and could therefore be considered for the monitoring-based exercise.

Table 6. Number of monitoring records and substances per matrix and fraction in the initial dataset.

	Inland "whole" water	Inland "dissolved" water fraction	Transitional, coastal, and marine waters (whole water)	Transitional, coastal, and marine waters (dissolved)	Sediment	Biota
Number of records	18.909.791	1.436.022	167.522	4.833	395.094	284.244
Number of substances	1390	389	170	8	619	226
Number of substances in more than 3 countries	481	91	56	7	70	60 (fish +mollusc)

For biota, the received data are mainly from transitional, coastal, and marine waters (271.360 records; 95.5% of total). Only 12.884 records (4.5 % of total) correspond to inland water bodies (lakes; rivers). The biota records were subdivided into different species groups (Table 7) according to the given species name. Samples without species name and group were discarded.

Table 7. Number of monitoring records for different biota species groups

Species groups	Number of records
Fish	153.086
Mollusc	124.457
Algae	1.318
Benthos	998
Crustacean	473
Cetacean	1.225
Other mammals	764
Birds	1.875

2.2.2. Missing information and modifications to the monitoring database

There was a high variation in the names given to the substances by different MS, many were spelled in different languages or different synonyms were used. To facilitate the analysis, the monitoring database was modified and a single name was assigned to each substance. Similarly, a single CAS value was assigned if the substance possessed several CAS from different sources. In a few cases, a single CAS was applied to stereoisomers of

the same substance. For a few substances, groups of similar substances were formed and analysed together in the STE (Table I-1). This was particularly relevant when there were indications that the available EQS/PNEC value was related to a group of substances.

The analysed fraction was sometimes not clearly identified in the data sets (or sometimes missing). In case of "whole water" analysis it was generally not specified if the fractions were analysed separately. Polar water-soluble substances are generally analysed by solid-phase extraction (SPE) of whole non-filtered water samples (or the water samples are filtered and only the filtrate is analysed). Conventional SPE however does not ensure the extraction of particle-bound substances. For polar substances this procedure can be accepted because only very small amounts will adsorb on the suspended particulate matter (SPM) of a water sample. However, it would be more correct to declare these measurements as "dissolved" fraction, which was done by some laboratories. Therefore it was necessary for our statistical evaluations to combine these "dissolved" fraction measurements for polar substances with the "whole water" results. The selection criterion for polar substances was their log K_{OW} value. Initially, the substances with a log $K_{OW} \leq 3.5$ were defined to be polar water-soluble. In addition, for some carboxylic acids with log K_{OW} higher than 3.5, the data from the dissolved fraction were merged with the "whole water" dataset because these acids are present in the deprotonated form and therefore will dissolve in the water sample (e.g. diclofenac, fenofibrate, etc). This was done also for 17β-estradiol (log $K_{OW=}$4.0) and 17α-ethinylestradiol (log $K_{OW=}$3.7). However, following the decisions of the 5th meeting of the SG-R the trigger value for merging the "dissolved" fraction with "whole water" was extended to substances with a log $K_{OW} \leq 5$, because according to the TGD-EQS, discrepancies between total and dissolved concentrations will generally become apparent at log K_{OW} =6. This merging of monitoring records allowed the assessment of a few additional substances (e.g. Triclosan, Ethion, Gemfibrozil, etc.). The polar, water soluble substances from the inland water in the dissolved fraction that have been merged with inland whole water are listed in Table I-2.

For metals, however, a strict separation between "whole water" and "dissolved phase" was performed by JRC because in the case of metals the EQS refers to the dissolved concentration, i.e. the dissolved phase of a water sample obtained by filtration through a 0,45 µm filter or any equivalent pre-treatment (Directive 2008/105/EC). Some EQS are expressed however as bioavailable metal, e.g. for nickel and zinc. STE for metals was run in the dissolved phase, and for those metals lacking monitoring data for the dissolved phase the STE was run for "whole" water" instead.

In some cases, mg/L or ng/L units had to be converted.

Whenever only the name or the CAS number of the substance were provided, the missing information was filled in.

An artificial CAS (e.g. "#noCAS-JRC-001") was given when originally no CAS number existed (e.g. for transformation products), including mixtures of chemicals (e.g. "chloronitrotoluenes" or "trichlorophenols").

The biota records (in total 284.244) were given on a wet weight, dry weight or lipid weight basis. For consistency, all data had to be converted to wet weight. This conversion however was only possible for the records given in dry weight (41.524), by using the dry-wet-weight ratio. The records given on a lipid weight basis (25.173) or with missing information (153 records) were discarded. The dry-wet-weight ratio was missing for 13.121 of the 41.524 dry weight records (31.6 %). For these records the average dry-wet-weight ratio of 5.5 (18.2 %) for molluscs and 4.2 (23.9 %) for fish was used. 253.473 records for fish and molluscs remained, most of them from coastal and transitional waters (246.057 records; 126.193 for fish, and 119.865 for mollusc).

2.2.3. Requirements to the monitoring data

The records for environmental concentrations of substances collected from different sources and databases were subject to data quality assessment as outlined in Figure 1.

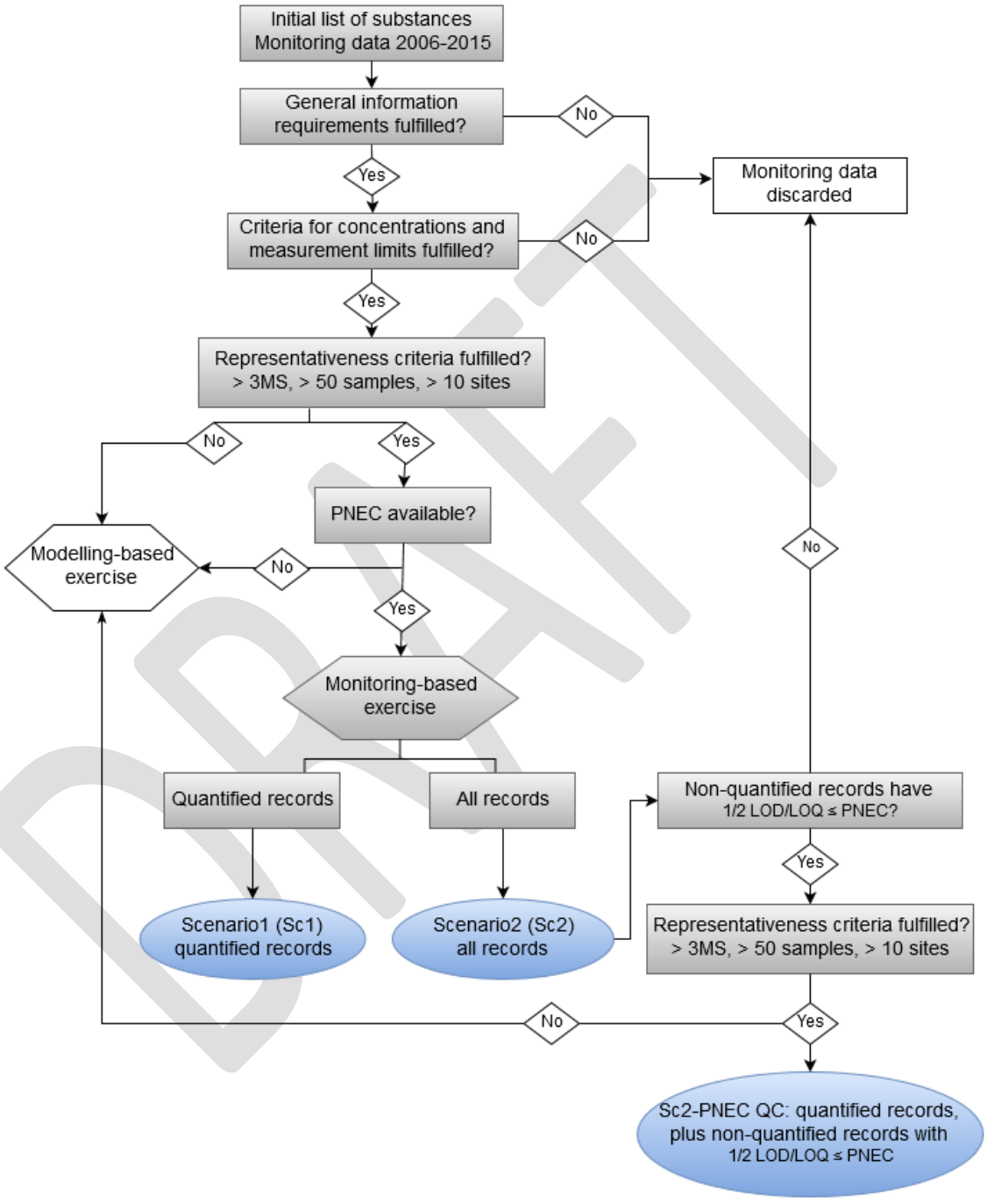


Figure 1. Decision tree for quality checks and selection of monitoring data for different scenarios. Sc2-PNEC QC was the one selected finally for the risk-based ranking of substances in the monitoring-based exercise.

The criteria applied in the assessment of data quality are structured in 3 specific groups as follows:

General requirements:

- Clear substance identification (CAS number and name of determinant).
- Country code (ISO 3166)
- Clear sampling station identification – name (coordinates optional)
- Date (yyyy/mm/dd)
- Matrix (surface water, sediment, biota)
- Water body (WB) type (river, lake, artificial, transitional and coastal)
- Clear identification of fraction (whole water, dissolved).
- Clear measurement unit (µg/L or µg/kg).

Criteria for concentrations and measurement limits:

- Exclusion of records when simultaneously the concentration is zero (or blank) and both LOD and LOQ are zero or blank (or combination of zero and blank)
- Keeping records when the concentration is quantified (specified as "individual value" or "above measurement limits") even though the measurement limits are missing
- Retaining records if the concentration is "less-than value" (marked "below measurement limits") when LOQ exists (LOD could be missing or should be coherent with LOQ (LOD<LOQ)) by setting concentrations equal to half of LOQ (according to Directive 2009/90/EC). In addition, following the procedure for data gathering in the first prioritisation excercise (James et al., 2009), the non-quantified records below LOD aslo were set to a half of LOD and kept in the dataset, when LOD was reported thoroughly.

  (Note: the non-quantified records below LOD are ca.3% from the total number of samples in the most abundant dataset of inland whole water before applying the outliers' procedure described under section 2.2.4).

Representativeness criteria:

- Any substance to be monitored in at least 4 countries among the 28 EU MS and 3 EFTA countries
- Time period of measurements: 2006-2015
- The total number of samples and sites per substance to be sufficient for statistical analyses (more than 50 samples and more than 10 sites).

The data records which were not fulfilling the aforementioned criteria for data quality (see the conditions above) were eliminated from the datasets.

Table 8 shows the summary information on the monitoring dataset for the substances included in the monitoring-based exercise, after the application of the above criteria, except for the representativeness criteria.

Table 8. Summary statistics of the initial monitoring dataset after the general requirements and the criteria for concentrations and measurement limits were verified (no limitations of representativeness applied)

	Inland whole water	Inland dissolved	Coastal whole water	Coastal dissolved	Sediment	Biota (fish)	Biota (mollusc)
Number of substances	1390	388	170	8	619	181	203
Number of countries per substance	1 - 28	1 - 24	1 - 19	3 - 8	1 - 13	1 - 20	1 - 22
Number of sites per substance	1 - 9121	1 - 7251	1 - 586	17 - 112	1 - 2530	1 - 404	1 - 1146
Records per substance	1 - 152775	1 - 104512	1 - 6646	74 - 962	1 - 4406	1 - 6745	1 - 5019
Total number of samples	16698442	1184035	167282	4833	371195	113268	109169
Non-quantified records per substance (%)	0 - 100 (mean 89.1%)	0 - 100 (mean 80.4%)	0 - 100 (mean 81.5%)	18 - 82.1 (mean 51.9%)	0 - 100 (mean 86.7%)	0 - 100 (mean 73.8%)	0 - 100 (mean 68.6%)

The monitoring dataset summarised above has suffered additional modifications, such as the compliance check for the representativeness criteria (described above) and the removal of outlier records as described below.

2.2.4. Discarding outliers from dataset

Originally, the STE method was developed intending to use maximum concentrations per observation station for the calculation of both $F_{spatial}$ and F_{extent}, assuming that datasets are "cleaned" of outliers ($F_{temporal}$ considers all records per site). However, after performing initial statistical analysis for each substance in the datasets, it became clear that sometimes there were extremely high concentrations – for example in a range of g/L or several orders of magnitude higher than the limits of solubility of the substances. While the extreme example above represents clear outliers in the dataset that are easily identified and removed, other potential outliers may be real values explained by the variability in the measured concentrations at different sites or days. Alternatively, they may indicate experimental error or even a reporting error. Possible explanations could be a wrong reporting of the unit of measurement, typos, secondary contamination of samples, sampling or analytical problems, etc. For this reason, the JRC has introduced an additional verification to the quality of the data in order to identify and eventually remove obvious outliers in the dataset.

Intuitively, an outlier is an observation point that is distant from other observations. There is however no rigid mathematical definition of what constitutes an outlier and therefore, determining whether or not an observation is an outlier is ultimately a subjective choice. Nevertheless, there are various methods of outlier detection - some are graphical such as normal probability plots, others are model-based. Box plots are a hybrid of both.

The hybrid methods for the outlier's identification are usually built on the interquartile range. For example, if Q1 and Q3 are the lower and upper quartiles respectively, then one could define an outlier to be any observation outside the range [Q1 - k (Q3 - Q1), Q3 + k (Q3 - Q1)] for a given positive constant k.

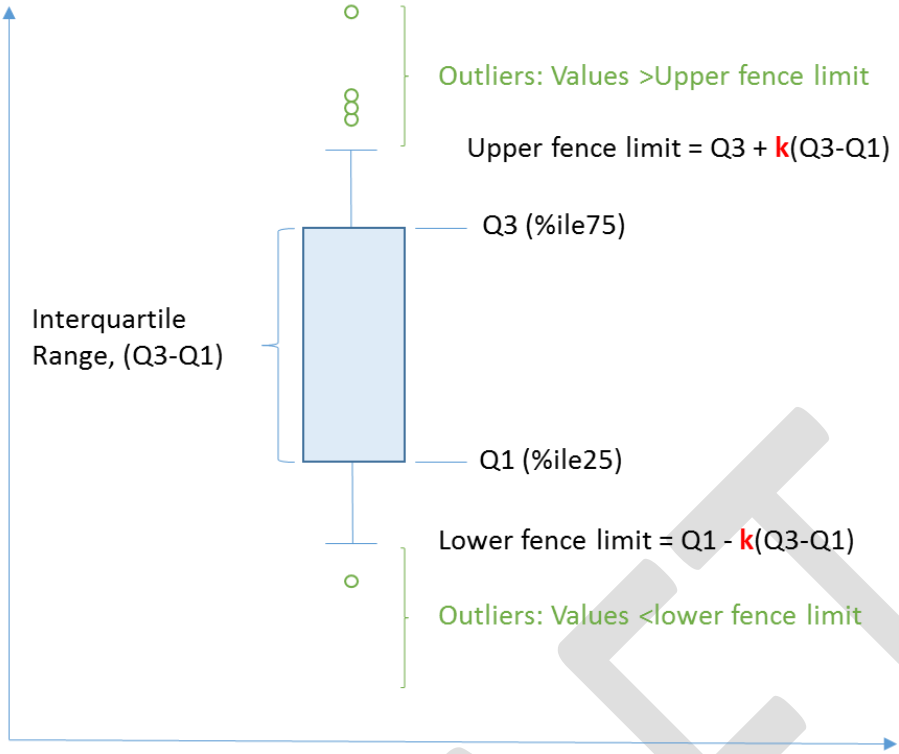


Figure 2. Scheme for the distribution of measurements in a boxplot, and the identification of outliers by defining the upper fence limits (UFL) with respect to the interquartile range. The outliers are identified as those for which the concentration is higher than 1000×UFL.

For the identification of outliers in the monitoring-based prioritisation exercise, the interquartile range was used, which is of box plot type (Chambers et al., 1983; Becker et al., 1988; Murrell, 2005), schematically displayed in Figure 2. This is a simple and clear method that can be applied easily in R scripts. Moreover, this method is used originally in R itself for making box-whiskers (by choosing the constant k=1.5).

Different scenarios for outlier identification have been tested by varying the value of the constant k, thus changing the fence limits according to the equation displayed above.

A procedure for elimination of outliers has been proposed by JRC to the experts during the 3rd SG-R meeting in September 2015. Although the initial proposal considered quite a high k-value (k = 1000) for the calculation of the fence limits, there were concerns that true peak concentrations would be discarded, a situation that should be avoided particularly for plant protection products for which seasonal peak releases are not unexpected. Finally, it was decided that in the monitoring-based exercise the defininition of the Upper Fence Limit (UFL) = Q3 +k*(Q3 - Q1) with k = 1000 would be followed by the calculation of a threshold corresponding to 1000×UFL above which the outliers were identified. Accordingly, these samples were deleted from the original dataset. In this way the outlier procedure is practically only targeting the erroneous reporting of the unit of measurement, typos, secondary contaminated samples, and wrong records resulting from problematic sampling or analytical problems, etc. The Figure 3 presents as an example the application of the outlier procedure for the case of glyphosate.

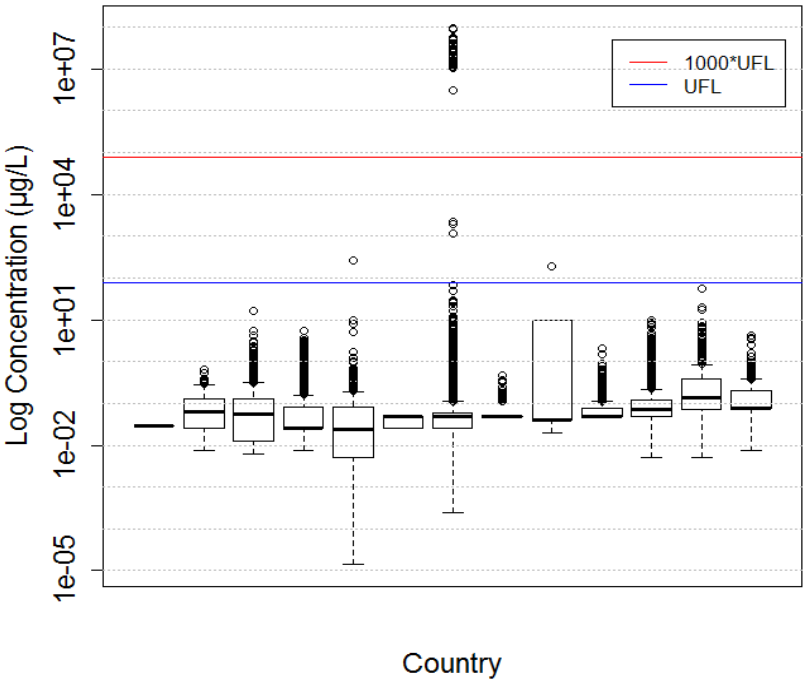


Figure 3. Example of the application of the outliers' procedure to the monitoring data of a substance containing likely outliers. The blue line corresponds to the upper fence limit (UFL) calculated with a constant k=1000, while the red line corresponds to the 1000×UFL threshold, above which all the records have been deleted from the dataset.

For the inland whole water dataset in Scenario 2 the number of the impacted substances (with monitoring records above 1000 × UFL) was 44 (Table 9). These substances are listed in Table 10 and the percentage of discarded records per substance vary from 0.001% up to 20.3% (the latter is a very specific case that corresponds to a significant number of wrong records in one MS for hexachlorocyclohexane) with an average=0.6%.

Table 9. Number of substances from inland whole water (Sc2) which max concentration exceeding considerably (10-1000) the UFL specified by the outliers' procedure.

Number of substances		
(max/UFL)>10	(max/UFL)>100	(max/UFL)>1000
104	70	44

Finally, the use of such a conservative approach for the treatment of outliers cannot exclude that the dataset still contains some problematic records. However, the contribution of "the unrealistic" samples to the final scoring is partly overcome by the use of 95 percentiles in the STE instead of maximal concentrations. Nevertheless, caution should be taken in the interpretation of the STE results, and the outlier procedure described above did not replace a thorough check of the dataset, particularly for those substances showing the highest risk in the STE that were therefore the potential candidates for moving forward in the prioritisation exercise.

Table 10. List of 44 substances from inland whole water (Sc2: all monitoring records) which max concentration exceeding 1000 times the UFL specified by the outliers' procedure (all concentrations in µg/L).

CAS	Substance	Max concentration	UFL	Max/UFL
1066-51-9	Aminomethylphosphonic acid (AMPA)	98999996	345.4	286649
1071-83-6	Glyphosate	96400003	75.1	1283622
107534-96-3	Tebuconazole	14400001	15.0	958402
117-81-7	Di(2-ethylhexyl) phthalate (DEHP)	796000	375.5	2119
118-74-1	Hexachlorobenzene (HCB)	25700	2.0	12834
120-12-7	Anthracene	33600	1.3	26826
122-34-9	Simazine	27000	5.0	5389
133-07-3	Folpet	20999999	15.0	1397670
140-66-9	4-tert-Octylphenol	99000	12.5	7904
15545-48-9	Chlorotoluron	98999996	15.0	6589018
1582-09-8	Trifluralin	21100	1.3	16812
1912-24-9	Atrazine	69600	10.0	6949
191-24-2	Benzo(g,h,i)perylene	51030	3.8	13589
205-99-2	Benzo(b)fluoranthene	160180	3.7	43233
206-44-0	Fluoranthene	67100	6.5	10308
207-08-9	Benzo(k)fluoranthene	70810	1.3	56534
25057-89-0	Bentazone	50999999	9.0	5657238
2921-88-2	Chlorpyrifos	19030	5.0	3800
309-00-2	Aldrin	10200	4.5	2264
330-54-1	Diuron	87100	10.0	8697
330-55-2	Linuron	20999999	5.0	4191617
333-41-5	Diazinon	58164	15.0	3872
34123-59-6	Isoproturon	96700	5.0	19301
40487-42-1	Pendimethalin	83999996	20.0	4194756
470-90-6	Chlorfenvinphos	12000	5.0	2395
50-29-3	DDT, p,p'	3000	2.0	1498
50-32-8	Benzo(a)pyrene	110840	3.9	28384
51218-45-2	Metolachlor	96999998	15.0	6458056
58-89-9	gamma-HCH (Lindane)	2500	2.3	1109
60-00-4	Edetic acid (EDTA)	96999998	4605.6	21061
60-57-1	Dieldrin	5000	4.0	1248
608-73-1	Hexachlorocyclohexane (HCH)	4400	2.5	1756
61-82-5	Aminotriazole	65999999	25.1	2634730
62-73-7	Dichlorvos	55787	9.5	5866
67129-08-2	Metazachlor	34000001	15.8	2155719
72-20-8	Endrin	1600	1.3	1277
7439-97-6	Mercury	22000	20.0	1098
77-47-4	Hexachlorocyclopentadiene (HCCP)	51630001	7415.5	6962
80-05-7	Bisphenol A	88000002	87.6	1004566

CAS	Substance	Max concentration	UFL	Max/UFL
84852-15-3	Nonylphenol	99900	37.6	2660
87674-68-8	Dimethenamid	40999999	15.0	2728785
87-86-5	Pentachlorophenol	85400	23.8	3591
91-20-3	Naphthalene	416000	10.6	39189
94-74-6	2-Methyl-4-chlorophenoxyacetic acid (MCPA)	86999998	2.5	34626865
94-75-7	2,4-Dichlorophenoxyacetic acid (2,4-D)	43000002	7.5	5723794
138261-41-3	Imidacloprid	10700001	15.0	712146

2.2.5. Selection of monitoring data as input to the STE

As described under Section 2.2.3 and illustrated in Figure 1, three different scenarios for monitoring data have been initially considered for each water type/fraction/matrix (Scenario1, Scenario2 and Scenario2-PNEC QC):

- **Scenario 1** considered only quantified monitoring records for the calculation of the STE score;
- **Scenario 2** includes all monitoring records (quantified and non-quantified) as input into the STE runs
- **Scenario2-PNEC QC** comprised quantified samples plus non-quantified for which ½ LOD/LOQ ≤ PNEC.

The comparison of STE scores obtained by the three data scenarios has been very informative and provided an overview of the general quality of the data. However, after a wide discussion during the 4th meeting of the SG-R, the Scenario2-PNEC QC was finally selected for the evaluation of substances aiming to ensure a bigger confidence in the results. The reasoning is that in Scenario1 for some susbtances the number of quantified samples (on average for all substances about 13.5% of the total number of samples) is not sufficient for statistical analyses. Scenario1 also could overestimate the risk linked to the presence of the chemicals, by considering only quantified records and disregarding to account the situations when the chemicals are not quantified because they are absent from the monitored waters or present at negligible concentrations. Furthermore, caution is warranted if Scenario2 (all records, including non-quantified) is used for risk-based calculations since non-quantified records (replaced by LOD/2 or LOQ/2) are artificial values and not real measurements. This is particularly relevant if these theoretical values are measured with an analytical method that is not sensitive enough and is not able to quantify the substance at least close to its PNEC value. In these situations, the inclusion of those non-quantified records potentially introduces artificial PNEC exceedances, which are excluded in Scenario2-PNEC QC. However, it should be highlighted that for substances that have a significant number of non-quantified records in the vicinity of the PNEC, it is expected that any change of the PNEC will change the number of records that will be considered for the STE SC2PNEC QC analysis, and therefore impact the STE score.

Summary monitoring information and statistics per substance for Scenario2 and Scenario2-PNEC QC are shown in Section 3.2 and Annex II.

The STE scores calculated for both Scenario2 and Scenario2-PNEC QC are presented in Annex IV, even though only those for the Scenario2-PNEC QC are used for the ranking of substances, under Section 3.5.

For metals, the STE analysis for surface water was run on the dissolved phase when monitoring data were available, otherwise results are presented for whole water. Table 11 shows the list of metals from the dataset for inland water that were scored considering the dissolved fraction. All other metals were ranked based on measurements in whole water.

Table 11. List of metals in dataset for inland water scored considering dissolved fraction (all other metals were evaluated by records for whole water).

Metals scored in Inland water dissolved fraction
Aluminum
Arsenic
Barium
Boron
Chromium
Cobalt
Copper
Iron
Manganese
Molybdenum
Selenium
Vanadium
Zinc

2.3. Hazard information

Environmental quality standards (EQS) or Predicted no-effect concentrations (PNEC) should protect freshwater and marine ecosystems from possible adverse effects of chemicals as well as human health via drinking water or ingestion of food originating from aquatic environments. Several different types of receptors potentially at risk need to be considered in the risk assessment, i.e. the pelagic and benthic communities in freshwater, brackish or saltwater ecosystems, the top predators of these ecosystems and human health (TGD-EQS, 2011).

QSs to protect human health utilise information about effects on mammals from oral exposure, repeated dose toxicity, carcinogenicity, mutagenicity and effects on reproduction. Typically, "No Observable Adverse Effect Level" (NOAEL), "Acceptable Daily Intake" (ADI) and "Tolerable Daily Intake" (TDI) values identified in the human health section of risk assessments performed under the REACH regime are used. Oral Reference Doses (RfD), ADI or TDI values adopted by national or international bodies such as the World Health Organization may also be used (TGD-EQS, 2011).

For the freshwater compartment, PNEC values have been collated or derived considering toxicity effects to aquatic freshwater organisms ($PNEC_{fw,\ eco}$), effects to human health from consumption of drinking water ($PNEC_{dw,\ hh}$) and, whenever derivation trigger values were met, PNEC values were also considered for sediment organisms ($PNEC_{eco,\ sed}$), for predators considering secondary poisoning route ($PNEC_{biota,\ secpois}$) and for human health through the consumption of fishery products ($PNEC_{biota,\ hh\ food}$).

Furthermore, $PNEC_{biota,\ secpois}$ and $PNEC_{biota,\ hh\ food}$ were converted (back calculated) into equivalent water concentrations, so they could be compared directly with other water column quality standards (QS) (TGD-EQS, 2011).

2.3.1. Sources of Hazard information

Hazard information has been collected from different sources (Table 12) for all the substances going through the monitoring-based exercise.

First, Environmental Quality Standards (EQS) for River Basin Specific Pollutants (RBSP) at the single country level have been collected from reports or online databases (Irmer et al. 2014; Ecotox, 2015; UK TAG, 2013). EQS for Dutch specific pollutants were provided directly to the JRC by e-mail correspondence in June 2015, and substance datasheets were retrieved from INERIS (FR), some containing also country-specific EQS values (http://www.ineris.fr/substances/fr/).

Secondly, PNEC values have been collected, with particular focus on the substances where no EQS value was available. A request for PNECs derived in the different countries was made to the experts of the SG-R group in July 2015, upon distribution of the preliminary list of substances going through the monitoring-based exercise. Furthermore, PNEC values were searched in the literature, with preference given to those used already in European monitoring campaigns or prioritisation exercises, such as the Joint Danube surveys (Liška et al. 2014), the NORMAN risk assessment prioritisation (Van der Ohe et al. 2011) and the datasheets produced under the development of the first Watch List (Carvalho et al. 2015).

Thirdly, PNECs have been collected from ECHA dossiers (http://echa.europa.eu/) and EFSA risk assessment reports (http://www.efsa.europa.eu/), when available.

Fourthly, when dossiers from ECHA or EFSA were available, but no PNECs were given, the ecotoxicity studies listed were used by the JRC to derive the PNEC, using only studies that were considered reliable or reliable with restrictions. Other literature has been screened, particularly those following the TGD-EQS (2011) for their PNEC derivation.

Finally, for those substances where information was not available from any of the sources listed above, available studies have been searched for in the US-EPA ECOTOX database

(http://cfpub.epa.gov/ecotox/) and the ETOX database from UBA Germany (https://webetox.uba.de), that the JRC used for PNEC derivation according to the TGD-EQS (2011).

Table 12. Sources for EQS/PNEC values

Sources	Description
ECHA DOSSIER	Value taken from ECHA dossier
Swiss ECOTOX Centre	Proposals for Acute and Chronic Quality Standards http://www.ecotoxcentre.ch/
NL Specific Pollutants	NL EQS values kindly provided to the JRC in July 2015
EFSA	Dossiers on chemicals from the European Food Safety Authority (EFSA)
ETOX	Information System Ecotoxicology and Environmental Quality Targets (UBA, DE)
EU RAR	European Union Risk Assessment Report (2001-2008)
EU_REPO	European Assessment Reports (Dir. 98/83/EC)
INERIS	Dossiers on chemicals from the Institut National de l'EnviRonnement Industriel et des Risque (INERIS, France)
JDS3	Joint Danube Survey 3
JRC	Joint Research Center PNEC derivation
RIVM	National Institute for public Health and the Environment (Netherland)
SE Chem Agency	Swedish Chemicals Agency (Sweden)
RBSP database WRc, 2012	Comparative Study of Pressures and Measures in the Major River Basin Management Plans - Task 2c (Comparison of Specific Pollutants and EQS): Final Report and database. Contract No. 070311/2011/603663/ETU/D1 to DG Environment, WRc Ref: UC8981/1
RBSP ECOSTAT report UBA, 2014	Technical Report for the WFD CIS Working Group A Ecological Status (ECOSTAT). Irmer et al. 2014 Ecological Environmental Quality Standards of "River Basin Specific Pollutants" in Surface Waters - Update and Development Analysis of a European Comparison between Member States.
Italian EQS Working Group, 2015	EQS for perfluoroalkyl substances (PFAS)
UK TAG	UK Technical Advisory Group on the Water Framework Directive - Updated Recommendations on Environmental Standards River Basin Management (2015-21) Final Report November 2013

Sources	Description
SEPA 2014	Scottish Environment Protection Agenc (SEPA) Supporting Guidance (WAT-SG-53) Environmental Quality Standards and Standards for Discharges to Surface Waters. V5.1 - Revised to reflect the *Standards Directions 2014.*
WHO, 2011	World Health Organization - Guidelines for drinking-water quality
BASF	PNEC derivation kindly provided by BASF to the JRC in July 2015
Peer-reviewed publications	Verbruggen et al. 2008; Von der Ohe et al. 2011
COMMPS database	Fraunhofer-Institut (1999) Revised proposal for a list of priority substances in the context of the Water Framework Directive (COMMPS procedure). COMMPS stands for Combined Monitoring-based and Modelling-based Priority Setting Scheme.
Stakeholders	Different stakeholders have provided PNECs or commented on those proposed (BASF, Syngenta, Eurometeaux, European Aluminium , EPMF, IZA, DuPont, Bayer CropScience, Dow AgroSciences, Sumito Chemical Agro Europe S.A.S, ADAMA Deutschland GmbH, Cheminova A/S, Currenta GmbH & Co. OHG, CEFIC).

2.3.2. Criteria for the initial selection of EQS/PNEC values

The criteria followed to select the PNEC value for the STE calculations, when several values were available, were the following:

- when different EQSs were available for a same country, the most recent EQS was selected. This was the case for EQS from NL, where values were available both from RBSP ECOSTAT report (Irmer et al., 2014) and were also received directly from the MS;

- EQS values for long-term toxicity effects (AA, annual average) were preferred to those for short-term toxicity effects (MAC, maximum allowed concentration);

- EQS values were preferred to PNEC values;

- following a conservative approach, when different EQS values were available from different countries, the lowest was provisionally selected;

- for the $PNEC_{dw,hh}$, following the TGD-EQS (2011), WHO guideline values (WHO, 2011) were selected over limit values from Directive 98/83/EC, in case both values were available, since the first is health-based. When no value was available, a precautionary value of 0.1 µg/L was used for pesticides, according to Directive 98/83/EC, unless existing evidence supported the derivation of a new $PNEC_{dw,hh}$ following the TGD-EQS (2011).

The list of EQS/PNEC values was subsequently updated following access to improved ecotox datasets for several substances and thorough discussion with SG-R members.

The list of EQS/PNEC collected (and associated sources) are summarised in Annex III, as well as the final PNEC value selected to run the STE method.

Note: The EQS/PNEC values selected and reported in Tables in Annex III are values chosen following the above mentioned criteria for the sake of STE exercise, and they are not to be intended as reference values for any other purpose.

2.3.3. PNECs for Sediment

The derivation of $EQS_{sed, eco}$ for the protection of freshwater benthic organisms is explained in the EQS guidance document (TGD-EQS, 2011; page 93). Sediment PNECs are available for some substances in EQS substance datasheets / dossiers (from the year 2005 or 2011) or from ECHA substance dossiers. In some cases, the marine water sediment PNECs are different from the freshwater PNECs.

If no reliable sediment toxicity data are available, Equilibrium Partitioning (EqP) can be used to estimate the $PNEC_{sed, eco}$, based on the REACH Guidance (ECHA, 2008; TGD-EQS, 2011; page 96-99). The INERIS prioritisation report (James et al., 2009) gives in Annex VII.2 PNECs for protection of sediment dwelling organisms ($PNEC_{sediment}$), which have been derived from $PNEC_{water}$ via the EqP approach using the K_{OC} values of the substances. This EqP approach appears to be a reasonable and convenient compromise for assessing ecotoxicity for sediments (see pages 38-40 of the INERIS report; James et al., 2009), but the assumptions and uncertainties inherent in the equilibrium partitioning approach have to be acknowledged (TGD-EQS, 2011).

The K_{OC} values were retrieved by INERIS from the PCKOC of EPISUITE v1.66 software (EPISUITE).

First, $K_{sediment-water}$, the partition coefficient between sediment and water is calculated according to TGD-EQS (2011), using the following formula. Input parameter is the K_{OC}, the partition coefficient between organic carbon and water.

$$K_{\text{sed-water}} = F\text{air}_{\text{sed}} \times K_{\text{air-water}} + F\text{water}_{\text{sed}} + F\text{solid}_{\text{sed}} \times \frac{K\text{p}_{\text{sed}}}{1000} \times RHO\text{solid}$$

with

$$K\text{p}_{\text{sed}} = F\text{oc}_{\text{sed}} \times K_{\text{oc}}$$

and

$$K_{\text{sed-water}} = \frac{C\text{total}_{\text{sed}}}{C\text{porew}_{\text{sed}}}$$

		Default value
$K_{sed-water}$	Partition coefficient between sediment and water	
$F_{air-sed}$	Fraction air in sediment	0
$K_{air-water}$	Air-water partition coefficient	
$F_{water-sed}$	Fraction water in sediment	0.8
$F_{solid-sed}$	Fraction solids in sediment	0.2
K_{p-sed}	Partition coefficient solid-water in sediment	
F_{OC-sed}	Weight fraction of organic carbon in sediment	0.05
RHO_{solid}	Density of the solid phase	2500
K_{OC}:	Partition coefficient between organic carbon and water	
$C_{total-sed}$	Total concentration in sediment	
$C_{porew-sed}$	Total concentration in pore water of sediment	

Then, $PNEC_{sediment}$ (= QS; wet or dry weight) is calculated according to TGD-EQS (2011), using the following formula.

$$QS_{\text{sediment, EqP, ww}} = \frac{K_{\text{sed-water}}}{RHO_{\text{sed}}} \times QS_{\text{fw, eco}} \times 1000$$

$$CONV\text{sed} = \frac{RHO_{sed}}{Fsolid_{sed} \times RHOsolid}$$

$$QS_{sediment,\,EqP,\,dw} = CONV\text{sed} \times QS_{sediment,\,EqP,\,ww}$$

		Default value
$QS_{sediment,EqP,ww}$	Wet weight quality standard for sediment based on equilibrium partitioning ($PNEC_{sed}$)	
$K_{sed\text{-}water}$	Partition coefficient between sediment and water	
RHO_{sed}	Bulk density of wet sediment	1300
$QS_{fw,eco}$	Quality standard for direct ecotoxicity on freshwater aquatic organisms ($PNEC_{water}$)	
$CONV_{sed}$	Conversion factor for sediment concentration wet-dry weight sediment	
$F_{solid\text{-}sed}$	Fraction solids in sediment	0.2
RHO_{solid}	Density of the solid phase	2500
$QS_{sediment,EqP,dw}$	Dry weight quality standard for sediment based on equilibrium partitioning ($PNEC_{sed\ dw}$)	

When the $QS_{sediment}$ has been calculated using EqP and log K_{OW} is > 5 for the compound of interest, $QS_{sediment}$ is divided by 10. This correction factor is applied because EqP only considers uptake via the water phase. Extra uncertainty due to uptake by ingestion of food should be covered by the applied assessment factor of 10.

The calculated PNEC values from the INERIS report (James et al., 2009) were compared with our calculations applying the formulas given above (taken from the TGD-EQS, 2011). The results of the calculations were not identical, but very similar. The conversion factor of the wet weight to dry weight ratio was 4.6 for suspended matter and 2.6 for wet sediment (personal communication by Els Smit). The difference of the calculations is shown in Table 13.

Table 13. Comparison between available PNEC values for sediment

Substance	$PNEC_{sed\ dw}$ (INERIS) (µg/kg)	$PNEC_{sed\ dw}$(JRC) (µg/kg) Calculated with $CONV_{sed}$
DDD - o,p'	0.99	0.50
Benzo(a)anthracene	27.7	13.9
Phenanthrene	2708	1356
Tetrabutyltin	0.202	0.101
Indeno(1,2,3-c,d)pyrene	72.1	36.1
Triphenyltin	2.9	14.4
Monobutyltin	1.17	0.57
Dicofol	1.05	0.53

For dibutyltin, the ECHA dossier gives a $PNEC_{sed}$ of 7.0 µg/kg (for dibutyltin dichloride). INERIS gives a $PNEC_{sed}$ of 3.09 µg/kg. Our calculated PNEC is 15.46 µg/kg (using the same $PNEC_{water}$ and K_{OC}) (Table 14).

Table 14. PNEC sediment for dibutyltin (dichloride)

	$PNEC_{sed\ dw}$ (ECHA) (µg/kg)	$PNEC_{sed\ dw}$ (INERIS) (µg/kg)	$PNEC_{sed\ dw}$ (JRC) (µg/kg)
Dibutyltin (dichloride)	7.0	3.09	15.46

In case of 2,2',3,4,4',5',6-heptabromodiphenyl ether (BDE-183), the calculated PNEC (266 µg/kg) was preferred over the non-specific PNEC of 49000 µg/kg given in the EQS data sheet from 2005. Also for the priority BDEs 2,2',4,4',5,5'-hexabromodiphenyl ether (BDE-153), 2,2',4,4',5,6'-hexabromodiphenyl ether (BDE-154), 2,2',4,4'-tetrabromodiphenyl ether (BDE-47) and hexachlorobenzene (HCB) there is a large difference between the PNEC given in the EQS data sheet from 2005 and the calculated PNECs (Table 15).

Table 15. PNEC sediment for BDEs and HCB

Substance	$PNEC_{sed\ dw}$ (EQS data sheet 2005) (µg/kg)	$PNEC_{sed\ dw}$ (JRC) (µg/kg)
2,2',4,4',5,5'-Hexabromodiphenyl ether (BDE-153)	310	1.34
2,2',4,4',5,6'-Hexabromodiphenyl ether (BDE-154)	310	52.5
2,2',4,4'-Tetrabromodiphenyl ether (BDE-47)	310	0.0979
2,2',3,4,4',5',6-heptabromodiphenyl ether (BDE-183)	49000	266
Hexachlorobenzene (HCB)	16.9	0.392

2.3.4. PNECs for Biota

The biota PNECs were mainly retrieved from the document of Johnson et al. (2012), which collects information from EU Member States (Tables III-7 and III-8). For the fish monitoring data of PCBs, several mollusc PNECs were used because no PNEC for fish was available. Zinc and copper should be excluded from the biota risk assessment because they are essential elements and do not pose a risk to secondary poisoning.

2.3.5. PNEC for effects on human health from drinking water ($PNEC_{dw,\ hh}$)

According to TGD-EQS (2011), the QS for the abstraction of drinking water ($QS_{dw,hh}$) needs to be derived as follows:

If an EU drinking water standard (from Directive 98/83/EC) or a WHO drinking water standard is available, they are adopted as $QS_{dw,hh}$. The WHO drinking water standard is preferred over the precautionary value for pesticides in Directive 98/83/EC, because it is human's health-based.

If the drinking water standard is less stringent than the other QSwater values already derived (i.e. $QS_{fw,\ eco}$, $QS_{sw,\ eco}$, $QS_{fw,\ ,secpois}$, $QS_{sw,\ secpois}$, $QS_{water,\ hh\ food}$), it could be decided that the $QS_{dw,\ hh}$ do not need to be derived but anyway JRC decided to keep these substances in the monitoring exercise for comparison of the risk to different receptors.

If the drinking water standard is more stringent than the other QSwater values already derived (i.e. $QS_{fw,\ eco}$, $QS_{sw,\ eco}$, $QS_{fw,\ secpois}$, $QS_{sw,\ secpois}$, $QS_{water,\ hh\ food}$), the $QS_{dw,\ hh}$ is derived as follows:

First, the substance-specific removal efficiencies are estimated. This may require consultation with drinking water experts. The removal efficiency is expressed as the fraction not removable by treatment ($F_{not\ removable\ by\ treatment}$). For substances considered in the monitoring exercise the parameter $F_{not\ removable\ by\ treatment}$ was provided by RIWA (NL) (see Table 16 and Table III-3) depending from the substances' physical-chemical properties (volatility and hydrophobicity).

Table 16. Look-up table for estimation of substance-specific removal efficiencies by treatment according to the substance physical-chemical properties.

Volatility	Henry's law constant	Log Kow	$F_{not\ removable\ by\ treatment}$
Not volatile	< 0.01	< 5	1
Not volatile	< 0.01	> 5	0.05
Volatile	> 0.01	< 5	0.05
Volatile	> 0.01	> 5	0.05 For these substances no need to derive $QS_{dw,\ hh}$ since they are totally removed by the treatment, however for completeness, these substances were kept in DW scenario

Then, the $QS_{dw,\ hh}$ is calculated using the following equation. In this way the purification efforts of the drinking water suppliers are taken into account in the monitoring prioritization.

$$QS_{dw,hh} = \frac{drinking\ water\ \text{standard}\ (98/83/EC)}{F_{not\ removable\ by\ treatment}}$$

2. If neither an EU nor WHO drinking water standard is available, we followed the procedure described below:

A provisional drinking water standard is calculated according to the equation:

$$QS_{dw,hh} = \frac{0.1 \cdot TL_{hh} \cdot bw}{uptake_{dw}}$$

Using a human body weight (bw) of 70 kg and a daily uptake of drinking water ($uptake_{dw}$) of 2 litres (ECHA, 2008). By default, a fraction of 0.1 of the human toxicological standard

(TL_{hh}) is allocated to intake of the substance via drinking water. This default may be adapted, but this should only be done when sufficiently underpinned data (e.g. total diet studies and total coverage of possible intake routes) are available demonstrating that either a higher or lower value is justified. The value for TL_{hh} should be the acceptable daily intake (ADI) or tolerable daily intake (TDI) if these are available, a reference dose (RfD) or a benchmark dose. The relevant ADI/TDI for 86 substances were provided by RIVM (NL) (33 out of these 86 have also $QS_{dw,hh}$ from WHO or Directive 98/83/EC), while the reference values ADI/TDI from www.popstoolkit.com/tools/HHRA/TDI_USEPA.aspx were used for the another 74 substances (40 out of these 74 have $QS_{dw,hh}$ from WHO or Directive 98/83/EC). The ADI/TDI data for 40 substances were found in both sources – RIVM and US EPA. If ADI/TDI values were available from both RIVM and USEPA the lower one was chosen.

If no ADI or TDI is available, the TL_{hh} could be calculated from the NOAELmin (the lowest no observed adverse effect level value from a review of mammalian toxicology data) but this option was not used to derive $QS_{dw,hh}$ in the monitoring exercise, since the needed $QS_{dw,hh}$ were derived by the other choices.

In total, from the 323 substances (including metals in dissolved) assessed in STEfw, eco for Sc2-PNEC QC, 276 substances were considered for the running of the STEdw, hh. For the remaining 47 substances, the $PNEC_{dw,\ hh}$ were missing. Details about the sources of $PNEC_{dw,\ hh}$ and the corresponding number of substances are provided in Table 17.

Table 17. Summary of the sources of $PNEC_{dw,\ hh}$ used in the $STE_{dw,\ hh}$ calculations and corresponding number of substances.

Source	# substances	RIVM	US EPA	RIVM/US EPA
DWD	160	27	19	3
WHO	47	3	17	1
no DWD/WHO	69	36	18	16
total	276	66	54	20

2.3.6. PNEC for effects on human health from contaminated fishery products ($PNEC_{biota,\ hh\ food}$)

Where no established $QS_{biota,\ hh\ food}$ value exists, the procedure described in TGD-EQS (2011) is recommended (described below). It assumes that the uptake of a substance from fishery products does not exceed 10% of the relevant threshold level (TL), estimated from experimental data and expressed in $\mu g \cdot kg^{-1}$ bw$\cdot d^{-1}$ for humans. For practical purposes, the acceptable daily intake (ADI), tolerable daily intake (TDI) or $NOAEL_{oral}$ (the latter divided by an assessment factor) provides such an estimate.

The $QS_{biota,\ hh\ food}$ (expressed as $\mu g \cdot kg^{-1}$) is calculated using defaults for human bw (70 kg) and for the consumption of fishery products (0.115 $kg \cdot d^{-1}$) as follows:

$$QS_{biota,\ hh\ food} = \frac{0.1 \cdot TL \cdot 70}{0.115}$$

This approach does not specifically consider possible sensitive groups, such as the developing foetus or subpopulations that consume more fishery products than the European average. However, the assumption that fishery products make up no more than

10% of the threshold level value (0.1·TL) at the European average level of compound uptake provides a margin of safety.

In the monitoring exercise the biota standards were converted into a water column concentration standard ($QS_{fw/sw,\ hh\ food}$) using the bioaccumulation factor (BAF) by

$$QS_{water} = \frac{QS_{biota}}{BAF}$$

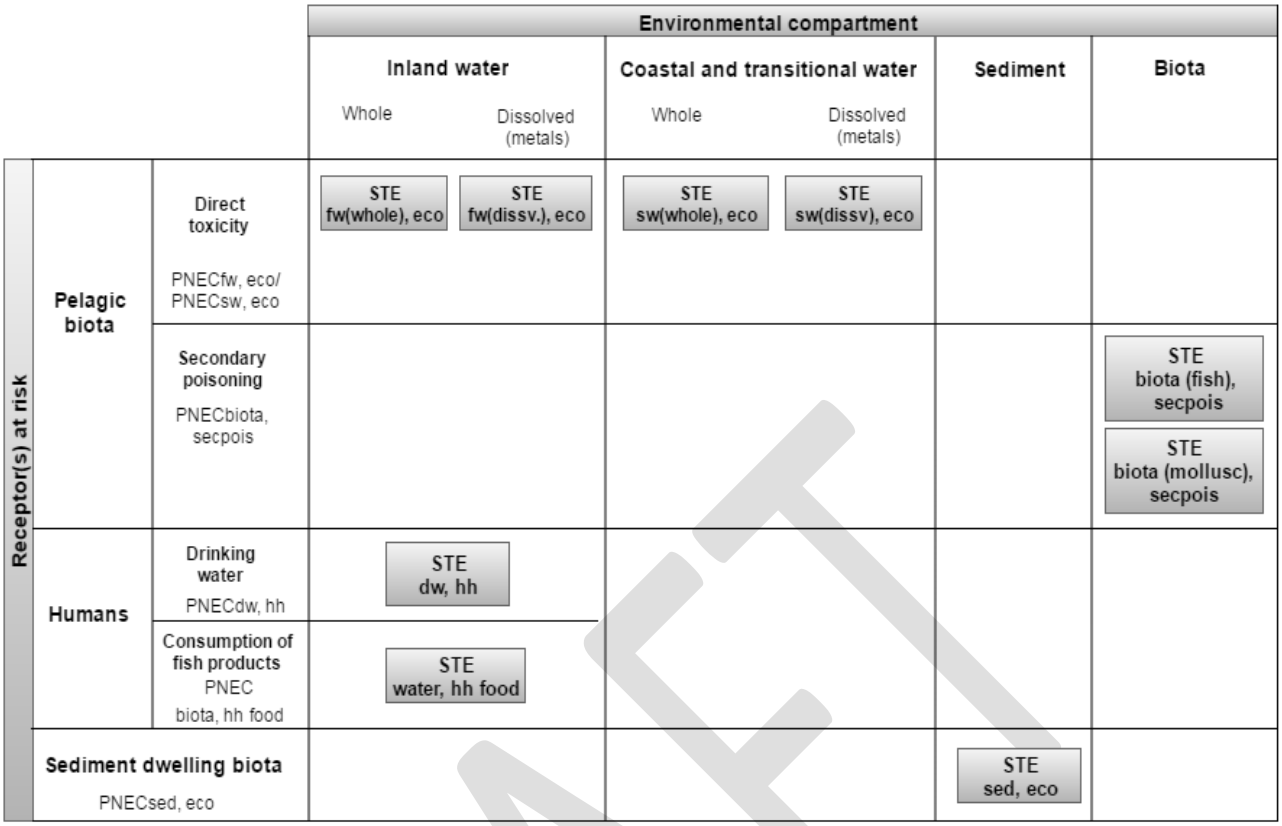
For fw,hh food scenario the tentative $PNEC_{fw,\ hh\ food}$ for 46 substances were provided by RIVM (NL).

2.4. Risk-based ranking of substances

Using the exposure and hazard data collected or derived as described in the previous sections, an assessment of the risk posed by each substance was done using the STE method described in Section 2.1.

2.4.1. Comparison of STE from different compartments and receptors at risk

Several STE runs were performed, following the scheme in Figure 4, assessing the risk in different environmental compartments and receptors at risk. For the water compartments, STE for metals was run preferably in the dissolved fraction (Table IV-3). For some metals, however, the final STE scores for inland water were based on the results for "whole water" (Table IV-2), if dissolved measurements were not available.



Note: The evaluation of risk for human health from the consumption of contaminated aquatic and aquaculture products was done for some substances by $STE_{water,hh\ food}$ (by using information for BAF and TDI/ADI) where human health standards were back-calculated to equivalent water PNECs (see Table III-4 and Table IV-6) since only very little biota monitoring data were available.

Figure 4. Scheme of the STE runs according to the environmental compartments and receptors at risk.

2.4.2. Short-listing of substances

For each substance, the STE scores from different compartments and receptors at risk have been compared and the highest of these values has been selected as final STE score which was used for the risk-based ranking of all substances in the monitoring-based exercise. The substances with the highest rank based on the final STE score (from 3.0 to 1.8) have been considered to move forward in the prioritization process. From this list of substances, additional relevant information was considered on uses, persistency in the environment, quality of the monitoring data, particular toxicological concern and uncertainty in the PNEC calculation (discussed under Section 4.1), for the selection of the list of substances for the preparation of detailed factsheets.

3. Results from monitoring-based exercise

3.1. Substances excluded from the monitoring-based exercise

Enough data was available in Scenario 2 (Sc2) for 354 substances (i.e. monitoring data in at least 4 countries, more than 10 sites and more than 50 samples). Twenty-eight of these substances have been excluded from the monitoring-based exercise after the application of the PNEC quality criterion and the successive additional check of representativeness (availability of monitoring data from at least 4 countries, more than 10 sites and 50 samples). Thus, 326 substances were considered in Sc2 PNEC QC (the scenario chosen by the SG-R as the basis for the final ranking). The excluded substances are listed in Table 18. This information was however available as supporting evidence whenever the substance ranked high in the modelling-based exercise (Lettieri et al. 2016).

Table 18. Substances excluded from the monitoring-based exercise after application of the representativeness criteria

CAS	Substance	Type	STE	Risk score	PNEC	Countries	Sites	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
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	Banned
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	Approved
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

CAS	Substance	Type	STE	Risk score	PNEC	Countries	Sites	Samples	Status
									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
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

3.2. Starting list of substances going through the monitoring-based exercise

Table 19 shows the summarising statistics for sampled substances considered in Scenario2 (Sc2), for which EQS or PNECs are available, in different compartments after the application of the criteria for data quality assessment (General requirements, Criteria for concentrations and measurement limits, Representativeness criteria, Section 2.2.3).

Table 19. Summary information for monitored substances in the different environmental compartments for Scenario 2 (quantified plus all non-quantified samples; a duplication of substances in different compartments is possible).

	InlWh [1]	InlDis [2]	TrCstWh [3]	TrCstDis [4]	Sediments	Bio_mollusc [5]	Bio_fish [6]
Number of substances	338	13	6	3	13	7	1
Number of countries per substance (range)	4-23	5-24	4-10	6-7	9-12	11-14	6
Number of sites per substance (range)	48-7429	60-7251	33-225	69-74	254-2462	336-749	84
Records per substance (range)	51-147284	855-104254	885-2176	462-475	300-3884	1483-3410	1995
Total number of samples	8245692	432712	10010	1403	29879	17364	1995
Non-quantified records per substance (%) (range)	0-100	0.2-86.3	60-95.6	18-82.1	0.1-98	1.2-56.9	73.4
Mean of non-quantified records per substance (%)	89.2	48.5	78.4	45.7	52.7	13.6	73.4

[1] Inland whole water; [2] Inland dissolved; [3] Transitional /coastal water; [4] Transitional/coastal water; [5] Biota mollusc; [6] Biota fish

Similar general statistics are presented for Scenario2–PNEC QC (Sc2-PNEC QC) in Table 20. For this scenario, all the criteria for data quality assessment have been applied (Section 2.2.3), including a PNEC quality criteria.

Table 20. Summary information for monitored substances in the different environmental compartments for Sc2-PNEC QC (quantified samples plus non-quantified records for which ½ LOD/LOQ ≤ PNEC; a duplication of substances in different compartments is possible).

	InlWh [1]	InlDis [2]	TrCstWh [3]	TrCstDis [4]	Sediments	Bio_mollusc [5]	Bio_fish [6]
Number of substances	310	13	6	4	13	7	1
Number of countries per substance (range)	4-23	4-24	4-10	3-6	9-12	11-14	6
Number of sites per substance (range)	38-7390	60-7009	33-225	11-68	142-2462	302-744	84
Records per substance (range)	51-147220	855-97036	885-2176	68-461	144-3884	1427-3410	1955
Total number of samples	6593615	372675	9680	1290	25093	16833	1955
Non-quantified records per substance (%) (range)	0-100	0.2-79.5	59.1-95.6	2.3-77	0.1-98	1.2-49.2	73.4
Mean of non-quantified records per substance (%)	83.8	36.6	77.3	34.9	44.8	10.9	73.4

[1] Inland whole water; [2] Inland dissolved; [3] Transitional /coastal water; [4] Transitional/coastal water; [5] Biota mollusc; [6] Biota fish

3.2.1. Inland whole water

The distribution of the monitoring records by country and year for Sc2-PNEC QC inland whole water is displayed in Figure 5.

Figure 5. Number of samples for inland whole water in Sc2-PNEC QC per country (top) and per year (bottom).

3.2.2. Inland dissolved water

The distribution of the monitoring records by country and year for Sc2-PNEC QC inland dissolved water is displayed in Figure 6.

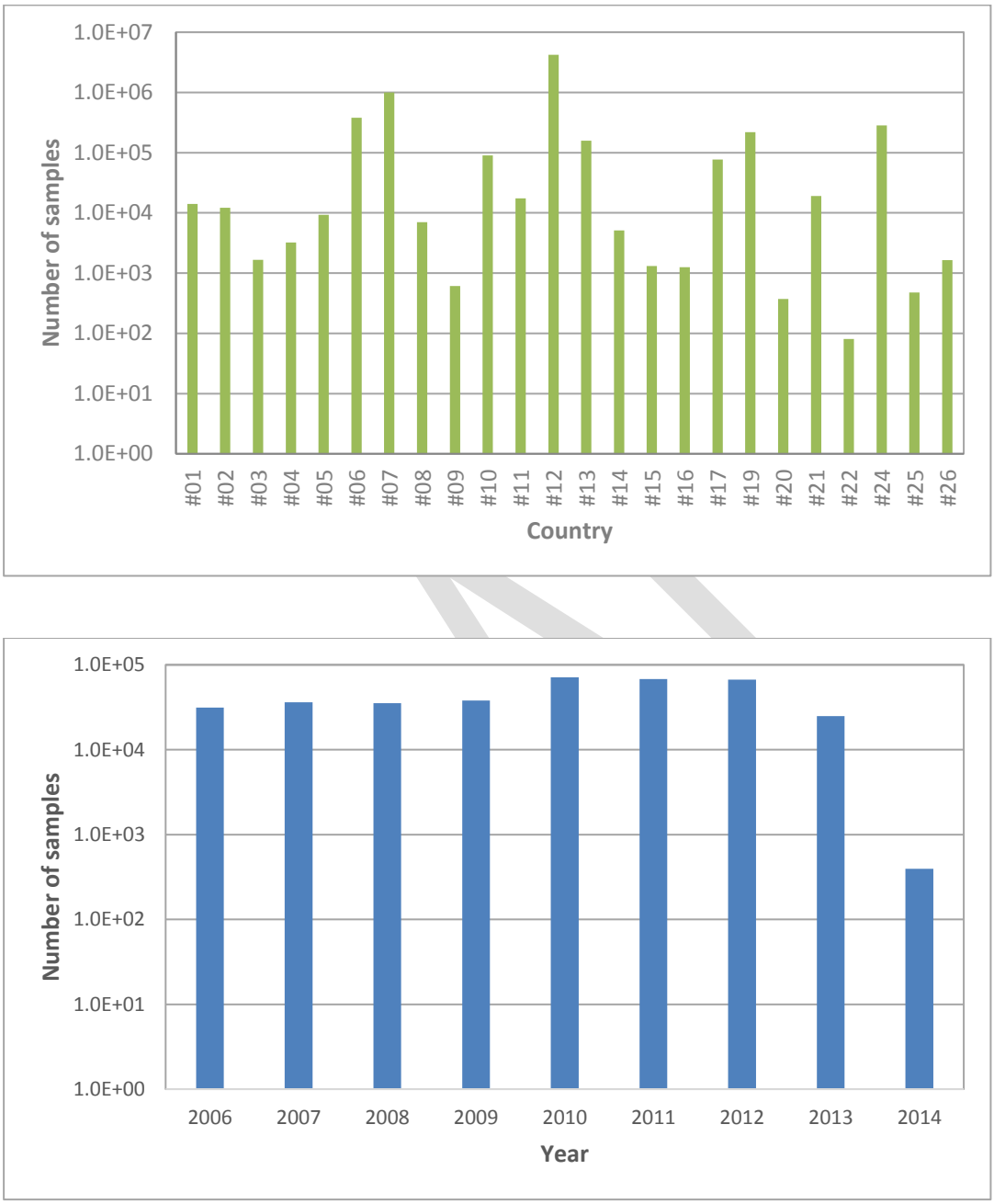


Figure 6. Number of samples for inland dissolved water in Sc2-PNEC QC per country (top) and per year (bottom).

3.2.3. Transitional and coastal whole water

The distribution of the monitoring records by country and year for Sc2-PNEC QC transitional and coastal water is displayed in Figure 7.

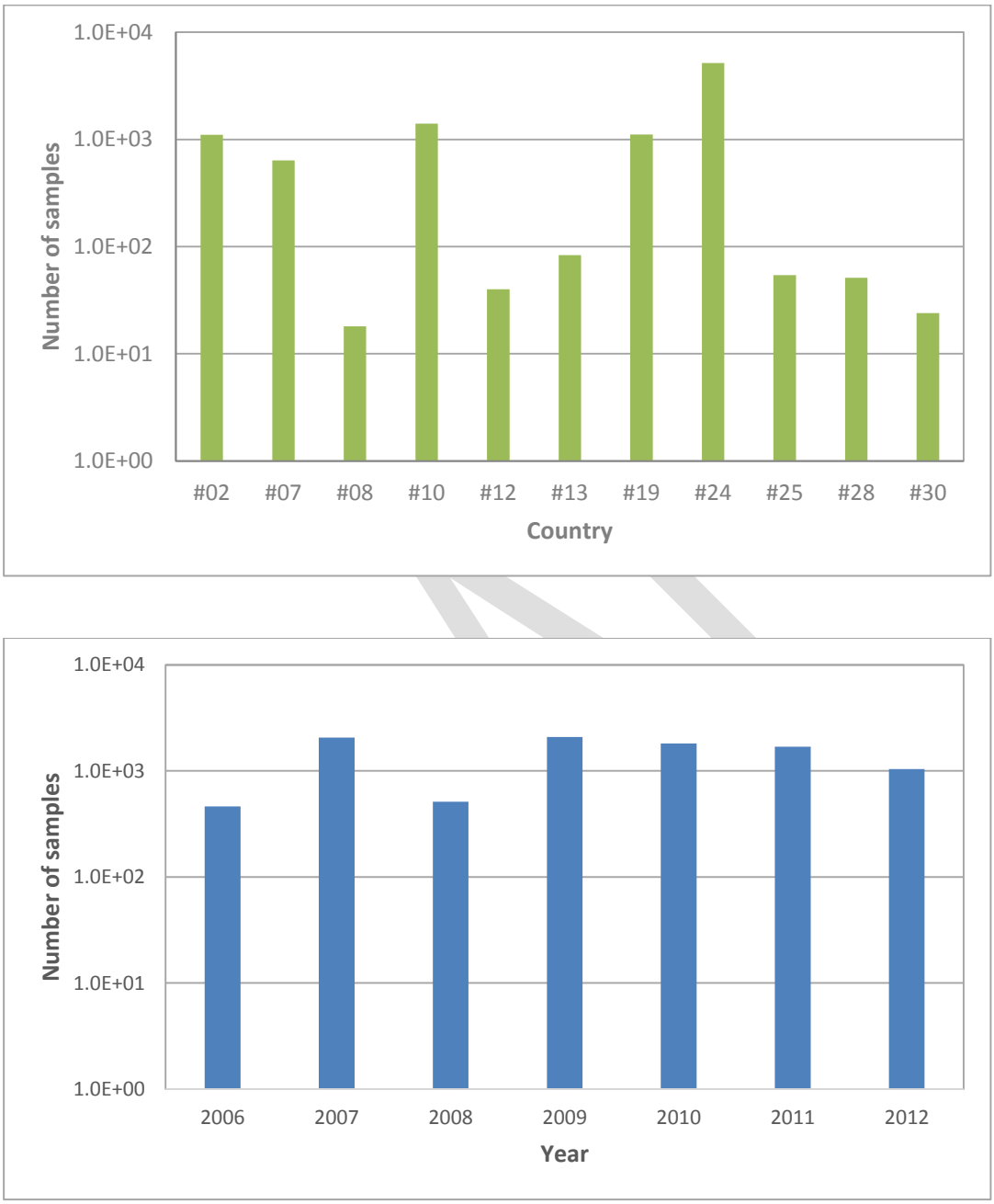


Figure 7. Number of samples for coastal and transitional whole water in Sc2-PNEC QC per country (top) and per year (bottom).

3.2.4. Sediments

The distribution of the monitoring records by country and year for Sc2-PNEC QC sediments is displayed in Figure 8.

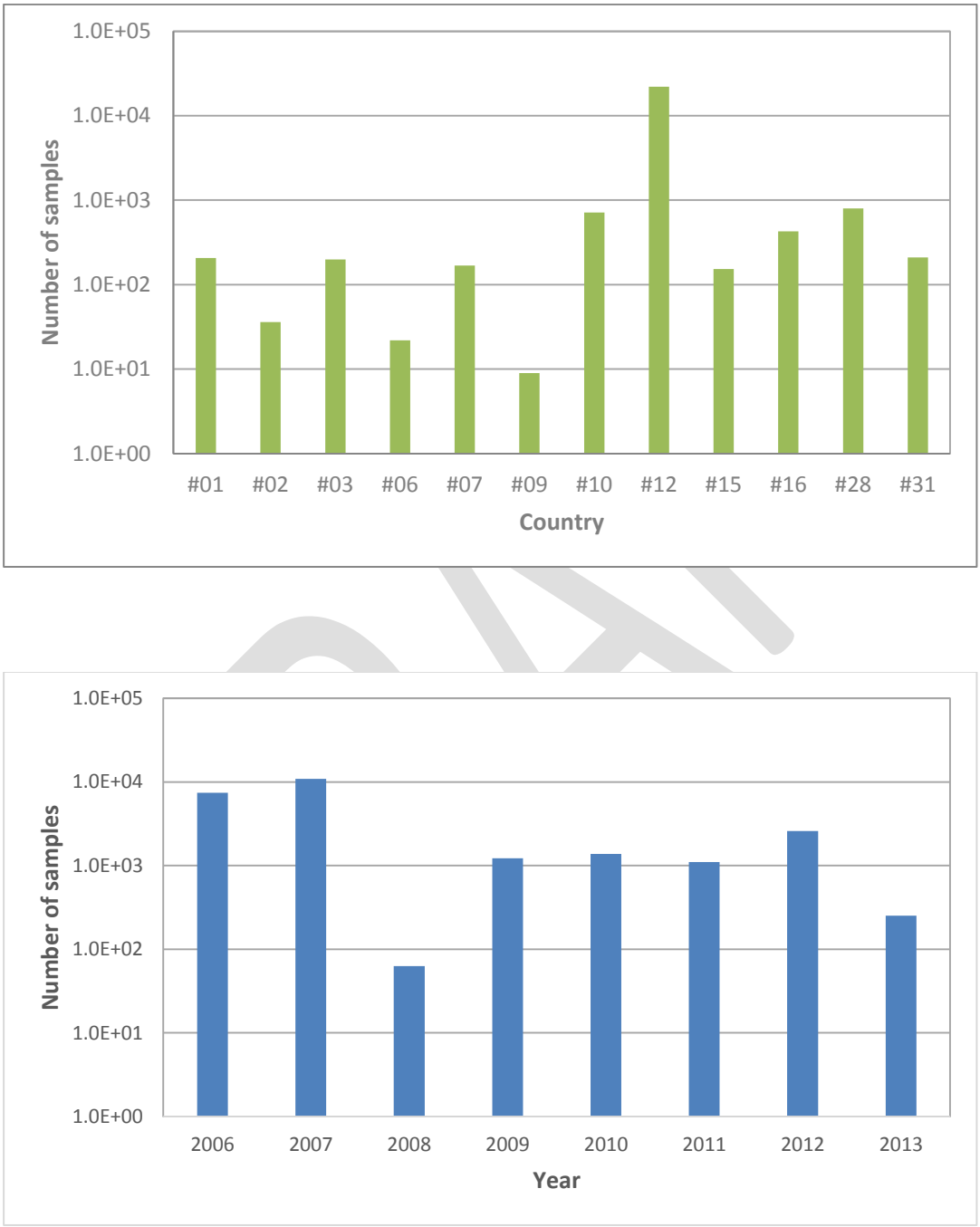
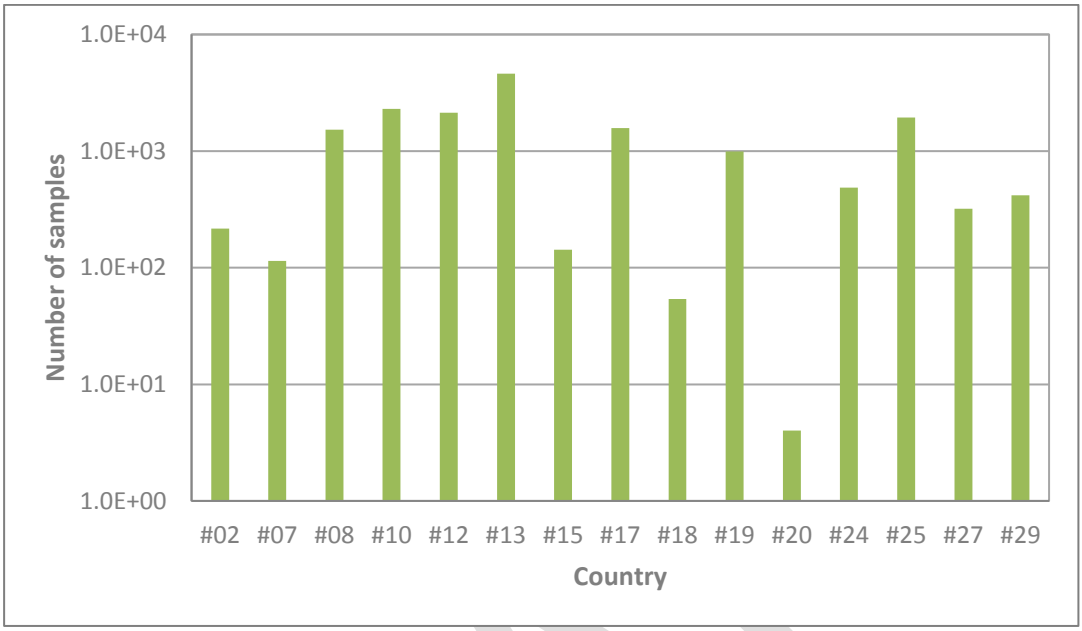


Figure 8. Number of samples for sediments in Sc2-PNEC QC per country (top) and per year (bottom).

3.2.5. Biota

The distribution of the monitoring records by country and year for Sc2-PNEC QC biota (molluscs) is displayed in Figure 9. No figures for biota fish are presented since only one substance was considered in Sc2-PNEC QC.



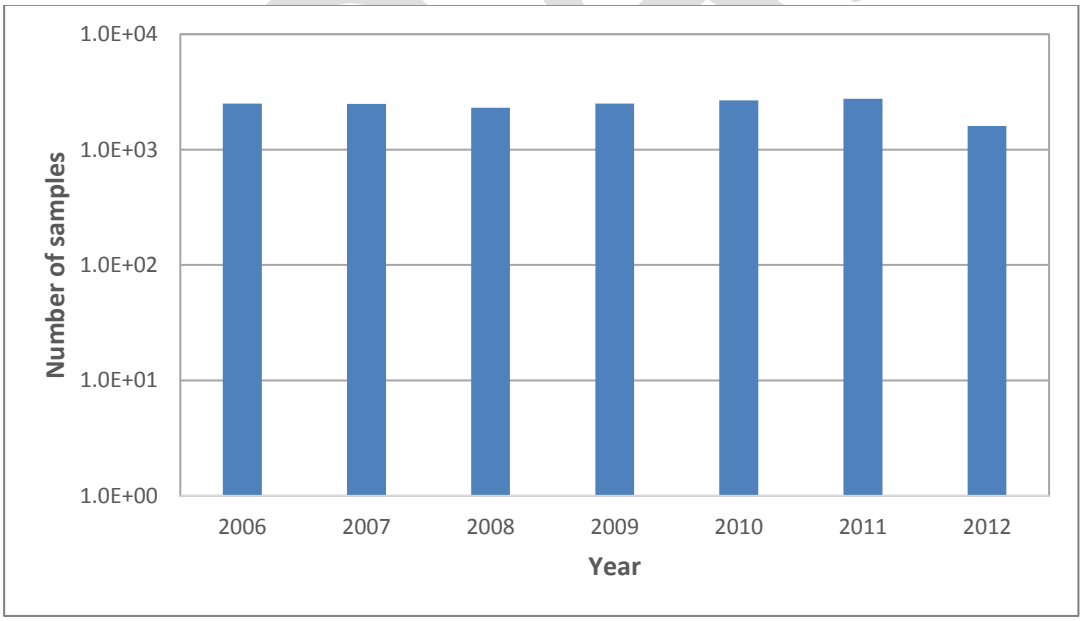


Figure 9. Number of samples for biota (molluscs) in Sc2-PNEC QC per country (top) and per year (bottom).

3.3. Robustness and Sensitive analysis of STE approach

3.3.1. Spatial factor

$F_{spatial}$ is a product of the multiplication of the spatial indicator for exceedances by site ($F_{s,site}$; the first term in the formula) and the correction coefficient for exceedances by country ($F_{s,country}$; the second term in the formula), as described in Section 2.1.1. The $F_{s,site}$ is intended to be the core part of $F_{spatial}$ while the $F_{s,country}$ is making an adjustment to the European scale according to the percentage of the impacted countries. $F_{s,country}$ aims to prevent the attribution of a high $F_{spatial}$ to the substances causing exceedances in a low proportion of countries where they are measured. In other words, thanks to this correction coefficient, substances causing many exceedances in a low proportion of countries will be attributed a lower spatial relevance at EU level.

Most of the monitored substances showed low values of the $F_{s,site}$. For instance, the STE run for inland whole water in Sc2-PNEC QC indicated: 110 substances with $F_{s,site}$ =0; 152 cases when $F_{s,site}$ ≤0.1; 32 cases when 0.1< $F_{s,site}$ ≤0.5 and 30 substances with $F_{s,site}$ >0.5 (in total 324 substances were considered; all metals were included in this exercise; Triclosan, Ethion, and Gemfibrozil, for which supplementary data were collected by additional merging of the dissolved and whole water datasets after the 5th SG-R meeting, also participated).

In addition, for the substances with higher spatial frequency of exceedance per site ($F_{s,site}$ >0.5), the correction coefficient per country is close to one (on average $F_{s,country}$ =0.9), while for those having lower frequency of exceedance per site (range from 0.1 up to 0.5) the correction per country displays a lower value (on average $F_{s,country}$=0.47). An overall good correlation between the values of $F_{s,site}$ and $F_{s,country}$ was found in the STE runs (e.g. R^2=0.83 in the example for the inland whole water Sc2-PNEC QC on Figure 10).

To understand better the link between the country and site indicators in $F_{spatial}$ a frequency analysis of the $F_{s,country}$ was performed excluding zeros (see Table 21). This evidenced that the lower values of $F_{s,country}$ (0< $F_{s,country}$ ≤0.5) are more frequently observed than the higher ones (0.5< $F_{s,country}$ ≤1) (lower $F_{s,country}$ were observed for 74 substances vs. 41 with higher ones).

Thus, the majority of the substances seem to show exceedances from a single or a few countries. Then, if only $F_{s,site}$ was used, it could be expected that some substances would have a high $F_{spatial}$, even though the spatial risk is limited to only a few countries. To make sure that only substances showing a high risk at EU level are identified by STE, the correction of $F_{spatial}$ by $F_{s,country}$ coefficient is required for making a proper evaluation of substances.

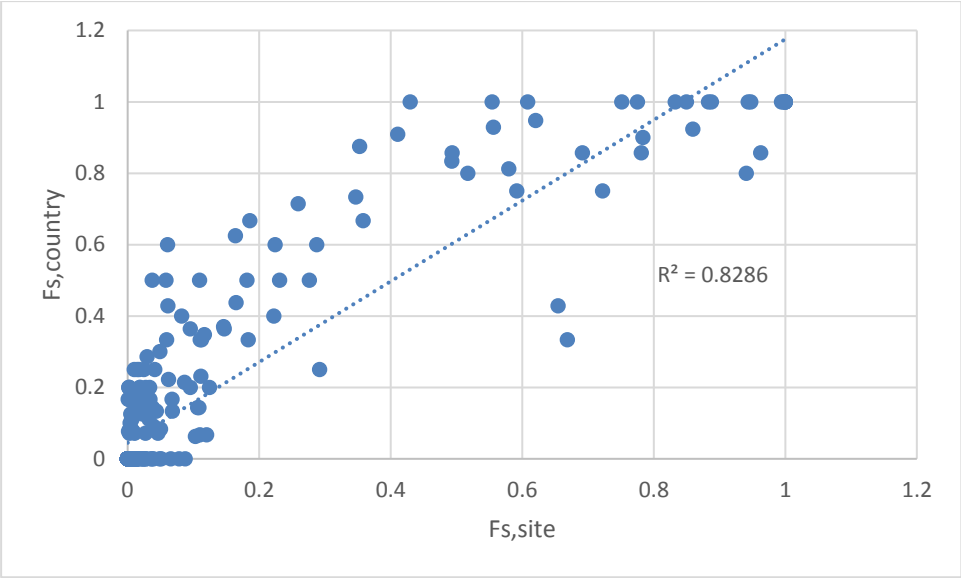
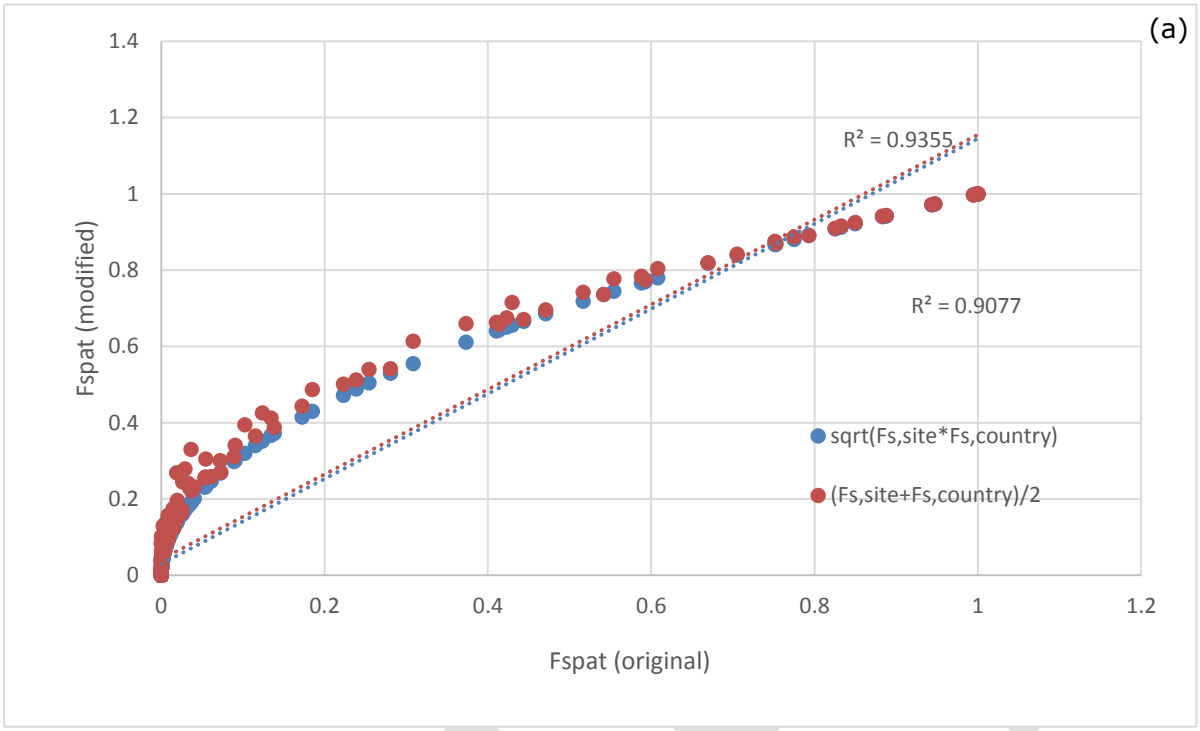


Figure 10. Accordance between the spatial indicator by country (*Fs,country*) and the spatial indicator by site (*Fs,site*) found in the STE run for the Inland whole water Sc2-PNEC QC.

Table 21. A frequency analysis of the country correction coefficient (Fs,country) for Inland whole water Sc2-PNEC QC.

Range of Country correction coefficient ($F_{s,country}$)	Number of substances
$F_{s,country}$ =0	209
0 < $F_{s,country}$ ≤0.5	74
0.5 < $F_{s,country}$ ≤1.0	41

Different formulae could be used to calculate $F_{spatial}$ based on $F_{s,country}$ and $F_{s,site}$ (as suggested by the experts and widely discussed at the 5th SG-R meeting) while still keeping the corrective effect of $F_{s,country}$. Thus, $F_{spatial}$ was tentatively calculated as i) half of the sum of $F_{s,site}$ and $F_{s,country}$ (($F_{s,site}$ + $F_{s,country}$)/2), or ii) equal to the squared root of their product: (sqrt($F_{s,site}$*$F_{s,country}$)). These alternative calculations have been compared with the formula of the spatial factor, presented in the section 2.1 of this report (see Figure 11). The impact of these different formulas on the STE approach was investigated to make sure that they produce concordant outcomes with respect to the STE scores, especially for the highly ranked substances, which are the preferential candidates to be short-listed and move forward in the prioritisation (see Figure 11). Although some minor deviations were observed in the low and intermediate range of STE scores (as expected the new formulae give a slightly higher STE values), it was found that the different approaches for calculation of $F_{spatial}$ showed comparable and quite similar STE scores (R^2=0.988 for the half of the sum and R^2=0.992 for the square root; see the scatter plot shown in Figure 11).



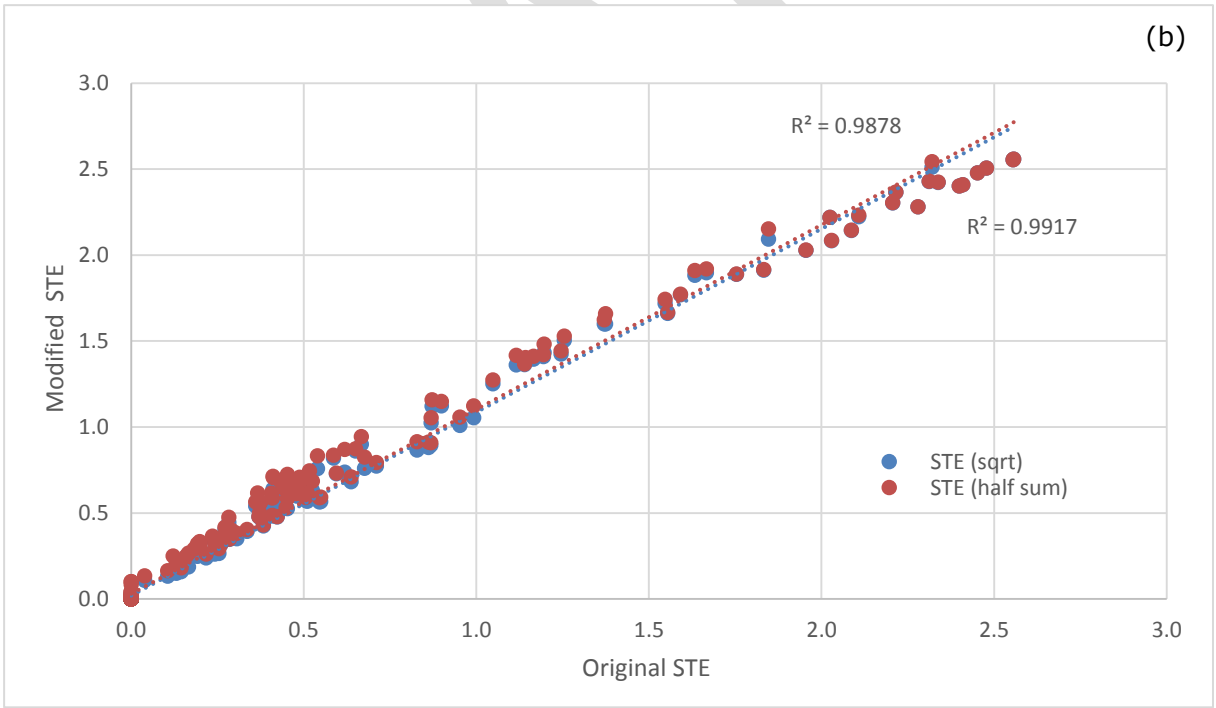


Figure 11. Comparison of $F_{spatial}$ (a) and STE scores (b) obtained by different formulae – the original formula (section 2.1.1), the half of the sum of *Fs,site* and *Fs,country* (*Fs,site*+*Fs,country*)/2) and the squared root of their product sqrt(*Fs,site*Fs,country*).**

In addition, we checked a possible change of the risk-based rank of substances for the most abundant dataset of inland whole water Sc2-PNEC QC according to STE scores

calculated using different formulae of $F_{spatial}$ (the distribution by risk-based rank is shown in Table 22). It was found that some substances will be shifted to a higher risk rank (in particular those with lower values of $F_{spatial}$ and respectively lower STE score). The detailed list of substances that increase their STE score and shift to higher risk rank when square root or mean of $F_{s,site}$ and $F_{s,country}$ is applied in $F_{spatial}$ of STE method is presented in Table 23. For instance, two substances (Mevinphos and Uranium), among those selected for a preparation of detailed factsheets, slightly increased their STE scores, but more impacted are some substances positioned in the low range of the risk rank (they are highlighted in blue in the Table 23) since they will increase their rank to intermediate. However, this will not change at all the selection of the top-ranked substances proposed for short-listing and eventual prioritization.

Table 22. Risk rank distribution according to STE scores calculated using different formulae of $F_{spatial}$ (original and square root or half of the sum of *Fs,site* and *Fs,country*) for substances in inland whole water Sc2-PNEC QC.

Risk rank	Number of substances		
	STE(original)	STE(sqrt)	STE(half sum)
Very high	6	10	10
High	14	13	13
Intermediate	10	14	14
Low	21	27	33
Very low	273	260	254

Table 23. List of substances that increase their STE score and shift to higher risk rank when square root or half of *Fs,site* and *Fs,country* is applied in $F_{spatial}$ of STE method (Note: the table considers only substances with very high, high and intermediate risk ranks; the substances that will move from low to intermediate risk rank are highlighted in blue).

Substance	STE(original)	STE(sqrt)	STE(half sum)
2-Hydroxyatrazine	2.400	2.403	2.403
Chrysene	2.338	2.422	2.423
Uranium	2.321	2.511	2.544
Mevinphos	2.313	2.428	2.430
Aluminium	1.753	1.888	1.890
Chlorpyriphos methyl	1.667	1.897	1.919
Triphenyltin	1.633	1.882	1.911
Dibenz(a,h)anthracene	1.196	1.434	1.483
Iron	1.195	1.410	1.420
Ammonia	1.166	1.395	1.410
Diclofenac	1.142	1.392	1.403

Permethrin	1.140	1.363	1.368
Thallium	1.116	1.361	1.417

In conclusion, the above comparison confirms the robustness of the original formula for the $F_{spatial}$ (Section 2.1.1) and completely motivates the usage of the country correction coefficient in its original form (section 2.1.1) in the STE scoring system.

3.3.2. Temporal factor

For a given substance $F_{temporal}$ estimates the frequency of exceedances (i.e. the average of the percentages of samples with exceedance per site) for the entire time-period of assessment. Thus, the purpose of $F_{temporal}$ is to identify the substances that frequently (or permanently) showed exceedances during the time-interval considered: given two substances with similar extents of exceedance (calculated by F_{extent}) and a similar spatial distribution of the exceedances (represented by $F_{spatial}$), it seems relevant to give a higher score to the substance for which the PNEC is exceeded more frequently.

The statistical analysis of $F_{temporal}$ for substances in inland whole water Sc2-PNEC QC showed 2.2 times more cases with lower (≤0.5) than higher (>0.5) values of $F_{temporal}$ (160 vs. 73 excluding zeros). This means that the high temporal exceedances do not happen so frequently. On the other hand, there are substances which are ranked spatially as intermediate or even low but their concentrations exceed very frequently the toxicological limit during the time period considered. Since each substance is measured in at least 4MS, the lower $F_{spatial}$ is not a guarantee for no concern and therefore the additional temporal scoring points assigned to these substances are important.

In the STE method, $F_{spatial}$ relies on the P95 of the concentrations while $F_{temporal}$ includes all measurements. For this reason, some inconsistency may appear between $F_{spatial}$ and $F_{temporal}$ ($F_{spatial}$ may be equal to 0 while $F_{temporal}$ does not). To solve this issue, a further adjustment (harmonization) was made by setting $F_{temporal}$=0 when $F_{spatial}$ =0. This modification was introduced into STE assessment tool after the 5th meeting of SG-R. The harmonisation correction has impacted only the low scored substances and doesn't change the top-ranked ones.

Finally, as decided at the 5th meeting of SG-R, the $F_{temporal}$ (see section 2.1.2) will continue to be calculated only for sampling stations that have at least 2 measurements for a given substance (this is the minimum number of records that allows consideration of a temporal trend; for instance, the request to increase the limit to 4 samples per site, or more, will be a quite severe restriction to short time series). Also the minimum limit of 2 samples per site is consistent with the monitoring requirement for substances included in the first watch list: these substances have to be monitored at least once a year, two years in a row, to generate data to inform the prioritisation.

3.3.3. Extent factor

The assessment of the extent of PNEC exceedances, as performed in the STE approach, has been applied previously for the risk-based prioritisation of substances (von der Ohe et al., 2011); Slobodnik et al. 2012). The use of the extent of exceedance factor F_{extent} (section 2.1.3) allows to differentiate the scale/size of the impact that the substances can have.

For example, a 1000-times exceedance, even being only a single event, could make an irreversible change in any aquatic system and will impact the species drastically on a long term. Therefore, the substances which largely exceed the toxicological threshold (PNEC or EQS) should obtain additional scoring points. This is the rationale behind the applicability of the F_{extent} in its current form in STE scoring tool.

The analysis performed for inland whole water in Sc2-PNEC QC indicated that 79 substances have an EXC_{extent} index between 1 and 100, compared to 20 substances with an EXC_{extent} superior to 100 (see Table 24). For that reason, the JRC has refined the evaluation (normalization) table that transforms the parameter EXC_{extent} to F_{extent}. The proposed modification includes additional reference levels in the lower range of EXC_{extent} values (see Section 2.1.3).

Table 24. Range of exceedance extent and corresponding number of samples for inland whole water in Sc2-PNECQC.

EXC_{extent} (range)		Number of substances
≤1		254
<1	≤10	47
<10	≤100	32
<100	≤1000	15
1000<		5

Finally, the F_{extent} was also harmonized/synchronized with $F_{spatial}$ similarly to the temporal factor - when $F_{spatial}$ =0 then F_{extent} =0. Likewise to the temporal factor the introduction of the harmonisation correction has no impact on the top-ranked substances.

3.3.4. Independence of STE factors

At first glance the STE factors may seem correlated since all of them are based on the measured concentrations and on exceedances of toxicological threshold. Indeed, one could argue that P95 of concentrations used in the spatial and extent factors contains indirectly the temporal pattern for each monitoring site. However, the STE factors assess the substances from completely different perspectives:

- $F_{spatial}$ shows how large (wide) is the impact spatially by accounting the number of sites (as percentage from total) where exceedances are observed at least once (P95 of concentrations per site is used)
- F_{extent} specifies the size (scale) of exceedance taking P95 of all individual Risk Quotients (RQ_{P95}) per site
- $F_{temporal}$ quantifies how frequently (as average percentage) the exceedances happened per site (all concentrations per site are considered).

In addition, the detailed investigation done on the monitoring dataset for the existing Priority Substances (Carvalho et al., *in preparation*; results presented at the 4th SG-R meeting in September 2015), concluded that the three STE factors are satisfactory independent from a statistical point of view (low correlation coefficients were observed).

The validity of these conclusions is confirmed once again for the wider dataset of emerging substances considered in this report. For instance using the results of STE run for the inland whole water Sc2-PNEC QC, Figure 12 demonstrates a low correlation between the Temporal and Spatial factors, and Figure 13 evidenced low link between the Extent and Temporal factors. A similar low correlation was found for F_{extent} and $F_{spatial}$ (not shown). In addition, these scatter plots show the capability of the STE factors to grasp the specific

cases of frequent temporal exceedances or the extreme extent of exceedances. All these evidences strengthened the confidence about the independence of the STE factors.

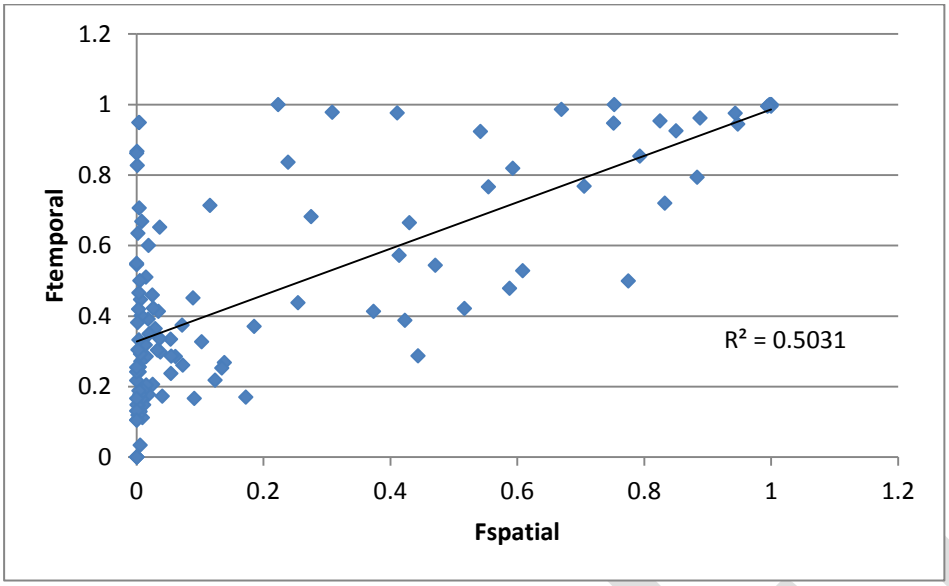


Figure 12. Example of low connectivity of the Spatial and Temporal factors (the zero values of $F_{spatial}$ were excluded).

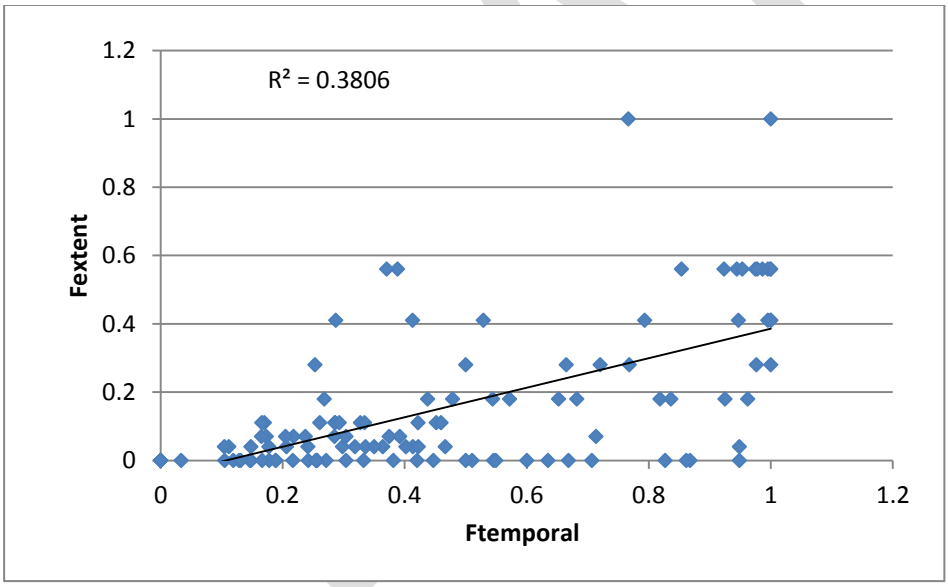


Figure 13. Example of low connectivity of the Extent and Temporal factors (the zero values of $F_{temporal}$ were excluded).

Finally, since the different STE factors were found to be independent from statistical point of view, it is reasonable/acceptable to sum these three different estimates and to establish a single and representative STE score (assessment) for each substance.

3.3.5. Sensitivity analysis of STE

The numerous STE runs performed showed that the method is sensitive to the number of samples and sites where the substances are measured (see for example in section 3.4.1 the comparison of results between the different data scenarios for inland whole water obtained either by all monitoring records (Sc2) or with the reduced monitoring records that fulfil the PNEC quality check, i.e. ½ LOD/LOQ ≤ PNEC (Sc2-PNEC QC). Therefore, before applying the STE a detailed statistical analysis of datasets is always needed in order to avoid inconsistent and unrealistic outcome. In particular, it is important to check that a sufficient number of measurement stations and records per substance are available while discarding records of a given substance, for example, measured occasionally or just once at individual sites. This was done by setting requirements on data for the minimum number of countries and sites with measurements, a minimum overall number of samples, and a minimum number of samples per site (at least 4 countries, more than 10 sites, more than 50 samples overall, and more than 2 samples per site).

Expectedly, the STE method is also very sensitive to the PNEC (EQS) values. Therefore, a special attention should be paid to this very important input parameter in the prioritisation process, as the uncertainty leveln in the PNEC derivation could have a significant inpact in the number and extent of exceedances (Carvalho et al., 2016, *in preparation*).

3.4. Assessment of metals

Metals, because of their unique properties, are critical to many of the technologies that modern society relies on. Metals are naturally present in the aquatic environment, but can also be released to it as a consequence of industrial manufacturing, consumer use and recycling. Metals, though naturally present in surface waters, can represent a threat to freshwater organisms. They are therefore an important group of compounds for chemical risk assessment. In Europe, these risks are managed by several pieces of legislation including REACH and the Water Framework Directive. The risk is difficult to assess however, because surface waters differ in observed toxicity of metals due to differences in water characteristics and consequently in speciation of metals. Total or dissolved metal concentrations only give a crude impression of potential effects of metals on aquatic organisms. Only a portion of the total amount of metal in the environment can be taken up by organisms and cause adverse effects, and toxicity is dependent on other factors, such as the characteristics of the water. Recognition of this complexity led to techniques that predict toxicity based on more than just metal concentration, using the concept of bioavailability. A metal is bioavailable when it is free for uptake by an organism and can react with its metabolism, possibly causing a toxic effect. This concept recognises that the toxic effect of a metal depends not only on its concentration, but also interactions with chemical and biological factors. Based on this understanding, Biotic Ligand Models **(BLMs)** have been developed to predict metal bioavailability in aquatic environments and their ability to cause effects in living organisms. Although the first tier assessment consists of comparison of total dissolved water concentrations with generic environmental quality standards, it is recognized that this is only a first step in risk assessment. The risk assessment may be refined, and the concept of bioavailability of toxic compounds is adopted for the second tier risk assessment. The BLM approach has been described in many peer-reviewed publications. Recently developed user-friendly BLM-based software tools can assess the toxicity of metals using a basic set of easy to measure water parameters, such as pH, hardness and dissolved organic carbon (DOC). These simplified tools are more appropriate for routine site-specific water quality assessments and can be used by non-experts. Thanks to these developments, BLMs can now be used effectively for regulatory risk assessment purposes. Compared to the traditional approach, based on total or dissolved concentration, BLMs provide a more realistic assessment of the effects metals may have on aquatic communities. The EQS Directive (2008/105/EC, amended by Directive 2013/39/EU) now includes bioavailable EQSs, for certain substances, and specifies that "Member States may, when assessing the monitoring results against the relevant EQS, take into account: hardness, pH, dissolved organic carbon or other water quality parameters that affect the bioavailability of metals, the bioavailable concentrations being determined using appropriate bioavailability modelling". Examples of this approach are reported by www.bio-met.net; Rüdel et al., 2015; Verschoor et al., 2011.

Following the implementation of the WFD some European countries (DE, NL, UK) began to feature BLMs in their regulations for monitoring water quality and risk assessment. So far, only a few countries have adopted the BLM-based water quality assessments. The UK and the USA have legally implemented tools at least for single metals (e.g., M-BAT in the UK), while in The Netherlands a tool is endorsed by the administration (i.e., PNEC.pro by the Dutch Ministry of Infrastructure and the Environment) (Rüdel et al., 2015).

3.4.1. Biomet software tool

Bio-met bioavailability tool is a free online resource for assessing the risk of metals in the freshwater aquatic environment, particularly within the EU Water Framework Directive. The bio-met site is currently focussed on copper, nickel and zinc, but may be extended in the future to include other metals. The biomet-model calculates for copper, nickel and zinc site-specific quality standards (expressed as dissolved metal concentrations) for the combination of site-specific pH as well as Ca and DOC concentrations, as well as the bioavailable metal concentration from the measured dissolved metal concentration (www.bio-met.net).

3.4.2. Zinc: a case study to implement the bioavailable concentration in STE methodology

The JRC received directly from 2 countries zinc (dissolved) monitoring data matched with supporting data on pH, DOC and calcium. In addition, the EEA provided to the JRC excel files with supporting data on Ca, Mg, hardness, DOC, and pH. All data were checked for completeness in order to run the biomet-model. Unfortunately, the necessary information on pH, DOC, and Ca (or hardness) was available only from very few countries. These supporting data were then matched with the available monitoring data for Zn (dissolved) by comparing the sampling stations and monitoring dates. However, matching data could be found only for 2 additional countries.

The Table 25 shows the number of samples and sampling stations for the four countries (#01; #12; #13; #20). Since for the last two countries only few data are available and the sampling period in the country #01 is longer than for countries #13 and #20, for the pilot study only the countries #01 and #12 have been used.

Table 25. Summary of the number of samples and sampling stations for the four countries for which supporting data for pH, DOC and hardness could be matched with the monitoring data.

	Country #01	Country #12	Country #13	Country #20
Number of samples	1.522	242	14.331	86 (quantified 37)
Number of sampling stations	40	124	1.353	16 (quantified 15)
Sampling period	2007-2014	2010-2012	2012-2014	2009, 2011, 2012

The bioavailable concentration has been calculated with the biomet-software-tool and the STE runs have been performed by using either the dissolved or the bioavailable concentration. In the case of country #01, for 114 of the 1.522 samples the supporting data were out of the validated range of the biomet-model, and in the case of country #12, 2.455 of the 14.331 samples. In addition, the records from stations with single measurements were discarded, so that in total 11.556 samples remained for these two countries. The results for the countries #01 and #12 are summarised in Table 26, showing dissolved and bioavailable concentration; the pH, DOC and hardness are shown as well. The values out of applicability of the biomet-model have been excluded, because the biomet-model is valid only in a certain range of pH, DOC and Ca concentrations.

Table 26. Results for the countries #1 and #12 for which more robust data were available to derive the bioavailable concentration. The table shows the concentration for dissolved and bioavailable concentrations.

	Measured Zn (dissolved) (µg/L)	pH	DOC (mg/L)	Ca (mg/L)	Zn (bioavailable) (µg/L)
Min	0.5	5.5	0.5	6.5	0.07
Median	**7.3**	7.9	2.1	49.2	**2.3**
Average	**47.3**	7.8	3.1	60.8	**27.4**
90th P	66.6	8.2	6.1	111	27.7
95th P	174	8.3	7.5	164	111
Max	3710	8.5	122	268	2574

The average Zn (dissolved) concentration is reduced from 47.3 µg/L to 27.4 µg/L (bioavailable), and the median from 7.3 µg/L to 2.3 µg/L.

The raw data of scenario 2 for countries #1 and #12 have been then used to run the STE; the results are given in Table 27. As expected, the STE score is lowered from 1.46 (dissolved) to 0.6 (bioavailable) Zn, respectively, which represents approximately a 59% of reduction. Also a comparison with the generic non-bioavailable PNEC of 20.6 µg/L is shown, which gives a STE score of 0.69 for dissolved and 0.39 for the bioavailable zinc (44% reduction). The comparison with the higher generic PNEC is done in order to investigate the need for the bioavailability correction approach.

Table 27. Comparison of the STE scores for countries #1 and #12 for dissolved zinc or bioavailable zinc (scenario2).

Substance	Fspat	Ftemp	Fext	Final Score	PNEC (µg/L)
Zinc dissolved	0.78	0.57	0.11	**1.46**	10.9
Zinc dissolved	0.31	0.31	0.07	**0.69**	20.6
Zinc bio	0.21	0.32	0.07	**0.60**	10.9
Zinc bio	0.04	0.31	0.04	**0.39**	20.6

Table 28 shows the score values for Zn considering the whole European data set, which suggests that the two countries #01 and #12 provide a robust and representative data as first pilot study.

Table 28. Comparison between the STE scores for Zn calculated from all samples in inland dissolved water in Europe considering the bioavailable and non-bioavailable PNEC values.

Scenario	Substance	Fspat	Ftemp	Fext	Final Score	PNEC (µg/L)
Sc2	Zinc dissolved	0.44	0.57	0.11	**1.12**	10.9
Sc2	Zinc dissolved	0.20	0.52	0.11	**0.82**	20.6
Sc2-PNEC QC	Zinc dissolved	0.39	0.50	0.18	**1.07**	10.9
Sc2-PNEC QC	Zinc dissolved	0.17	0.44	0.11	**0.72**	20.6

In conclusion, this exercise is the first pilot study to run and compare the STE analysis by using either the dissolved or the bioavailable concentration for Zn. Good datasets for Zn (dissolved), pH, DOC, and calcium were available from two countries. The results showed that the STE score is reduced (by approximately 59%) by using the bioavailable Zn. However to evaluate the European scenario more data on pH, DOC and hardness across Europe is needed together with the zinc monitoring data.

For metals that have well developed bioavailability models available, such as Cu, Zn, and Ni, it is generally preferred to use dissolved concentrations, and to calculate the bioavailable concentrations with a bioavailable PNEC. However, if for some reason the bioavailability correction cannot be estimated, then the use of the dissolved concentrations and a non-bioavailable but reliably derived dissolved PNEC/EQS could be considered as a reasonable approximation in the risk assessment of metals.

3.5. Outcome of the STE analysis

The STE approach was applied to all substances with monitoring data that passed the criteria laid out under Section 2.2. A separate STE was run for each environmental compartment and receptor at risk, as described in section 2.4.1:

i) fresh whole (or dissolved) water - risk to aquatic organisms (eco, fw)

ii) fresh water - risk to humans via consumption of drinking water (hh, dw)

iii) fresh water - risk to humans via consumption of fish products (hh, food)

iv) salt whole (or dissolved) water - risk to aquatic organisms (eco, sw)

v) sediment - risk to benthic organisms (eco, sed)

vi) biota - risk to aquatic organisms from secondary poisoning (eco, secpois)

The STE analysis was run, after the additional quality check of data, for quantified records plus non-quantified excluding those for which 1/2 LOD/LOQ>PNEC (Scenario2-PNEC QC) and additionally (only for completeness) for all monitoring samples (Scenario 2). The total number of substances considered in the monitoring-based exercise is 326 in Sc2-PNECQC and 354 in Scenario 2. The results from the STE runs are presented in Annex IV. The highest ranked substances are shown in Table 29.

3.5.1. Comparison between the different STE analyses

The STE analysis was run for different scenarios, corresponding to differently-treated monitoring datasets, as well as different statistical measures (95th percentile or max values). The different scores obtained have been compared, to verify how consistent the rankings based on the different calculations are.

Figure 14 shows the comparison between the scores using the 95th percentile and the max concentration in the STE calculations for inland whole water in Sc2-PNEC QC. It is observed that the scores obtained with either the 95th percentile or the max values are quite consistent. Particularly for the top ranked substances with very high, high and intermediate risk classifications (STE score > 1.2) the average deviation is 1.1% with a range from 0% up to 7.4% (for lower scored substances - STE≤ 1.2, the average deviation is 14.7% with a range from 0% to 100%). This suggests that the selection of the 95th percentile over the max for the substance assessment is not critical for the final outcome of the monitoring-based exercise. This analysis confirmed again the suitability of using 95th percentile of sampled concentrations per site or per country. The decision of the application of 95th percentile in the STE tool was approved during the 4th and 5th meetings of SG-R.

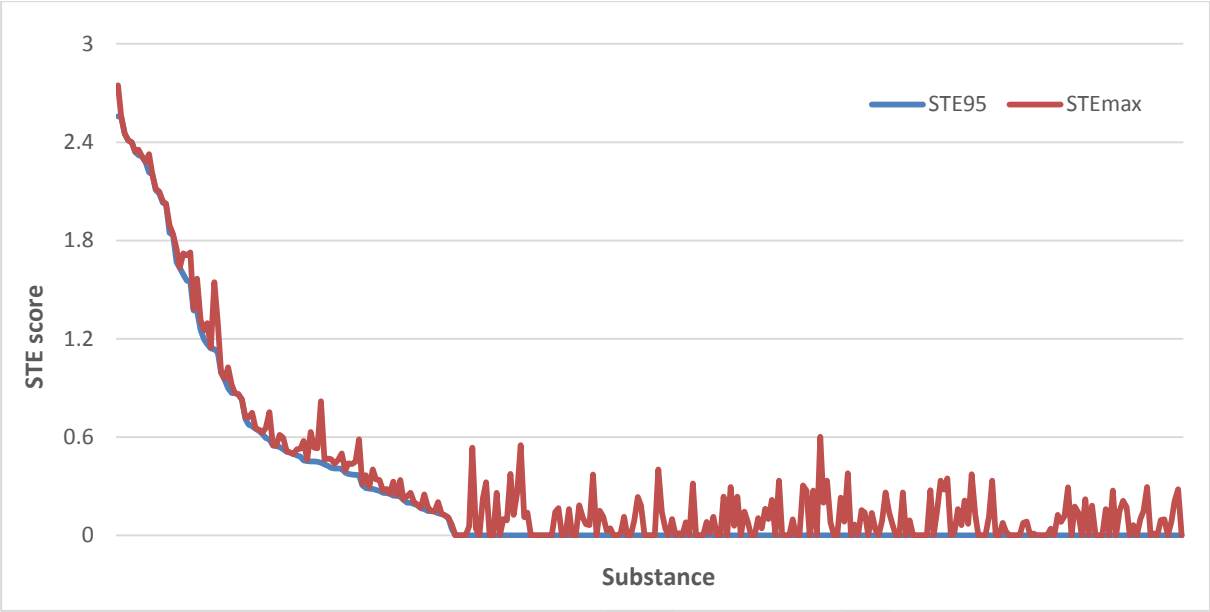


Figure 14. Comparison between the STE scores obtained by using either the 95th percentile or the max concentration at each monitoring site for substances into the STE calculation for inland whole water, and the monitoring data scenario Sc2-PNEC QC.

Figure 15 present the comparison of STE scores for the inland whole water under two different data scenarios (Sc2 and Sc2-PNEC QC). As expected, the Sc2 leads sometimes to an increase in the number of exceedances (that obviously increases the STE scores). This is explained by the assignment in Sc2 of the artificial concentration of ½ LOD/LOQ to all non-quantified values, while part of these values are excluded from Sc2-PNEC QC if the analytical method is not able to detect the substance close to its PNEC.

It can be seen from Figure 15 that the magnitude of the deviations between the two scenarios increases from the group of the top-ranked substances (STE>1.2; average deviation of 9.9% with a range from -5.4% up to 36.9%) to the low-scored substances (STE<1.2; on average 93%; a range from -11% to 683%). However, the second group is of less interest in the monitoring-based prioritization because of the lower calculated risk. Considering the above, it was justified to perform the ranking of substances by Sc2-PNEC QC. This conclusion was supported by the experts participating to the 4th meeting of SG-R.

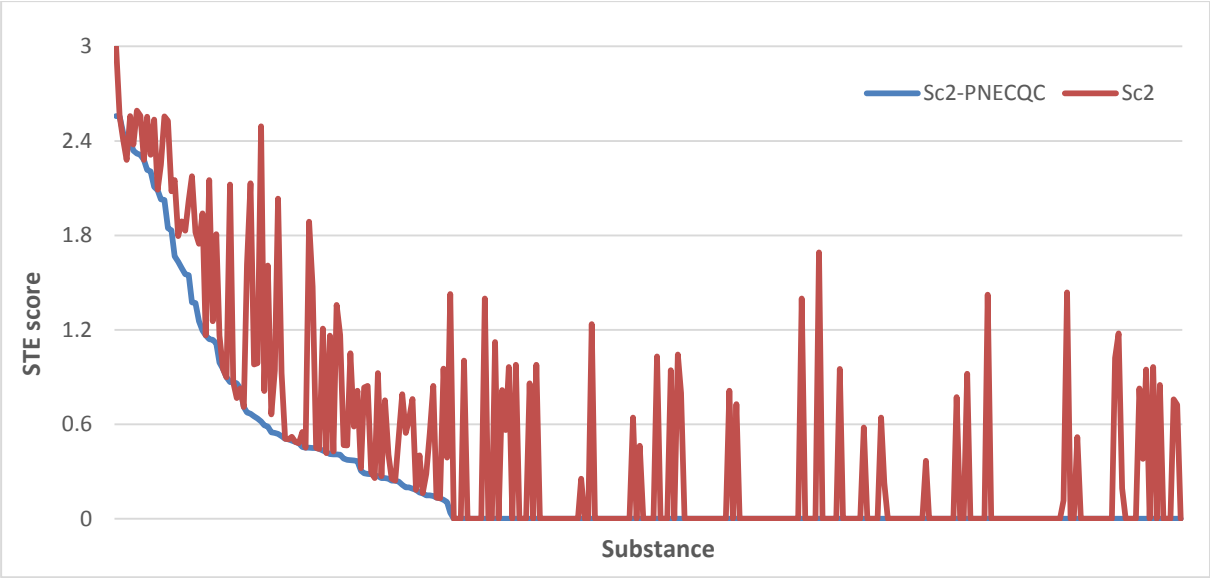


Figure 15. Comparison between the STE scores for inland whole water obtained by using the 95th percentile of concentration at monitoring stations for 2 data scenarios: either all monitoring records (Sc2) or a reduced dataset that that fulfils the PNEC quality check (Sc2-PNECQC) i.e., quantifed samples plus non-quantifed samples when PNEC ≤ ½ LOD/LOQ.

3.5.2. Ranking of substances

For ranking substances, the highest STE score derived from all compartments, has been selected. As a graphical illustration, only the results from the STE analysis in inland whole water (InlWh) Sc2-PNEC QC are presented. For instance Figure 16 shows the ranking for substances in the group classified as posing very high, high and intermediate risk while Figure 17 shows the ranking for the substances classified as posing low or very low risk, but excluding those for which the STE score was zero.

Then, the STE scores obtained for the different environmental matrices and receptors at risk are presented in Table 29. The details, related to STE factors, risk quotients, etc., are provided in Annex IV. The monitoring data used to score the substances are from Scenario2-PNEC QC (summarised under Annex II) while the applied PNEC values are summarised in Annex III. Substances are only shown if their final STE score > 0.

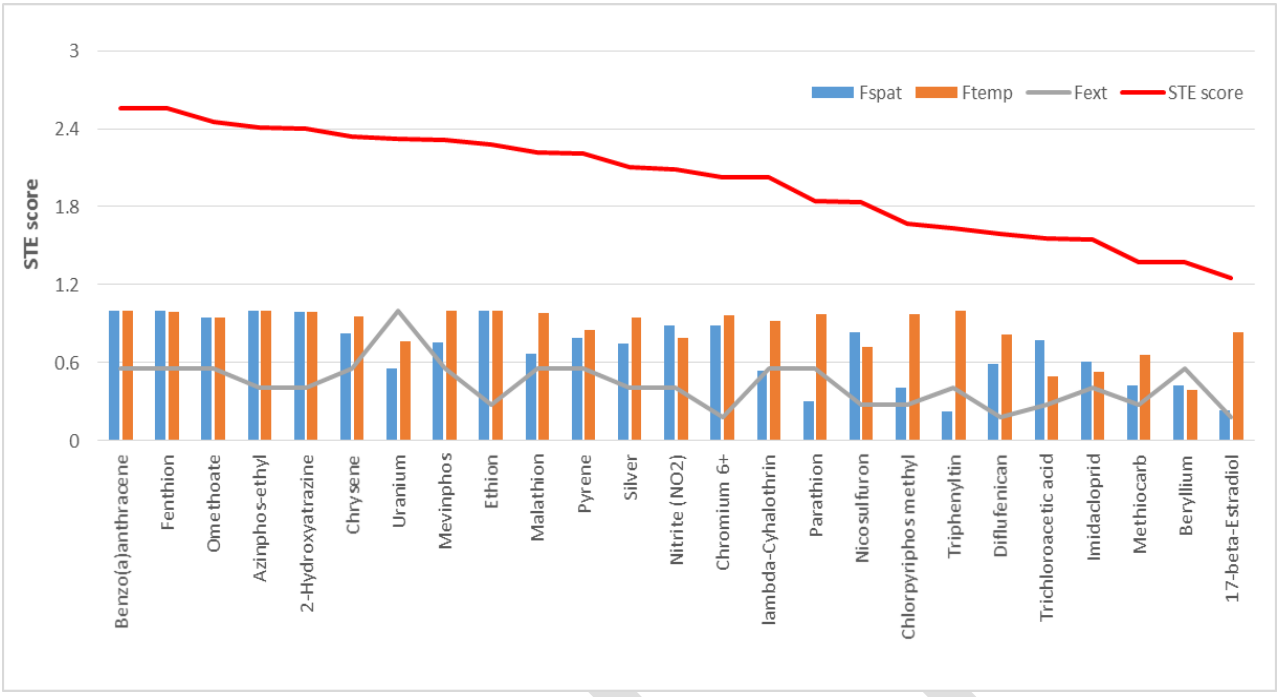


Figure 16. STE scores for substances in inland whole water, using the 95th percentile of concentrations at monitoring stations in STE run for Sc2-PNEC QC. Only substances which risk is classified as very high, high or intermediate are shown.

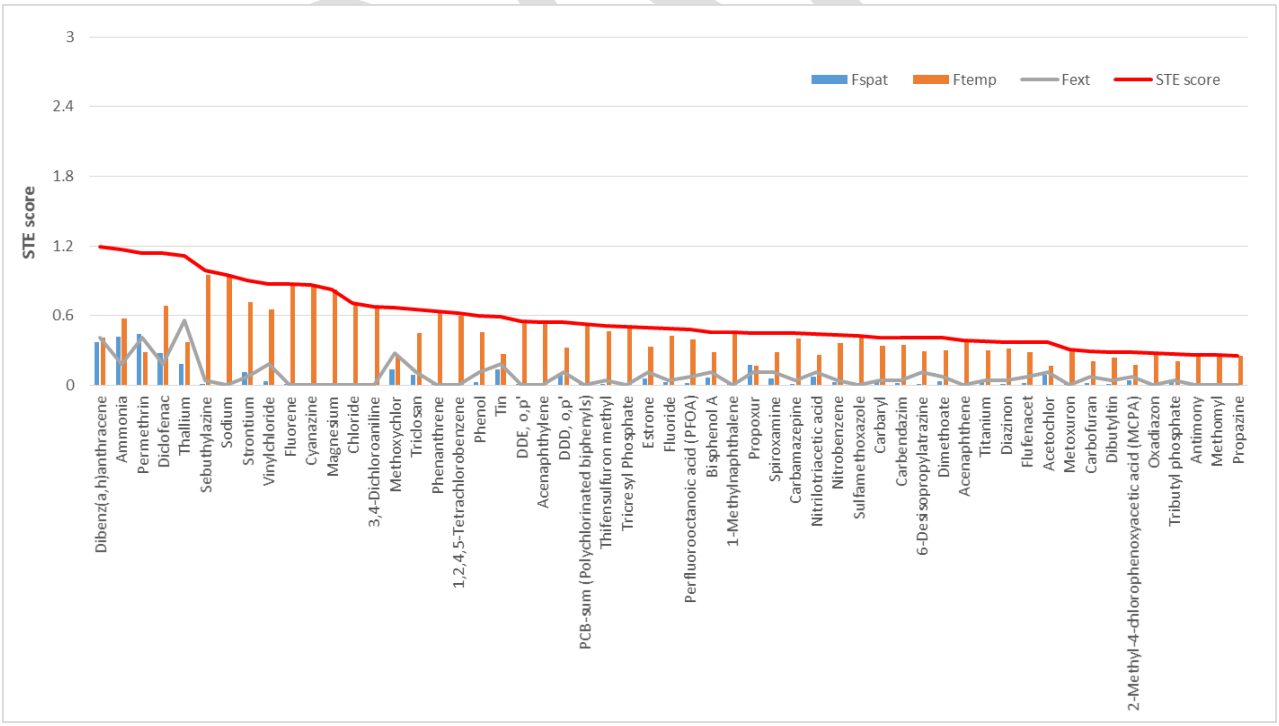


Figure 17. STE scores for substances in inland whole water, using the 95th percentile of concentrations at monitoring stations in STE run for Sc2-PNEC QC. Only substances which risk is classified as low or very low, but not zero are shown.

Table 29. Comparison of STE results in different environmental matrices and receptors at risk when the final STE score > 0 (the individual scores are listed in Annex IV). In the STE runs the selected monitoring data refers to Scenario2-PNEC QC (summarised under Annex II) while the PNEC values are summarised in Annex III.

CAS number	Substance	STEfw whole,eco	STEfw dissv, eco	STEsw whole,eco	STEsw dissv,eco	STEsed, eco	STEbiota (mollusc), sec pois	STEbiota (fish), secpois	STEwater, hh food	STEfw dissv dw,hh	STEfw whole dw,hh	STE score
56-55-3	Benzo(a)anthracene	2.557		0.000		1.443	1.966		1.088		0.578	2.557
55-38-9	Fenthion	2.555									0.000	2.555
1113-02-6	Omethoate	2.452									0.000	2.452
2642-71-9	Azinphos-ethyl	2.410									0.253	2.410
2163-68-0	2-Hydroxyatrazine	2.400									0.000	2.400
218-01-9	Chrysene	2.338		0.000			2.229					2.338
7440-61-1	Uranium	2.321									1.220	2.321
7786-34-7	Mevinphos	2.313									0.000	2.313
563-12-2	Ethion	2.280									0.000	2.280
121-75-5	Malathion	2.216									0.000	2.216
129-00-0	Pyrene	2.207		0.388			2.094		0.515		0.247	2.207
7782-49-2	Selenium		2.206							0.000	0.000	2.206
85-01-8	Phenanthrene	0.637		0.129		0.000	2.177				0.000	2.177
7440-22-4	Silver	2.108									0.000	2.108
14797-65-0	Nitrite (NO2)	2.087									0.000	2.087
18540-29-9	Chromium 6+	2.030									1.023	2.030
91465-08-6	lambda-Cyhalothrin	2.025									0.000	2.025
7440-39-3	Barium		1.931							0.000	0.000	1.931
56-38-2	Parathion	1.846									0.000	1.846
111991-09-4	Nicosulfuron	1.833									0.520	1.833
5598-13-0	Chlorpyriphos methyl	1.667							0.000		0.000	1.667
668-34-8	Triphenyltin	1.633				0.000					0.001	1.633
83164-33-4	Diflufenican	1.592							1.003		0.000	1.592

CAS number	Substance	STEfw whole,eco	STEfw dissv, eco	STEsw whole,eco	STEsw dissv,eco	STEsed, eco	STEbiota (mollusc), sec pois	STEbiota (fish), secpois	STEwater, hh food	STEfw dissv dw,hh	STEfw whole dw,hh	STE score
76-03-9	Trichloroacetic acid	1.555									0.000	1.555
138261-41-3	Imidacloprid	1.547									0.473	1.547
7429-90-5	Aluminium		1.457							0.581	0.715	1.457
78763-54-9	Monobutyltin					1.398						1.398
2032-65-7	Methiocarb	1.374									0.539	1.374
7440-41-7	Beryllium	1.371									1.014	1.371
108-42-9	3-Chloroaniline	0.167									1.357	1.357
53-70-3	Dibenz(a,h)anthracene	1.196					1.266		0.701		1.004	1.266
67-72-1	Hexachloroethane	0.000							1.255		0.000	1.255
50-28-2	17-beta-Estradiol	1.255									0.000	1.255
7439-96-5	Manganese		0.931							0.931	1.246	1.246
7439-89-6	Iron		0.833							0.833	1.195	1.195
95-51-2	2-Chloroaniline	0.000									1.177	1.177
7664-41-7	Ammonia	1.166									0.603	1.166
52645-53-1	Permethrin	1.140							0.000		0.000	1.140
106-47-8	4-Chloroaniline	0.000									1.140	1.140
7440-66-6	Zinc		1.069		1.138	0.898				0.000	0.000	1.138
15307-86-5	Diclofenac	1.137									0.000	1.137
7440-28-0	Thallium	1.116									0.926	1.116
106-89-8	Epichlorhydrin (1-Chloro-2,3-epoxypropane)	0.000									1.086	1.086
120-32-1	Chlorophene	0.000									1.070	1.070
16887-00-6	Chloride	0.711									1.002	1.002
142459-58-3	Flufenacet	0.370							0.940		1.001	1.001
208-96-8	Acenaphthylene	0.546							1.000		0.000	1.000
7286-69-3	Sebuthylazine	0.993									0.599	0.993

CAS number	Substance	STEfw whole,eco	STEfw dissv, eco	STEsw whole,eco	STEsw dissv,eco	STEsed, eco	STEbiota (mollusc), sec pois	STEbiota (fish), secpois	STEwater, hh food	STEfw dissv dw,hh	STEfw whole dw,hh	STE score
7440-23-5	Sodium	0.952									0.952	0.952
17254-80-7	Chloridazon methyl-desphenyl	0.000									0.937	0.937
21725-46-2	Cyanazine	0.862									0.934	0.934
94-81-5	4-(4-Chloro-o-tolyloxy) butyric acid	0.000									0.900	0.900
7440-24-6	Strontium	0.899									0.000	0.899
75-01-4	Vinylchloride	0.869									0.655	0.869
86-73-7	Fluorene	0.868							0.795		0.000	0.868
1002-53-5	Dibutyltin	0.285				0.865						0.865
53-19-0	DDD, o,p'	0.540				0.863					0.480	0.863
19666-30-9	Oxadiazon	0.278							0.362		0.849	0.849
7439-95-4	Magnesium	0.828									0.000	0.828
7440-38-2	Arsenic		0.000			0.817	0.333			0.323	0.374	0.817
80-05-7	Bisphenol A	0.457							0.664		0.737	0.737
59-50-7	Chlorocresol (3-Methyl-4-chlorophenol)	0.000									0.699	0.699
1702-17-6	Clopyralid	0.000									0.677	0.677
95-76-1	3,4-Dichloroaniline	0.677										0.677
72-43-5	Methoxychlor	0.667							0.000		0.000	0.667
1698-60-8	Chloridazon	0.000									0.651	0.651
3380-34-5	Triclosan	0.650									0.000	0.650
133-06-2	Captan	0.000									0.636	0.636
7440-47-3	Chromium		0.345		0.564	0.623	0.400	0.000		0.000	0.095	0.623
95-94-3	1,2,4,5-Tetrachlorobenzene	0.619							0.619		0.000	0.619
7440-50-8	Copper		0.406		0.195	0.615				0.000	0.000	0.615

CAS number	Substance	STEfw whole,eco	STEfw dissv, eco	STEsw whole,eco	STEsw dissv,eco	STEsed, eco	STEbiota (mollusc), sec pois	STEbiota (fish), secpois	STEwater, hh food	STEfw dissv dw,hh	STEfw whole dw,hh	STE score
83-32-9	Acenaphthene	0.383									0.611	0.611
7440-42-8	Boron		0.598							0.000	0.000	0.598
108-95-2	Phenol	0.594									0.000	0.594
7440-31-5	Tin	0.586									0.000	0.586
7440-48-4	Cobalt		0.555							0.290	0.400	0.555
3424-82-6	DDE, o,p'	0.550									0.457	0.550
26225-79-6	Ethofumesate	0.000									0.533	0.533
1336-36-3	PCB-sum (Polychlorinated biphenyls)	0.525										0.525
7440-62-2	Vanadium		0.463							0.463	0.517	0.517
79277-27-3	Thifensulfuron methyl	0.510									0.513	0.513
1330-78-5	Tricresyl Phosphate	0.505							0.000		0.000	0.505
53-16-7	Estrone	0.497										0.497
16984-48-8	Fluoride	0.489									0.000	0.489
335-67-1	Perfluorooctanoic acid (PFOA)	0.480									0.292	0.480
90-12-0	1-Methylnaphthalene	0.453							0.000		0.000	0.453
114-26-1	Propoxur	0.452									0.044	0.452
118134-30-8	Spiroxamine	0.451							0.000		0.000	0.451
298-46-4	Carbamazepine	0.449									0.000	0.449
139-13-9	Nitrilotriacetic acid	0.444									0.000	0.444
7439-98-7	Molybdenum		0.000							0.437	0.254	0.437
10605-21-7	Carbendazim	0.409									0.433	0.433
98-95-3	Nitrobenzene	0.433									0.253	0.433
723-46-6	Sulfamethoxazole	0.423									0.000	0.423
63-25-2	Carbaryl	0.412									0.000	0.412

CAS number	Substance	STEfw whole,eco	STEfw dissv, eco	STEsw whole,eco	STEsw dissv,eco	STEsed, eco	STEbiota (mollusc), sec pois	STEbiota (fish), secpois	STEwater, hh food	STEfw dissv dw,hh	STEfw whole dw,hh	STE score
1007-28-9	6-Desisopropylatrazine	0.409									0.000	0.409
60-51-5	Dimethoate	0.407									0.000	0.407
307-24-4	Perfluorohexanoic acid (PFHxA)	0.000									0.396	0.396
7440-32-6	Titanium	0.375										0.375
333-41-5	Diazinon	0.372							0.313		0.323	0.372
34256-82-1	Acetochlor	0.367									0.000	0.367
171118-09-5	Metolachlor ethanesulfonic acid (ESA)	0.000									0.358	0.358
19937-59-8	Metoxuron	0.306									0.000	0.306
1563-66-2	Carbofuran	0.290									0.000	0.290
94-74-6	2-Methyl-4-chlorophenoxyacetic acid (MCPA)	0.284									0.000	0.284
126-73-8	Tributyl phosphate	0.272									0.000	0.272
139-40-2	Propazine	0.255									0.262	0.262
7440-36-0	Antimony	0.260									0.000	0.260
16752-77-5	Methomyl	0.259									0.000	0.259
15545-48-9	Chlorotoluron	0.243									0.000	0.243
121-73-3	1-Cloro-4-nitrobenzene	0.242										0.242
25057-89-0	Bentazone	0.000									0.240	0.240
111988-49-9	Thiacloprid	0.236									0.000	0.236
41394-05-2	Metamitron	0.000									0.217	0.217
108-90-7	Chlorobenzene	0.217									0.000	0.217
57837-19-1	Metalaxyl	0.000									0.216	0.216
104-35-8	4-Nonylphenol mono-ethoxylate (NP1EO)	0.199										0.199

CAS number	Substance	STEfw whole,eco	STEfw dissv, eco	STEsw whole,eco	STEsw dissv,eco	STEsed, eco	STEbiota (mollusc), sec pois	STEbiota (fish), secpois	STEwater, hh food	STEfw dissv dw,hh	STEfw whole dw,hh	STE score
50-00-0	Formaldehyde	0.199									0.000	0.199
121-14-2	2,4-Dinitrotoluene	0.192									0.113	0.192
117-84-0	Di-n-octyl phthalate	0.183										0.183
90717-03-6	Quinmerac	0.000									0.180	0.180
1194-65-6	Dichlobenil	0.000									0.166	0.166
67129-08-2	Metazachlor	0.161									0.155	0.161
330-55-2	Linuron	0.149		0.000							0.149	0.149
85-68-7	Butylbenzyl phthalate	0.148										0.148
100-41-4	Ethylbenzene	0.145									0.000	0.145
69377-81-7	Fluroxypyr	0.000									0.140	0.140
15687-27-1	Ibuprofen	0.135							0.000		0.000	0.135
88-73-3	1-Cloro-2-nitrobenzene	0.131										0.131
92-52-4	Biphenyl	0.122							0.000		0.000	0.122
23950-58-5	Propyzamide	0.000									0.116	0.116
100-42-5	Styrene	0.106									0.000	0.106
122931-48-0	Rimsulfuron	0.039									0.005	0.039
22204-53-1	Naproxen	0.001										0.001
108-60-1	Dichloroisopropyl ether (Propane)	0.001										0.001

Notes: The empty positions in the table indicate that the substances are not considered in these comparments.
Tentative PNEC value for ibuprofen; discussions are still ongoing regarding an agreement on $PNEC_{fw,\ eco}$. None of the proposed PNECs led to a high STE score.

4. Short-listing of substances

The substances with a risk classification of very high (STE score 2.4 - 3), high (STE score 1.8-2.4) and eventually intermediate (STE score 1.2 – 1.8), according to Table 4, have been selected to move forward in the monitoring-based prioritisation process. For these substances, additional information was collected and presented in Table 30 including the hazard properties such as P, B, T, C, M, R and ED, substances' type of usage and status.

For the PBT, the information was retrieved from ECHA (industrial chemicals), EFSA for pesticides, while the "2012-2015 Environmentally classified pharmaceuticals document" from the Stockholm County Council was the source for human pharmaceuticals. Carcinogenicity (C), Mutagenicity (M) and Reproduction Toxicity (R) are in accordance to GHS categories from ECHA dossiers. For EDs the EDS database and categorisation of the European Commission was used (EDS database, EC). Concerning pesticides, if EFSA dossiers were available, CMR scores were set accordingly.

In the current prioritisation exercise, the substances which are very high and highly ranked (STE score ≥ 1.8) include: pesticides or Plant Production Products (PPPs) (fenthion, omethoate, azinphos-ethyl, mevinphos, ethion, malathion, lambda-cyhalothrin, parathion, nicosulfuron), polycyclic aromatic hydrocarbons (PAHs: benzo(a)anthracene, chrysene, pyrene, phenanthrene), nitrite and metals (uranium, selenium, silver, chromium 6+, barium). 2-Hydroxyatrazine (STE=2.4) is not considered as a new candidate since it is a derivative of Atrazine (already a PS).

Table 30. Top-ranked substances following the STE approach. This list contains names of substances which scores are: very high, high and intermediate (STE range is from 1.2 up to 3).

CAS	Substance	STE score	Risk score	Type	Approval status	P	B	T	vP	vB	C	M	R	ED	Note
56-55-3	Benzo(a)-anthracene	2.557	1	Other	n.a.	yes	yes	yes	no	no	0.75: CAT.2 (1B)	0.5: CAT. 3 (2)	0.25	0.5	
55-38-9	Fenthion	2.555	1	PPP	severely restricted	no	no	yes	no	no	0	0.5: CAT. 3 (2)	0.25	0.25	1
1113-02-6	Omethoate	2.452	1	PPP	Banned	no	no	yes	no	no	0.5: CAT. 3 (2)	0.25	0.25	1	2
2642-71-9	Azinphos-ethyl	2.410	1	PPP	Banned	yes	yes	yes	yes	no	0.25	0.25	0.25	0.25	1
2163-68-0	2-Hydroxyatrazine	2.400	2	Other	n.a.	yes	yes	no data	no	no	0.25	0.25	0.25	0.25	
218-01-9	Chrysene	2.338	2	Industrial	n.a.	yes	yes	yes	no	no	0.75: CAT.2 (1B)	0.5: CAT. 3 (2)	0.25	0.25	
7440-61-1	Uranium	2.321	2	Other	n.a.	yes	no data	yes	no	no	1: CAT. 1 (1A)	1: CAT. 1 (1A)	0.25	0.25	1
7786-34-7	Mevinphos	2.313	2	PPP	Banned	no	no	yes	no	no	0.25	0.25	0.25	0.5	1
563-12-2	Ethion	2.280	2	PPP	Not approved	no data	yes	no data	no	no	0.25	0.25	0.25	0.25	
121-75-5	Malathion	2.216	2	Human medicine; PPP	Approved	no	no	yes	no	no	0	0	0.25	0.5	1
129-00-0	Pyrene	2.207	2	Industrial	n.a.	high concern									
7782-49-2	Selenium	2.206	2	Industrial	n.a.	yes	yes	yes	no	yes	0.25	0.25	0.25	0.25	1
85-01-8	Phenanthrene	2.177	2	other	n.a.	yes	no	yes	no	no	0.5: CAT. 3 (2)	0.25	0.25	0.25	
7440-22-4	Silver	2.108	2	Industrial; Biocide	Sodium silver thiosulfate is approved as PPP	yes	no	yes	no	no	0.25	0.25	0.25	0.25	

CAS	Substance	STE score	Risk score	Type	Approval status	P	B	T	vP	vB	C	M	R	ED	Note
14797-65-0	Nitrite (NO2)	2.087	2	Industrial	n.a.	no data	no data	no data	no	no	0.25	0.25	0.25	0.25	
18540-29-9	Chromium 6+	2.030	2	Industrial	Banned	no	no data	yes	no	no	1: CAT. 1 (1A)	0.5: CAT. 3 (2)	0.25	0.25	2
91465-08-6	lambda-Cyhalothrin	2.025	2	Biocide; PPP	Approved	yes	yes	yes	no	no	0.25	0.25	0.25	1	
7440-39-3	Barium	1.931	2	Industrial	n.a.	yes	no	yes	no	no	0.25	0.25	0.25	0.25	
56-38-2	Parathion	1.846	2	PPP	Banned	no	no	yes	no	no	0.25	0.25	0.25	0.5	1; 3
111991-09-4	Nicosulfuron	1.833	2	PPP	Approved	no	no	yes	no	no	0	0	0.25	0.25	
5598-13-0	Chlorpyriphos methyl	1.667	3	PPP	Approved	no	no	no data	no	no	0.25	0.25	0.25	0.25	1
668-34-8	Triphenyltin	1.633	3	PPP	Banned	no	yes	yes	no	no	0.25	0.25	0.25	0.25	1
83164-33-4	Diflufenican	1.592	3	PPP	Approved	yes	yes	yes	yes	no	0	0.25	0.25	0.25	
76-03-9	Trichloroacetic acid	1.555	3	Industrial	Banned as PPP	high concern									
138261-41-3	Imidacloprid	1.547	3	Biocide; PPP	Approved	yes	no	yes	no	no	0.25	0	0.25	0.25	
7429-90-5	Aluminium	1.457	3	Industrial	n.a.	yes	no	yes	no	no	0.25	0.25	0.25	0.25	
78763-54-9	Monobutyltin	1.398	3	Other	Banned	no data	no	no data	no	no	0.25	0.25	0.25	0.25	1
2032-65-7	Methiocarb	1.374	3	PPP	Approved	no	no	yes	no	no	0.25	0	0.25	0.25	1
7440-41-7	Beryllium	1.371	3	Industrial	n.a.	high concern									
108-42-9	3-Chloroaniline	1.357	3	Industrial	n.a.	high concern									
53-70-3	Dibenz(a,h)anthracene	1.266	3	Other	n.a.	yes	yes	yes	no	no	0.75: CAT.2 (1B)	0.25	0.25	0.25	
67-72-1	Hexachloroethane	1.255	3	Industrial	Restricted	no data	no	yes	no	no	0.5:CAT. 3 (2)	0.25	0.25	0.25	
50-28-2	17-beta-Estradiol	1.255	3	Industrial; Human medicine	Approved	no	no	yes	no	no	0.25	0.25	0.25	1	4

CAS	Substance	STE score	Risk score	Type	Approval status	P	B	T	vP	vB	C	M	R	ED	Note
7439-96-5	Manganese	1.246	3	Industrial	n.a.	no concern									

Notes:
(1) Substance ranked 'very high' or 'high' in the monitoring-based exercise of the last Review of PS but not taken forward in the prioritisation
(2) Substances short-listed during the last Review of PS list but not taken forward owing to a lack of evidence
(3) Highly ranked in the modelling-based exercise (Lettieri et al. 2016)
(4) Substances short-listed during the last Review of PS list but not taken forward and included in the first Watch list
n.a. – not applicable

4.1. Draft list of substances to be short listed as potential PS

Based on the above ranking, 14 substances (Table 31) have been selected to be short-listed based on their highest risk from the monitoring-based exercise and supporting evidence (the rationale for selection is given in section 4.2).

The short-listed substances are among the highest ranked substances (STE score >1.8, risk high or very high) in the monitoring-based excersice, with the exception of the substances mentioned in section 4.3. Factsheets have been drafted and presented in Annex V (except for Ethion). The factsheets gather a 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), 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 outcome of the STE analysis together with the detailed information in the factsheets allow experts to select the substances for which an EQS should be derived, for inclusion in the list of proposed candidate priority substances.

Table 31. List of highest ranked monitoring based substances (STE > 1.8) for which a factsheet has been developed (see Annex V)

No.	Substance
1	Fenthion
2	Omethoate (plus Dimethoate)
3	Azinphos-ethyl
4	Uranium
5	Mevinphos
6	Ethion
7	Malathion
8	Selenium
9	Silver
10	Chromium 6+
11	lambda-Cyhalothrin
12	Barium
13	Parathion
14	Nicosulfuron

Note 1: **Permethrin** (although initially short-listed and and a factsheet for this substance was prepared) is not included in Table 31 since according to the initially selected PNEC=0.0015 µg/L, the score by the refined STE tool is intermediate (STE=1.14 in Sc2-PNECQC Inland whole water). However, after the revision of PNEC value of Permethrin (new PNEC=0.00047 µg/L), the STE score (refined) arose to STE=2.29 (indicating a high risk), thus Permethrin is still considered as a top-ranked substance.

Note 2: Initially, factsheets have been prepared also for thallium, propoxur and methoxychlor since they highly scored; however, after the STE script's refinement, the STE scores of these substances became below 1.8, so they are not considered anymore as candidates for short-listing.

Note 3: Considering the fact that Ethion is not approved as PPP in the EU (since 2006), it has been decided not to prepare a factsheet for this substance.

4.2. Rationale for the draft short-listing of the substances

The rationale and conclusions presented below are based on the analysis of the monitoring-based prioritisation results by the JRC. However, the decision on the selection of substances for which an EQS should be derived will be made upon agreement with the experts from the SG-R.

Fenthion. The STE score of Sc2-PNEC QC is very high (2.555 with PNEC=0.0002 µg/L), indicating a very high risk to the aquatic environment. The STE score for the PNEC of 0.0013 µg/L is 2.167 (Sc2). Fenthion has been analysed in 9 countries in Scenario2. In Sc2-PNEC QC samples were available in 5 countries (all quantified), however, a detailed check of the monitoring data revealed that the reported LOD of the quantified samples are over the PNEC (ca.72% of the records), so seemed to be in reality non-quantified samples. According to the harmonised classification and labelling approved by the EU, this substance is very toxic to aquatic life, with long lasting effects. Fenthion is not approved anymore as PPP in the EU (approval ceased in 2004) nor is it approved for use in biocidal products.

According to the JRC, the data quality for fenthion is not sufficient to propose as candidate for EQS derivation. In addition, it is not authorised for use in the EU.

Omethoate/Dimethoate. The STE score of Omethoate in Sc2-PNEC QC is very high (2.452 with PNEC=0.00084 µg/L), indicating a very high risk to the aquatic environment. The new proposed PNEC of 0.0042 µg/L, lowers the STE score to 2.157 (Sc2) indicating a high risk. Omethoate has been analysed in 5 countries in Sc2-PNECQC (8 in Sc2), however, a detailed check of the monitoring data for omethoate showed that in Sc2-PNEC QC, only around 12 records can be considered as quantified data above the PNEC (in 2 countries). Omethoate is not approved anymore as PPP in the EU; however, dimethoate is approved in EU as PPP and it may be expected that omethoate will therefore occur in the environment from its transformation/degradation. Given the apparent link between dimethoate and omethoate, the two substances should be looked at together. Neither dimethoate nor omethoate bioaccumulate, but both are highly toxic to freshwater invertebrates. According to the harmonised classification and labelling approved by the European Union, omethoate is very toxic to aquatic life.

According to JRC, omethoate together with dimethoate could be possible candidates for EQS derivation. Dimethoate is approved in EU as PPP and it may be expected that omethoate will occur in the environment.

Azinphos-ethyl. The STE score of Sc2-PNEC QC is very high (2.41 with PNEC=0.0011 µg/L), indicating a very high risk to the aquatic environment. A detailed check of the monitoring data showed that in Sc2-PNEC QC, samples were available in 6 countries and all of them were declared as quantified. Five countries provided quantified and detected exceedances in the majority of samples analyzed. According to the harmonised classification and labelling approved by the EU, this substance is very toxic to aquatic life and with long lasting effects. Azinphos-ethyl was found to be one of the responsible compounds for acute risk to macroinvertebrates in the Llobregat River (Catalonia; Spain) (Kuzmanović et al., 2016). Azinphos-ethyl is not approved as PPP in the EU nor is it approved for use in biocidal products (approval as a PPP ceased in 1995).

According to JRC, based on the available evidence, azinphos-ethyl could be a possible candidate for EQS derivation. Even though azinphos-ethyl is not currently authorised for use in the EU it should be taken into account that values in the environment continue to pose a risk many years after the ceasing of its use as PPP.

Uranium. The STE score of Sc2-PNEC QC is very high (2.545 with PNEC=0.5 µg/L), indicating a very high risk to the aquatic environment although due to the high natural background concentration, a threshold should be taken into account. Uranium has been analysed in five countries. In Sc2-PNEC QC, samples were available in five countries, 78 % of them quantified. The available monitoring data are from "whole water". A detailed check of the monitoring data showed that the quality of data for uranium is good; there is a high percentage of quantified exceedances of the PNEC. According to the harmonised classification and labelling approved by the EU, this substance may cause long lasting harmful effects to aquatic life. Agriculture activities (phosphate fertilizers) contribute to an increased presence of uranium in the environment. The EU Fertiliser Regulation 2003/2003 revision is currently in the discussion and preparation phase; however, it fails to address environmental concerns arising from uranium contamination.

According to the JRC, uranium could be a candidate for EQS derivation. However, the monitoring data are for "whole water", the natural background levels of uranium in EU surface waters are in the range of the PNEC of 0.5 µg/L, and its bioavailability and toxicity might be reduced due to complexing with phosphates or natural organic matter. In order to gather more monitoring data from dissolved fraction, uranium could be proposed for the watch list. Addiitonal comments and suggestions of the SG-R are reported in the factsheet.

Mevinphos. The STE score of Sc2-PNEC QC is high (2.313 with PNEC= 0.00017 µg/L), suggesting that a lot of exceedances occur in the aquatic environment. Mevinphos has been analysed in 9 countries in Scenario2. In Sc2-PNEC QC, samples were available in 5 countries, however, a detailed check of the monitoring data revealed that only nine quantified exceedances in 2 MS were available. According to the harmonised classification and labelling approved by the European Union, this substance is very toxic to aquatic life, and is very toxic to aquatic life with long lasting effects. Mevinphos is not approved as PPP in the EU (since 2002) nor is it approved for use in biocidal products.

According to JRC, data quality for mevinphos is not sufficient to propose it as a candidate for EQS derivation. Moreover, mevinphos is not currently authorised for use in the EU.

Malathion. The STE score of Sc2-PNEC QC with the lowest value of PNEC= 0.0002 µg/L is high (2.216), indicating a high risk to the aquatic environment. The STE score is however reduced to 1.398 (for Sc2) with the PNEC of 0.006 µg/L, indicating an intermediate risk. Malathion has been analysed in 11 countries in Sc2. In Sc2-PNEC QC, samples were available in 7 MS, and a detailed check of the monitoring data showed that the quality of data is good since 7 MS provided reliable quantified data displaying in their majority exceedance of the PNEC (0.0002 µg/L). According to the harmonised classification and labelling approved by the European Union, this substance is very toxic to aquatic life and with long lasting effects. Malathion is approved as PPP in the EU (date of approval: 01/05/2010; expiration of approval: 30/04/2020).

According to the JRC, the risk observed when the lowest PNEC is used would justify deriving an ESQ for Malathion. However, the final decision will depend on the value of the PNEC considered in the STE scoring.

Selenium. The STE score of Sc2-PNEC QC is high (2.206 with PNEC=0.05 µg/L), indicating a high risk to the aquatic environment. Selenium has been analysed in 7 countries in Sc2-PNEC QC, 4509 samples were available and 77% of them were quantified. The available monitoring data are for the "dissolved" fraction. A detailed check of the monitoring data showed that the quality of data for selenium is good, because the quantified records without information on LOD/Q seem to be real quantified measurements, and not false positive non-quantified records. According to the harmonised classification and labelling approved by the EU, this substance may cause long lasting harmful effects to aquatic life. Selenium is a bioaccumulative pollutant of substantial toxicity, if toxicity is determined

from diet, not dissolved exposure. Selenium pollution seems to be a worldwide phenomenon, with wide differences in regulations among jurisdictions and environments. According to the available scientific evidence, integrating the chemistry of selenium with its biology and ecotoxicology may give indications on how to regulate its environmental levels. In Austria, selenium was identified as one of the relevant substances with impact on good chemical status of surface water quality via the discharge of treated wastewater (Clara et al., 2012).

According to JRC, selenium could be a good candidate for EQS derivation with the considered PNEC value. However, the natural background levels and bioavailability issues should be taken into account locally.

Silver. The STE score of Sc2-PNEC QC is high (2.108 with PNEC=0.017 µg/L). In Sc2-PNEC QC, 1424 samples (whole water) were available in 7 countries, with only 18% of them not quantified. Silver with several additionally proposed PNEC values of 0.01, 0.02 and 0.04 µg/L has been analysed in 9 MS in Scenario2. These monitoring data are from "whole water"; however, the STE score is high (2.354 for Scenario2) even when the highest PNEC of 0.04 µg/L is used. The available monitoring data from dissolved fraction (from 2 MS) were analysed by STE with two PNECs (0.01 and 0.04 µg/L), and the STE score still shows high value (2.280 and 2.016, respectively). According to the classification provided by companies to ECHA in REACH registrations, silver is very toxic to aquatic life and with long lasting effects. This substance is manufactured and/or imported in the European Economic Area in 100 000 - 1 000 000 tonnes per year. Sodium silver thiosulfate is approved as PPP in EU, and silver is currently under review as Biocidal Active Substance for other types of applications.

According to JRC, silver could be a good candidate for EQS derivation.

Chromium 6+. The STE score of Sc2-PNEC QC is high (2.03 with PNEC=0.47 µg/L), indicating a high risk to the aquatic environment. However, the score is lowered to 1.393 (intermediate risk) when using PNEC=3.4 µg/L, recently agreed upon for the Watch List selection. A detailed check of the monitoring data showed that the quality of data is relatively good; in Sc2-PNEC QC 415 samples were available in four countries, 92.5% of them quantified. The available monitoring data are from "whole water". According to the harmonised classification and labelling approved by the EU, this substance is very toxic to aquatic life and is very toxic to aquatic life with long lasting effects. Chromium trioxide and other Cr(VI) compounds are now banned from all consumer uses, and all professional uses except as laboratory substance; the latest application date expected for chromium trioxide was 21 March 2016, with a "sunset date" of 21 September 2017 (COMMISSION REGULATION (EU) No 348/2013).

According to JRC, although the monitoring data are of good quality, this substance should not be considered for the EQS derivation, because when using the PNEC recently agreed upon for the watch list selection, the STE score would decrease from 2.03 down to 1.4 and the recent restrictions in its use will likely decrease the environmental concentrations.

Lambda-Cyhalothrin. The STE score of Sc2-PNEC QC is high (2.025 with PNEC=0.0002 µg/L), indicating a high risk to the aquatic environment. In Sc2-PNEC QC, 228 samples are available in 4 countries, however, a detailed check of the monitoring data revealed that for lambda-cyhalothrin there are practically no reliable quantified records, but "false positives" based on non-quantified measurements. Lambda-cyhalothrin has been analysed in 6 countries in Scenario2. According to the harmonised classification and labelling approved by the EU, this substance is very toxic to aquatic life and is very toxic to aquatic life with long lasting effects. Lambda-cyhalothrin is approved as PPP in the EU (date of approval renewal 01/04/2016, expiration of approval: 31/03/2023).

According to JRC, data quality for lambda-cyhalothrin is not sufficient to be proposed as candidate for EQS derivation.

Barium. The STE score of Sc2-PNEC QC is high (STE=1.931 with PNEC=9.3 µg/L), indicating a high risk to the aquatic environment. The PNEC value of 9.3 µg/L however has been derived for fish consumption according to the methodology of the WFD, but ends up clearly below the background value and thus cannot be set as a workable QS value. The STE score with a more realistic PNEC of 73 µg/L is 0.595 (Scenario2), indicating a low risk to the aquatic environment. The available monitoring data for barium are from dissolved fraction. For Sc2-PNEC QC, 855 samples from five countries have been analysed. A detailed check of the monitoring data showed that the quality of data is good. According to the harmonised classification and labelling approved by the EU, this substance may cause long lasting harmful effects to aquatic life. Due to increasing industrial use of barium, concentrations in the environment are rising.

According to JRC, barium could be a possible candidate for shortlisting and EQS derivation, depending on the choice of the PNEC.

Parathion. The STE score of Sc2-PNEC QC is high (1.844 with PNEC=0.0002 µg/L), indicating a high risk to the aquatic environment. Parathion has been analysed in 13 countries in Scenario2. In Sc2-PNEC QC, 8189 samples were available in 8 countries, 15% of them quantified. Although the majority of the data have been probably erroneously labelled as quantified (creating false positives), the remaining ca. 100 quantified samples from 6 MS are far above the PNEC. According to the harmonised classification and labelling approved by the EU, this substance is very toxic to aquatic life and with long lasting effects. Parathion is not approved anymore as PPP in the EU (since 2001) nor is it approved for use in biocidal products (but no clear downward time trend was found by annual mean ocncentrations).

According to JRC, based on the available evidence, parathion could be a possible candidate for EQS derivation. However, parathion (and parathion-methyl) is not currently authorised for use in the EU.

Nicosulfuron. The STE score of Sc2-PNEC QC is high (1.833 with PNEC=0.0087 µg/L), indicating a high risk to the aquatic environment. Nicosulfuron, with a proposed PNEC of 0.0087 µg/L, has been analysed in 5 countries in Scenario2 (18410 samples; 97% non-quantifed). In Sc2-PNEC QC, 1104 samples were available in 5 countries, 48% of them quantified. A detailed check of the monitoring data showed that there are quantified exceedances in many of the samples from all five MS, so the quality of data is good. According to the classification provided by companies to ECHA in CLP notifications, this substance is very toxic to aquatic life and with long lasting effects. Nicosulfuron is approved as PPP in the EU (since 01/01/2009; expiration of approval: 31/12/2018)

According to JRC, Nicosulfuron is a good candidate for EQS derivation.

Permethrin. The STE score of Sc2-PNEC QC is high (2.29 with the newly derived PNEC=0.00047 µg/L; calculated by the refined STE tool), indicating a high risk to the aquatic environment. Permethrin has been analysed in 7 countries in Scenario2. In Sc2-PNEC QC (0.00047 µg/L), 117 samples were available in 4 countries, 98.3% of them quantified. A detailed check of the monitoring data for permethrin showed minor problems of the monitoring data (75 reliable quantified samples from 2 countries were available). According to the harmonised classification and labelling approved by the EU, this substance is very toxic to aquatic life and is very toxic to aquatic life with long lasting effects. Permethrin is not approved anymore as PPP in the EU (in agriculture to protect crops or

kill livestock parasites). The authorisations for permethrin as a PPP were withdrawn by a Commission decision in 2000. Permethrin is explicitly approved as biocide only.

According to JRC, permethrin could be a candidate for EQS derivation.

4.3. Substances for which no factsheet was drafted

Following the comments from the experts during the 4th SG-R meeting, no factsheet was drafted for the following substances, depite the high ranking in the STE approach:

PAHs: The group of PAHs is already adequately covered by the present set of PS. PAHs, being mainly combustion by-products, occur as a relatively stable mixture in the environment. By already regulating the main components of this mixture (anthracene, fluoranthene; naphthalene; benzo(a)pyrene; benzo(b)fluoranthene; benzo(k)-fluoranthene; benzo(g,h,i)perylene; indeno(1,2,3-cd)pyrene), the other individual PAHs (benzo(a)anthracene; chrysene; pyrene; phenanthrene) do not need to be regulated separately. In addition, the PAHs already included in the PS List have a relative hazard scoring to benzo(a)pyrene, the most toxic one. Measures to reduce emissions of PAHs will obviously reduce levels of any individual PAH since they all have the same sources.

Therefore, it is not required to add other PAHs to the existing list of PS (Kim et al., 2013; Moeckel et al., 2014).

2-Hydroxyatrazine: 2-hydroxyatrazine is a metabolite of atrazine, which is already a PS. Atrazine is banned in the EU since 2009. 2-Hydroxyatrazine and atrazine can be released into water from contaminated sediments. The PNEC of 0.002 µg/L for 2-hydroxyatrazine from JDS3 has been questioned by experts.

Therefore, 2-hydroxyatrazine is not proposed to be short-listed.

Ethion: this substance has obtained a high STE score of 2.28 (*fw, eco*; Scenario 2-PNEC QC) when the extra data (additional merging of the polar substances in the inland dissolved with those in the inland whole water) were introduced into the analysis after the 5th meeting of SG-R. However, considering the fact that ethion is not approved as PPP in the EU (since 2006), it has been decided not to prepare a factsheet.

Therefore, Ethion is not proposed to be short-listed.

Nitrite (NO2): In the aquatic environment, nitrite (together with nitrate and ammonium) is a part of the nitrogen cycle and an important compound supporting the biological quality indicators. Nitrates are already regulated by the Nitrates Directive (1991) aiming to protect water quality across Europe by preventing nitrates from agricultural sources polluting ground and surface waters and by promoting the use of good farming practices (http://ec.europa.eu/environment/water/water-nitrates/index_en.html).

Under the Water Framework Directive, nitrite are not part of the chemical status but could be considered under the general physic-chemicals elements supporting the biological quality elements. They will therefore not be considered here, and no factsheet has been prepared for them.

5. Discussion

The report shows the results of the monitoring-based exercise and ranking of substances based on a new approach that considers the spatial, temporal and extent of PNEC exceedances (STE exercise) in surface water (fresh and transitional/coastal) and other compartments (sediments and biota) and receptors (drinking water and human health food).

After the criteria for data quality have been applied to the monitoring data in Scenario2 for freshwater (whole water and dissolved fraction) and transitional/coastal waters, we had 338, 13 and 9 substances, respectively (see Table 19). Twenty eight substances have been excluded from the inland whole water (see Table 18) in the STE exercise (Scenario2) because they were not fulfilling the set criteria of minimum number of MS (>3), or minimum number of 10 sampling sites (Decabromodiphenyl ether (BDE-209) was excluded from inland whole water but nevertheless participated in the monitoring exercise through the sediment compartment). These substances have been included in the screening phase of the modelling-based exercise. When Scenario2 monitoring data has been further processed by the additional criteria of the PNEC quality control (Sc2-PNEC QC) to remove the non-quantified data for which ½ LOD/LOQ > PNEC, the inland whole water substances were reduced to 310 while there was no reduction for freshwater dissolved and transitional/coastal waters (see Table 20). The total number of substances considered in the monitoring-based exercise is 326 in Sc2-PNECQC and 354 in Scenario 2.

The ranking based on the STE scores was the main criteria for selection of substances for short-listing and drafting of factsheet (section 4.1 and 4.2). For a few substances, additional information, briefly described under section 4.3, supported their exclusion from the short-list despite the high ranking.

Some substances with high or intermediate STE scores were already highly ranked in the previous exercise (see WFD scoping report, 2014). For instance, two substances, AMPA and chromium trioxide (Cr 6+) were short-listed but not taken forward in the last prioritisation exercise. AMPA again does not show a high score in our exercise while chromium trioxide obtained a high STE score (2.03), with monitoring data in "whole" water from four MS. Although chromium trioxide could have been a good candidate for the watch list, it was concluded that since, according to the ECHA registration the sunset date for this substance is in 2017 (Carvalho et al., 2015), a concentration reduction should be expected. However due to the high risk, a mechanism should be developed to keep under control the concentration over time to ensure its decrease. Other substances were ranked in the previous exercise as "very high" or "high" in the monitoring based exercised but not taken forward. Meanwhile two of these substances have been banned, azinphos-ethyl and omethoate. The substance tetrabutyltin showed a zero STE score in fw(whole),eco (the substance was excluded from STEsed,eco since the unsuffcient number of records for a proper calculation of $F_{temporal}$ factor) but actually has a very high screening score in the modelling exercise (Lettieri et al., 2016). Tetrabutyltin was ranked high in the last prioritisation exercise (scoping report, 2014), but not prioritised.

Interestingly, the ranks based on the risk quotient (RQ: 95th percentile/PNEC) are generally comparable to the ranks obtained from the calculation of the STE approach, see Figure 18 for inland whole water (Sc2-PNECQC). However, discrepancies equal or more than 15 possitions arose for a few substances. Considering the top 50-ranked substances, the RQ-based scoring shows a lower ranking position for uranium with respect to the ranking position obtained with the STE method. Conversely, other substances - for instance lambda-Cyhalothrin, got a higher ranking position with the RQ-based method than with STE. Despite the occasional discrepancies between the two ranking methods (STE and RQ_P95), both identify a considerable risk for the top 50 substances, including all those selected for short-listing.

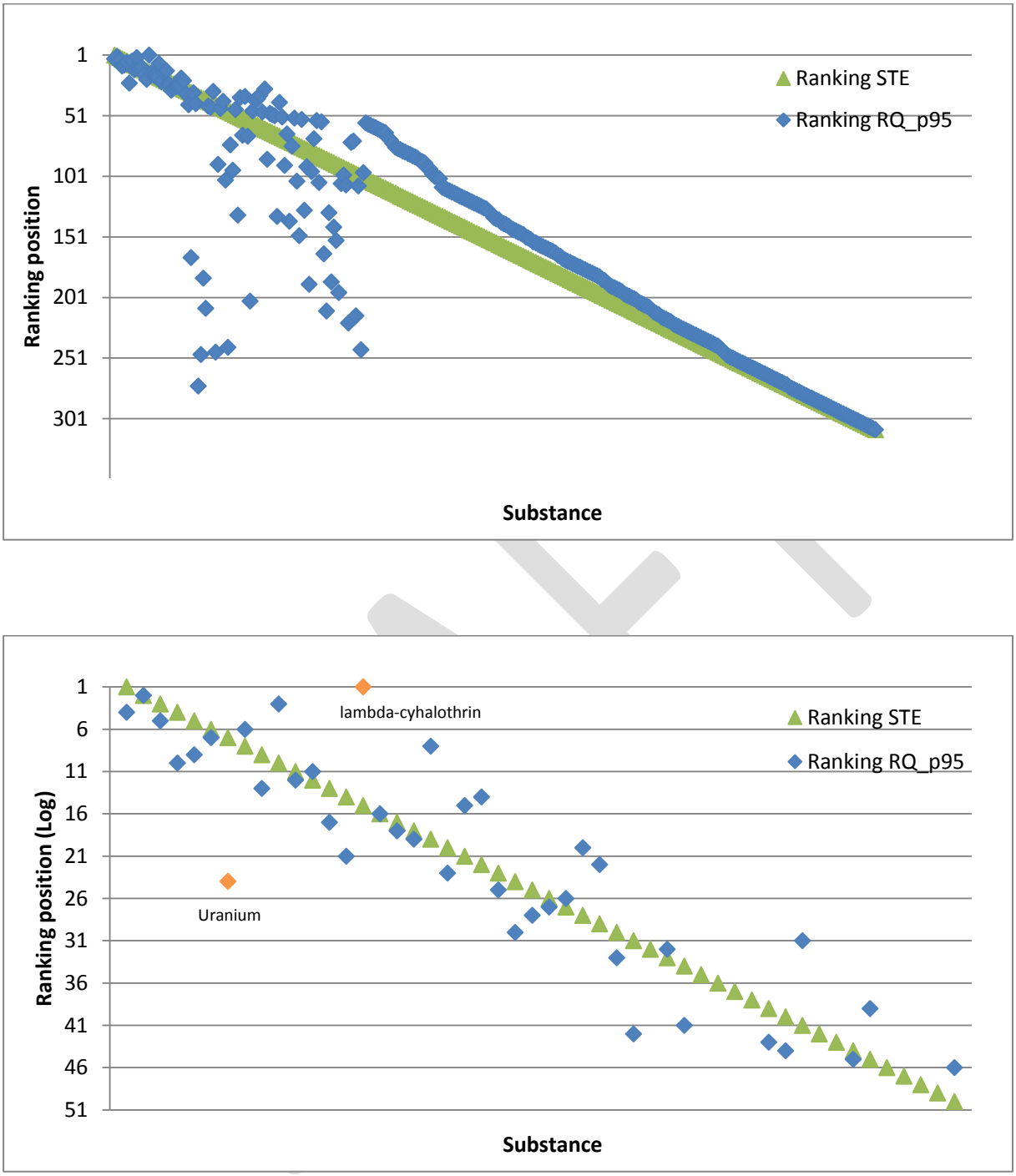


Figure 18. Comparison of the rankings obtained with the STE approach and the Risk quotient based on the 95th percentile of all records, for inland whole water. Top graph shows the ranking position of all substances, while the bottom graph shows only the top 50 substances. Substances for which their ranking position in the two approaches differ by more than 15 places are labelled in orange if they rank at the top 50 position in at least one of the ranking systems.

Twenty five metals were measured in inland water (12 in whole water and 13 in dissolved fraction), 3 in transitional/coastal water, 4 in sediments, 2 in biota and 23 were considered in the drinking water scenario. For most of the metals, the highest STE score was observed from inland water measurements with the exception of arsenic, chromium and copper from sediments and zinc from coastal/transitional water. The STE exercise did not consider the bioavailable fraction or information on background concentrations of metals since the MS usually do not report the necessary supporting information (e.g. pH, DOC, hardness, local natural background) together with the collected monitoring data. For inland water, 13 out of 25 metals (about half of the total) were measured and evaluated in dissolved fraction while the others (12 out of 25) were reported only in whole water fraction. As already discussed, the use of the dissolved concentration and the appropriate PNEC in the scoring of metals is a reasonable approximation respecting the limitation of data availability to estimate bioavailable fraction. However, the obtained high STE scores for the metals measured only in whole water fraction (for example uranium and chromium 6+) should be considered carefully before taking a decision for their possible listing as potential PS.

Finally, even though significant efforts were done to identify the substances posing the highest risk to or via the aquatic environment, it is difficult to argue that all substances posing a risk have been short-listed in the current monitoring-based exercise. Substances which STE score is below 1.8 (but higher than 1.2), together with the substances identified as highly risky in the previous prioritisation but not forwarded, should be considered relevant for a future assessment and eventual control measures at the country or river-basin level.

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List of abbreviations and definitions

AA	Annual average
ADI	Acceptable daily intake
B	Bioaccumulation
BAF	Bioaccumulation Factor
BDE	Brominated diphenylether
BLM	Biotic Ligand Model
C	Carcinogenicity
CAS	Chemical Abstract Service
CIS	Common Implementation Strategy
DG ENV	DG Environment
DOC	Dissolved organic carbon
DOM	Dissolved organic matter
ECHA	European Chemicals Agency
ECOSTAT	CIS Working Group on Ecological Status
ED	Endocrine disruptor activity
EEA	European Environment Agency
EFTA	European Free Trade Association
EMPODAT	Database on emerging pollutants from NORMAN
EqP	Equilibrium Partitioning
EQS	Environmental quality standard
$F_{spatial}$	Spatial factor in the STE approach
$F_{temporal}$	Temporal factor in the STE approach
F_{extent}	Extent factor in the STE approach
GHS	Globally harmonized system of classification and labelling
HH	Human health
IPCheM	Information Platform for Chemical Monitoring data
JDS	Joint Danube Survey
JRC	Joint Research Centre
LOD	Limit of Detection
LOQ	Limit of Quantification
M	Mutagenicity
MAC	Maximum allowable concentrations
MS	Member State
MSDAT	Data submitted by European countries
NOAEL	No Observable Adverse Effect Level

NORMAN	Network of reference laboratories, research centers and related organisations for monitoring of emerging environmental substances
P	Persistence
PAH	Polycyclic Aromatic Hydrocarbon
PEC	Predicted environmental concentration
PHS	Priority Hazardous Substance
PNEC	Predicted no-effect concentration
PPP	Plant Production Product
PS	Priority Substance
R	Reproduction toxicity
RBSP	River basin specific pollutant
REACH	Registration, Evaluation, and Authorisation of Chemicals
Sc	Scenario
secpois	Secondary poisoning
sed	Sediment
SG-R	Sub-group of experts for the review of PS
SoE	State of the Environment
SPM	Suspended particulate matter
STE	Spatial, temporal and extent of PNEC exceedances
STE dw, hh	STE score based on effects to human health from consumption of drinking water
STE fw, eco	STE score based on toxicity effects to aquatic freshwater organisms
STE secpois, eco	STE score based on risk to aquatic organisms from secondary poisoning
STE sed, eco	STE score based on risk to benthic organisms
STE sw, eco	STE score based on risk to aquatic salt water organisms
STE water,hh food	STE score based on risk for human health from the consumption of aquatic and aquaculture (fish) products
T	Toxicity
TDI	Tolerable Daily Intake
TGD-EQS	Technical Guidance Document on EQS derivation
UBA	Umweltbundesamt; Environment Agency of Germany or Austria
UFL	Upper Fence Limit
WFD	Water Framework Directive

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Figure 18. Comparison of the rankings obtained with the STE approach and the Risk quotient based on the 95th percentile of all records, for inland whole water. Top graph shows the ranking position of all substances, while the bottom graph shows only the top 50 substances. Substances for which their ranking position in the two approaches differ by more than 15 places are labelled in orange if they rank at the top 50 position in at least one of the ranking systems.

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Table 31. List of highest ranked monitoring based substances (STE > 1.8) for which a factsheet has been developed (see Annex V)

Annex I: Modifications to the monitoring database

Table I-1. Groups of substances merged prior to the STE runs

Existing identification of substances		Grouping of substances prior to the STE	
CAS number	Substance name	Merged CAS number	Merged Substance name
10061-02-6	trans-1,3-Dichloropropene	542-75-6	1,3-Dichloropropene
10061-01-5	cis-1,3-Dichloropropene		
542-75-6	1,3-Dichloropropene		
156-59-2	cis-1,2-Dichloroethylene	540-59-0	1,2-Dichloroethene
156-60-5	trans-1,2-Dichloroethylene		
5103-71-9	alpha-Chlordane	57-74-9	Chlordane
5103-74-2	trans-Chlordane		
5566-34-7	gamma-Chlordane		
51218-45-2	Metolachlor	51218-45-2	Metolachlor
87392-12-9	S-Metolachlor		
57837-19-1	Metalaxyl	57837-19-1	Metalaxyl
70630-17-0	Metalaxyl-M		
1330-20-7	Xylene	1330-20-7	Xylene (mixed isomers)
108-38-3	m-Xylene		
95-47-6	o-Xylene		
56-38-2	Parathion	56-38-2	Parathion/Parathion-methyl
298-00-0	Parathion-methyl		
7012-37-5	2,4,4'-Trichlorobiphenyl (PCB-28)	1336-36-3	Polychlorinated biphenyls (PCB) sum
35693-99-3	2,2',5,5'-Tetrachlorobiphenyl (PCB-52)		
37680-73-2	2,2',4,5,5'-Pentachlorobiphenyl (PCB-101)		
35065-27-1	2,2’,4,4’,5,5’-Hexachlorobiphenyl (PCB-153)		
35065-28-2	2,2’,3,4,4’,5’-Hexachlorobiphenyl (PCB-138)		
35065-29-3	2,2’,3,4,4’,5,5’-Heptachlorobiphenyl (PCB-180)		

Table I-2. List of substances for which the monitoring data in the dissolved phase have been merged with the whole water fraction

Note: For some compounds (mainly degradation products) it was not possible to find Kow values, but since they are polar water soluble compounds, their records for dissolved phase and whole water also were merged.

Substance	CAS	log Kow
1,1,1,2-Tetrachloroethane	630-20-6	2.5
1,1,2,2-Tetrachloroethane	79-34-5	2.4
1,1,2-Trichloroethane	79-00-5	1.9
1,1-Dichloroethane	75-34-3	1.8
1,1-Dichloroethylene	75-35-4	1.3
1,2,3-Trichloropropane	96-18-4	2.3
1,2,4-Trimethylbenzene	95-63-6	3.8
1,2-Dibromoethane	106-93-4	3.3
1,2-Dichloropropane	78-87-5	2
1,3,5-Benzenetriol	108-73-6	
1,3,5-Trimethylbenzene	108-67-8	3.6
1,3-Dichloropropene	542-75-6	1.6
1,4-Dichlorobenzene	106-46-7	3.4
10,11-Dihydro-10,11-dihydroxycarbamazepine	58955-93-4	
1H-Benzotriazole	95-14-7	1.4
2,3-Dichloroaniline	608-27-5	2.8
2,4,6-Trichlorophenol	88-06-2	3.4
2,4-Dichlorophenol	120-83-2	3.2
2,4-Dichlorophenoxyacetic acid (2,4-D)	94-75-7	2.8
2-Chlorophenol	95-57-8	2.1
2-Methyl-4-chlorophenoxyacetic acid (MCPA)	94-74-6	2.8
2-Nitrophenol	88-75-5	1.8
3,4-Dichloroaniline (3,4-DCA)	95-76-1	2.7

Substance	CAS	log Kow
3-Chloroaniline	108-42-9	1.9
4-Chloroaniline	106-47-8	1.8
4-Chlorophenol	106-48-9	2.3
4-Nonylphenoxy acetic acid	3115-49-9	
4-tert-Butylphenol	98-54-4	3.3
5-Methyl-1H-benzotriazole	136-85-6	1.2
6-Desisopropylatrazine	1007-28-9	
Acenaphthene	83-32-9	3.9
Acephate	30560-19-1	-1.87
Acetaminophen (Paracetamol)	103-90-2	0.34
Acetazolamide	59-66-5	0.13
Acetochlor	34256-82-1	3
Aldicarb	116-06-3	1.1
Alprazolam	28981-97-7	2.1
Ametryn	834-12-8	3
Aminomethylphosphonic acid (AMPA)	1066-51-9	-2.1
Aminotriazole	61-82-5	-0.1
Ammonium (NH4 - N)	14798-03-9	
Anthrachinone	84-65-1	3.4
Atenolol	29122-68-7	0.16
Azinphos-ethyl	2642-71-9	3.4
Azinphos-methyl	86-50-0	3
Azithromycin	83905-01-5	4
Bentazone	25057-89-0	2.8
Bezafibrate	41859-67-0	3.3
Biphenyl	92-52-4	3.7
Bisphenol A	80-05-7	2.2

Substance	CAS	log Kow
Bromacil	314-40-9	1.9
Bromazepam	1812-30-2	2.05
Caffeine	58-08-2	0.01
Carbamazepine	298-46-4	2.3
Carbaryl	63-25-2	2.3
Carbendazime	10605-21-7	1.5
Carbofuran	1563-66-2	2.4
Carbontetrachloride	56-23-5	2.6
Chlorate	14866-68-3	
Chlordiazepoxide	58-25-3	2.4
Chloridazon	1698-60-8	1.6
Chloridazon-desphenyl	6339-19-1	
Chloridazon-methyl-desphenyl	17254-80-7	
Chloride (Cl-)	16887-00-6	
Chlorocresol	59-50-7	3.1
Chlorothalonil	1897-45-6	2.9
Chlorotoluron	15545-48-9	2.4
Chlorpropham	101-21-3	3.5
Ciprofloxacin	85721-33-1	0.28
Clarithromycin	81103-11-9	3.2
Clobazam (Urbadan)	22316-47-8	1.7
Clofibric acid (metabolite of clofibrate)	882-09-7	2.9
Clonazepam	1622-61-3	2.4
Clotrimazole	23593-75-1	3.6
Cyanazine	21725-46-2	2.3
Cyanide (as total CN)	57-12-5	
Cyclophosphamide	50-18-0	0.63

Substance	CAS	log Kow
Cyproconazole	94361-06-5	3.1
Deltamethrine	52918-63-5	4.6
Desethylatrazine	6190-65-4	1.5
Desethylterbuthylazine	30125-63-4	
Desmetryn	1014-69-3	2.4
Diatrizoate	117-96-4	1.4
Diazepam	439-14-5	2.8
Diazinon	333-41-5	3.7
Dibutyltin-cation	1002-53-5	
Dicamba	1918-00-9	2.2
Dichlobenil	1194-65-6	2.7
Dichlofluanid	1085-98-9	2.8
Dichlorvos	62-73-7	1.4
Diclofenac	15307-86-5	4.5, but deprontonated
Diethyl phthalate	84-66-2	2.4
Diisobutyl phthalate	84-69-5	3.7
Dimethenamid	87674-68-8	2.6
Dimethoate	60-51-5	2.7
Dioctyltin-cation	94410-05-6	
Diphenylamine	122-39-4	3.6
Diphenyltin-cation	1135-99-5	
Disulfoton	298-04-4	4
Drospirenone	67392-87-4	4
Endosulfan-sulfate	1031-07-8	
Erythromycin	114-07-8	3.1
Estriol	50-27-1	2.5

Substance	CAS	log Kow
Estrone	53-16-7	3.1
Ethion	563-12-2	5
Ethofumesate	26225-79-6	2.7
Ethoprophos	13194-48-4	3.6
Ethylbenzene	100-41-4	3.1
Ethylenediaminetetraacetic acid (EDTA)	60-00-4	-3.3
Ethylparaben	120-47-8	3
Fenarimol	60168-88-9	3.7
Fenitrothion	122-14-5	3.3
Fenofibrate	49562-28-9	deprotonated
Fenofibric acid	42017-89-0	deprotonated
Fenthion	55-38-9	4.1
Flunitrazepam	1622-62-4	2.1
Fluorene	86-73-7	4.2
Fluoride	16984-48-8	
Fluroxypyr	69377-81-7	2.2
Flurtamone	96525-23-4	3.2
Flusilazole	85509-19-9	3.7
Flutriafol	76674-21-0	2.3
Fonofos	944-22-9	3.9
Formaldehyde	50-00-0	-0.83
Furosemide	54-31-9	2
Gemfibrozil	25812-30-0	4.7, but deprotonated
Glyphosate	1071-83-6	-3.2
Halazepam	23092-17-3	
Heptenophos	23560-59-0	2.3
Hexachlorocyclohexane (all isomers)	319-84-6	3.8

Substance	CAS	log Kow
Hexazinone	51235-04-2	1.2
Ibuprofen	15687-27-1	0.8
Imidaclopride	138261-41-3	0.5
Iohexol	66108-95-0	-2.3
Iomeprol	78649-41-9	<0
Iopamidol	60166-93-0	-2.4
Iopromide	73334-07-3	-2.3
Iprodione	36734-19-7	3
Ketoprofen	22071-15-4	3.1
Lead triethyl	5224-23-7	-1.76
Lindane (gamma-Hexachlorocyclohexane)	58-89-9	3.7
Linuron	330-55-2	3.2
Lorazepam	846-49-1	2.4
Malathion	121-75-5	2.7
Mecoprop	7085-19-0	2.9
Mecoprop	93-65-2	0.6
Mestranol	72-33-3	4.7
Metalaxyl	57837-19-1	1.7
Metaldehyde	108-62-3	0.12
Metamitron	41394-05-2	0.8
Metazachlor	67129-08-2	2.5
Metazachlor ESA	72960-62-2	
Metazachlor OA	1231244-60-2	
Methamidophos	10265-92-6	-1.74
Methidathion	950-37-8	2.2
Methiocarb	2032-65-7	3.1
Methomyl	16752-77-5	0.6

Substance	CAS	log Kow
Methoxychlor	72-43-5	4.7
Methyl-1H-benzotriazole / Tolyltriazole	29385-43-1	1.9
Methylparaben	99-76-3	2
Methyl-tert-butyl ether	1634-04-4	1.2
Metolachlor	51218-45-2	3.1
Metolachlor ESA	171118-09-5	
Metolachlor OXA	152019-73-3	
Metoprolol	37350-58-6	1.9
Metribuzin	21087-64-9	1.7
Mevinphos	7786-34-7	-0.24
Midazolam	59467-70-8	4.3
Molinate	2212-67-1	2.9
Monocrotophos	6923-22-4	0.4
N,N-Diethyl-m-toluamid (DEET)	134-62-3	2
Naproxen	22204-53-1	3.18
Nitrates (NO3-N)	7697-37-2	
Nitrite	14797-65-0	
Nitrobenzene	98-95-3	1.9
N-Nitrosomethylethylamine	10595-95-6	0.6
N-Nitrosopyrrolidine	930-55-2	-0.5
Norethindrone	68-22-4	3
Norfloxacin	70458-96-7	0.46
Ofloxacine	82419-36-1	0.4
Omethoate	1113-02-6	0.8
Oxadixyl	77732-09-3	0.65
Oxazepam	604-75-1	2.2
o-Xylene	95-47-6	

Substance	CAS	log Kow
Paclobutrazol	76738-62-0	3.2
Parathion	56-38-2	3.1
Parathion methyl	298-00-0	2.8
Paroxetine	61869-08-7	2.1
p-Cresol	106-44-5	1.9
Perfluorobutanesulfonate (PFBS)	375-73-5	
Perfluorodecanoic acid	335-76-2	
Perfluoro-dodecanoic acid	307-55-1	
Perfluoroheptanoic acid (PFHpA)	375-85-9	
Perfluorohexanoic acid (PFHxA)	307-24-4	
Perfluorononanoate (PFNA)	375-95-1	
Perfluorooctane sulfonate (PFOS)	45298-90-6	
Perfluorooctanoic acid (PFOA)	335-67-1	
Perfluoroundecanoic acid	2058-94-8	
Permethrin	52645-53-1	2.9
Phenazone	60-80-0	2.3
Phenol	108-95-2	0.62
Phosphate	14265-44-2	
Phoxime	14816-18-3	4.4
Pirimicarb	23103-98-2	1.7
Pirimiphos-methyl	29232-93-7	4.3
Potassium	9/7/7440	
Prazepam	2955-38-6	3.7
Primidone	125-33-7	0.9
Prochloraz	67747-09-5	4.1
Prometryn	7287-19-6	3.5
Propachlor	1918-16-7	2.2

Substance	CAS	log Kow
Propanil	709-98-8	2.9
Propazine	139-40-2	2.9
Propiconazole	60207-90-1	3.7
Propranolol	525-66-6	3
Propyzamide	23950-58-5	3.4
Quinmerac	90717-03-6	2.1
Quizalofop	32536-52-0	1.7
Roxithromycin	80214-83-1	2.7
Secbumeton	26259-45-0	3.6
Sodium	7440-23-5	
Sotalol	3930-20-9	0.24
Spiroxamine	118134-30-8	2.9
Sulfadiazine	68-35-9	-0.09
Sulfadimethoxin	122-11-2	1.6
Sulfamethazine	57-68-1	0.9
Sulfamethoxazole	723-46-6	0.9
Sulfapyridine	144-83-2	0.35
Sulphates (SO4--)	14808-79-8	
Tau-fluvalinate	102851-06-9	4.3
Tebuconazole	107534-96-3	3.7
Temazepam	846-50-4	
Terbumeton	33693-04-8	3
Terbuthylazine	5915-41-3	3
Tetrabutyl tin ion	1461-25-2	
Tetrachloroethylene	127-18-4	3.4
Tetraethyl lead	78-00-2	-1.76
Thiabendazole	148-79-8	2.5

Substance	CAS	log Kow
Thiodicarb	59669-26-0	1.7
Thiometon	640-15-3	3.15
Toluene	108-88-3	2.7
Tolylfluanid	731-27-1	3.9
Triadimefon	43121-43-3	3
Triadimenol	55219-65-3	3.1
Triallate	2303-17-5	4.6
Tributyl phosphate	126-73-8	4
Trichloroethylene	79-01-6	2.3
Triclosan	3380-34-5	4.7, but deprotonated
Trimethoprim	738-70-5	2.2
Triphenylphosphine oxide	791-28-6	2.9
Triphenyltin (cation)	668-34-8	
Vinyl chloride (Chloroethylene)	75-01-4	1.2
Xylene (mixed isomers)	1330-20-7	3.1
Zolpidem	82626-48-0	2.4

Annex II: Summary of monitoring data

Table II-1. Summary monitoring data - inland whole water.

For each substance, two scenarios are presented. Top/shaded: Sc2 (all monitoring records; non-quantified records set as half LOD/Q); Bottom/white: Sc2-PNEC QC (quantified records plus non-quantified samples excluding those for which ½LOD/Q > PNEC). Substances are sorted by CAS numbe; concentrations in µg/L.

Note: n/a for some substances in Sc2-PNECQC indicates that they are not considered in STE since did not fulfild the representativeness criteria

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
100-00-5	1-Chloro-4-nitrobenzene	4	1424	12554	38	12512	0.03	5.00E-05	1.77E-01	1.67E-01	1.50E-01	5.00E-01	5.00E-01	1.40E+00
		4	1424	12554	38	12512	0.03	5.00E-05	1.77E-01	1.67E-01	1.50E-01	5.00E-01	5.00E-01	1.40E+00
1002-53-5	Dibutyltin	12	2442	22448	171	21508	3.43	5.00E-05	2.85E-02	1.74E-01	5.00E-03	1.95E-02	2.50E-02	6.80E+00
		12	2034	17034	171	16094	4.51	5.00E-05	8.87E-03	9.87E-02	4.00E-03	7.50E-03	1.00E-02	6.80E+00
100-41-4	Ethylbenzene	14	3009	45750	429	45001	0.7	3.00E-06	3.65E-01	6.08E-01	2.50E-01	7.03E-01	2.50E+00	1.02E+01
		14	2852	42981	429	42232	0.74	3.00E-06	2.34E-01	3.12E-01	1.25E-01	5.00E-01	5.00E-01	1.02E+01
100-42-5	Styrene	9	1375	19934	988	18797	0.75	2.50E-03	2.01E-01	2.31E-01	1.25E-01	5.00E-01	5.00E-01	6.60E+00
		9	1374	19006	984	17873	0.78	2.50E-03	1.61E-01	1.43E-01	1.25E-01	2.50E-01	5.00E-01	5.33E+00
1007-28-9	6-Desisopropylatrazine	17	5691	79087	3547	74547	1.26	5.00E-06	2.51E-02	1.77E-01	1.25E-02	5.00E-02	5.00E-02	1.00E+01
		16	2800	37175	1407	34775	2.67	5.00E-06	9.62E-03	3.59E-02	1.00E-02	1.00E-02	1.00E-02	4.22E+00
101200-48-0	Tribenuron-methyl	4	154	2836	0	2784	1.83	1.00E-03	2.77E-02	2.12E-02	1.00E-02	5.00E-02	5.00E-02	1.90E-01
		4	154	2836	0	2784	1.83	1.00E-03	2.77E-02	2.12E-02	1.00E-02	5.00E-02	5.00E-02	1.90E-01
101205-02-1	Cycloxydim	4	230	3552	50	3467	0.99	1.00E-03	1.88E-02	6.32E-02	1.50E-02	2.50E-02	2.50E-02	3.70E+00
		4	230	3552	50	3467	0.99	1.00E-03	1.88E-02	6.32E-02	1.50E-02	2.50E-02	2.50E-02	3.70E+00
101-21-3	Chlorpropham	5	2947	36000	3501	31587	2.53	1.00E-03	3.62E-02	1.03E+00	2.50E-02	5.00E-02	5.00E-02	1.94E+02

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
		5	2947	35998	3501	31585	2.53	1.00E-03	3.57E-02	1.02E+00	2.50E-02	5.00E-02	5.00E-02	1.94E+02
1014-69-3	Desmetryn	5	2738	40261	2394	37643	0.56	2.50E-04	1.47E-02	2.49E-01	5.00E-03	1.25E-02	2.50E-02	1.00E+01
		5	2734	40173	2367	37582	0.56	2.50E-04	8.34E-03	9.45E-03	5.00E-03	1.25E-02	2.50E-02	1.30E+00
10265-92-6	Methamidophos	5	1584	23414	107	23287	0.09	2.50E-03	2.26E-02	1.52E-02	2.00E-02	5.00E-02	5.00E-02	1.30E-01
		4	983	9872	0	9852	0.2	2.50E-03	9.10E-03	4.26E-03	1.00E-02	1.25E-02	1.25E-02	1.30E-01
102851-06-9	Tau-fluvalinate	4	1107	7935	84	7849	0.03	3.00E-04	1.90E-02	6.82E-03	2.00E-02	2.50E-02	2.50E-02	2.50E-02
		n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
1031-07-8	Endosulfan sulfate	9	3366	31728	1572	29938	0.69	5.00E-05	7.84E-03	2.76E-02	5.00E-03	1.00E-02	2.50E-02	2.50E+00
		9	2519	20939	1233	19488	1.04	5.00E-05	3.79E-03	2.10E-02	5.00E-03	5.00E-03	5.00E-03	1.00E+00
103-65-1	n-Propylbenzene	6	539	6267	0	6238	0.46	2.50E-03	8.41E-01	1.73E+00	1.50E-01	5.00E+00	5.00E+00	5.00E+00
		6	539	6267	0	6238	0.46	2.50E-03	8.41E-01	1.73E+00	1.50E-01	5.00E+00	5.00E+00	5.00E+00
103-90-2	Acetaminophen (Paracetamol)	4	104	1301	16	1107	13.68	5.00E-04	2.17E-02	6.21E-02	1.00E-02	3.00E-02	6.00E-02	9.30E-01
		4	104	1301	16	1107	13.68	5.00E-04	2.17E-02	6.21E-02	1.00E-02	3.00E-02	6.00E-02	9.30E-01
104-35-8	4-Nonylphenol mono-ethoxylate (NP1EO)	19	2104	31638	1089	30113	1.38	2.50E-05	4.69E-02	4.78E-02	4.50E-02	1.50E-01	1.50E-01	3.00E+00
		18	2085	27029	1089	25504	1.61	2.50E-05	3.29E-02	3.36E-02	2.50E-02	5.00E-02	5.00E-02	3.00E+00
104-51-8	n-Butylbenzene	6	743	6160	0	6149	0.18	2.50E-02	3.42E-01	4.08E-01	2.50E-01	1.00E+00	1.00E+00	2.50E+00
		6	743	6160	0	6149	0.18	2.50E-02	3.42E-01	4.08E-01	2.50E-01	1.00E+00	1.00E+00	2.50E+00
10605-21-7	Carbendazim	6	4079	48648	3304	37198	16.74	5.00E-04	2.50E-01	3.52E+00	1.00E-02	5.00E-02	1.50E-01	4.40E+02
		6	4075	48567	3224	37197	16.77	5.00E-04	2.49E-01	3.52E+00	1.00E-02	5.00E-02	1.50E-01	4.40E+02
106-43-4	4-Chlorotoluene	8	1820	29657	116	29468	0.25	2.50E-04	5.23E-01	1.14E+00	2.50E-01	5.00E-01	5.00E+00	5.00E+00
		8	1615	26990	116	26801	0.27	2.50E-04	1.87E-01	1.11E-01	1.25E-01	2.50E-01	5.00E-01	2.00E+00

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
106-46-7	1,4-Dichlorobenzene	12	4148	53189	669	52306	0.4	2.50E-03	4.14E-01	1.09E+01	2.50E-01	5.00E-01	2.50E+00	2.50E+03
		12	4034	50360	606	49540	0.42	2.50E-03	2.32E-01	1.76E-01	2.50E-01	5.00E-01	5.00E-01	4.90E+00
106-47-8	4-Chloroaniline	5	2323	26925	1288	25421	0.8	5.00E-03	4.88E-02	5.28E-02	5.00E-02	5.00E-02	1.50E-01	5.00E-01
		5	2129	25240	709	24315	0.86	5.00E-03	3.64E-02	1.60E-02	5.00E-02	5.00E-02	5.00E-02	3.70E-01
106-48-9	4-Chlorophenol	8	2497	30558	510	29522	1.72	2.50E-03	6.54E-02	2.87E+00	5.00E-02	5.00E-02	1.00E-01	5.00E+02
		8	2497	30557	510	29521	1.72	2.50E-03	4.91E-02	2.75E-01	5.00E-02	5.00E-02	1.00E-01	4.70E+01
1066-51-9	Aminomethylphosphonic acid (AMPA)	15	3581	40873	1143	17252	54.99	2.50E-04	1.71E+00	5.50E+01	1.00E-01	1.00E+00	2.05E+00	4.55E+03
		15	3581	40873	1143	17252	54.99	2.50E-04	1.71E+00	5.50E+01	1.00E-01	1.00E+00	2.05E+00	4.55E+03
106-89-8	Epichlorhydrin (1-Chloro-2,3-epoxypropane)	5	928	6210	1150	4998	1	2.50E-02	8.08E-01	1.96E+00	2.50E-01	2.50E+00	5.00E+00	2.50E+01
		4	794	5563	1112	4389	1.11	2.50E-02	2.67E-01	1.74E-01	2.50E-01	5.00E-01	5.00E-01	1.00E+00
106-93-4	1,2-Dibromoethane	10	1820	28898	218	28662	0.06	1.00E-02	5.57E-01	1.04E+00	2.50E-01	1.25E+00	2.50E+00	5.00E+00
		n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
1071-83-6	Glyphosate	18	4154	45604	2987	28100	31.83	1.40E-05	4.33E-01	1.49E+01	5.00E-02	2.60E-01	5.30E-01	2.24E+03
		18	4154	45604	2987	28100	31.83	1.40E-05	4.33E-01	1.49E+01	5.00E-02	2.60E-01	5.30E-01	2.24E+03
107534-96-3	Tebuconazole	8	3370	38524	1945	33977	6.75	1.25E-03	2.39E-02	8.88E-02	1.25E-02	5.00E-02	5.00E-02	1.40E+01
		8	3370	38520	1941	33977	6.75	1.25E-03	2.38E-02	8.86E-02	1.25E-02	5.00E-02	5.00E-02	1.40E+01
108-41-8	3-Chlorotoluene	5	1278	13583	43	13540	0	1.00E-02	7.74E-01	1.50E+00	2.50E-01	5.00E+00	5.00E+00	5.00E+00
		5	1058	12068	43	12025	0	1.00E-02	2.44E-01	9.07E-02	2.50E-01	2.50E-01	5.00E-01	5.00E-01
108-42-9	3-Chloroaniline	5	2097	25145	228	24810	0.43	5.00E-03	4.73E-02	3.18E-01	5.00E-02	5.00E-02	5.00E-02	5.00E+01
		5	2096	25126	226	24793	0.43	5.00E-03	4.49E-02	4.29E-02	5.00E-02	5.00E-02	5.00E-02	1.18E+00
108-43-0	3-Chlorophenol	8	1388	12890	206	12464	1.71	2.50E-03	4.86E-02	7.22E-02	2.50E-02	1.00E-01	1.00E-01	5.00E-01

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
		8	1388	12890	206	12464	1.71	2.50E-03	4.86E-02	7.22E-02	2.50E-02	1.00E-01	1.00E-01	5.00E-01
1085-98-9	Dichlofluanid	6	1866	24105	845	23191	0.29	2.50E-03	1.01E-02	6.07E-03	1.00E-02	2.00E-02	2.00E-02	5.40E-02
		6	1866	24105	845	23191	0.29	2.50E-03	1.01E-02	6.07E-03	1.00E-02	2.00E-02	2.00E-02	5.40E-02
108-60-1	Dichloroisopropyl ether (Propane)	5	327	2789	25	2760	0.14	5.00E-02	2.23E+00	2.72E+00	1.00E+00	5.00E+00	5.00E+00	1.00E+02
		5	327	2789	25	2760	0.14	5.00E-02	2.23E+00	2.72E+00	1.00E+00	5.00E+00	5.00E+00	1.00E+02
108-67-8	1,3,5-Trimethylbenzene	8	926	9406	0	9360	0.49	2.50E-03	4.90E-01	5.48E-01	5.00E-01	1.00E+00	2.50E+00	2.50E+00
		8	888	8915	0	8869	0.52	2.50E-03	3.79E-01	2.85E-01	5.00E-01	1.00E+00	1.00E+00	2.00E+00
108-88-3	Toluene	17	5170	95445	2616	90530	2.41	5.00E-06	4.01E-01	3.28E+00	2.50E-01	5.00E-01	5.00E-01	1.00E+03
		17	5170	95444	2616	90529	2.41	5.00E-06	3.91E-01	5.55E-01	2.50E-01	5.00E-01	5.00E-01	4.10E+01
108-90-7	Chlorobenzene	12	2480	43579	73	43212	0.67	1.00E-06	2.29E-01	3.24E-01	2.50E-01	5.00E-01	5.00E-01	1.05E+01
		12	2433	43141	73	42774	0.68	1.00E-06	2.12E-01	2.66E-01	2.50E-01	5.00E-01	5.00E-01	1.00E+01
108-95-2	Phenol	6	931	7876	1078	4309	31.6	5.00E-04	6.82E-01	3.31E+00	5.00E-02	1.00E+00	3.00E+00	1.10E+02
		5	882	7428	762	4177	33.51	5.00E-04	4.77E-01	3.24E+00	2.50E-02	6.03E-01	1.00E+00	1.10E+02
110488-70-5	Dimethomorph	4	1583	16142	0	15495	4.01	2.50E-03	3.51E-02	7.18E-02	2.50E-02	5.00E-02	5.00E-02	5.50E+00
		4	1583	16142	0	15495	4.01	2.50E-03	3.51E-02	7.18E-02	2.50E-02	5.00E-02	5.00E-02	5.50E+00
1113-02-6	Omethoate	8	2747	34289	808	33404	0.22	1.00E-04	3.05E-02	1.02E-01	2.50E-02	5.00E-02	5.00E-02	1.00E+01
		5	38	77	0	0	100	1.00E-04	6.58E-02	1.20E-01	4.00E-02	1.00E-01	1.14E-01	7.63E-01
111988-49-9	Thiacloprid	6	713	6398	2167	3874	5.58	1.00E-03	1.57E-01	2.99E+00	5.00E-03	1.00E-02	1.00E-02	1.00E+02
		5	673	6301	2092	3852	5.67	1.00E-03	4.03E-02	1.78E+00	5.00E-03	1.00E-02	1.00E-02	1.00E+02
111991-09-4	Nicosulfuron	5	1794	18410	0	17879	2.88	1.50E-03	3.12E-02	4.25E-01	1.50E-02	2.50E-02	2.50E-02	1.60E+01
		5	197	1104	0	573	48.1	1.50E-03	2.23E-01	1.73E+00	5.00E-03	8.97E-02	1.97E-01	1.60E+01
114-26-1	Propoxur	5	883	7246	112	6962	2.37	2.50E-03	1.62E-02	9.25E-03	2.00E-02	2.50E-02	2.50E-02	4.60E-01

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
		5	174	3646	0	3474	4.72	2.50E-03	1.07E-02	1.01E-02	1.00E-02	1.00E-02	1.00E-02	4.60E-01
115-86-6	Triphenyl phosphate (TPT)	8	425	4923	825	3577	10.58	5.00E-06	5.19E-02	7.92E-02	2.00E-02	2.50E-01	2.50E-01	4.60E-01
		8	425	4923	825	3577	10.58	5.00E-06	5.19E-02	7.92E-02	2.00E-02	2.50E-01	2.50E-01	4.60E-01
115-96-8	Tris(2-chloroethyl)phosphate (TCEP)	8	453	6696	326	2723	54.47	3.40E-03	6.44E-02	9.89E-02	3.30E-02	1.60E-01	2.50E-01	4.10E+00
		8	453	6696	326	2723	54.47	3.40E-03	6.44E-02	9.89E-02	3.30E-02	1.60E-01	2.50E-01	4.10E+00
116-06-3	Aldicarb	6	2992	33434	3676	29621	0.41	1.00E-03	2.04E-02	6.08E-02	1.00E-02	5.00E-02	5.00E-02	5.00E+00
		6	2982	32299	3676	28486	0.42	1.00E-03	1.62E-02	1.89E-02	1.00E-02	5.00E-02	5.00E-02	1.50E+00
116-29-0	Tetradifon	4	825	5619	210	5408	0.02	1.60E-05	4.17E-02	1.40E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02
		4	825	5619	210	5408	0.02	1.60E-05	4.17E-02	1.40E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02
1163-19-5	Decabromodiphenyl ether (BDE-209)	4	2412	38856	0	37362	3.84	7.50E-05	3.75E-01	1.80E+01	1.00E-02	2.50E-01	1.00E+00	1.25E+03
		n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
117428-22-5	Picoxystrobin	4	547	6020	0	5929	1.51	1.00E-03	2.18E-02	1.62E-02	1.25E-02	5.00E-02	5.00E-02	8.90E-02
		4	547	6020	0	5929	1.51	1.00E-03	2.18E-02	1.62E-02	1.25E-02	5.00E-02	5.00E-02	8.90E-02
117-84-0	Di-n-octyl phthalate	5	109	636	173	452	1.73	2.50E-03	2.39E+00	5.99E+00	4.10E-02	8.50E+00	8.50E+00	1.00E+02
		5	109	636	173	452	1.73	2.50E-03	2.39E+00	5.99E+00	4.10E-02	8.50E+00	8.50E+00	1.00E+02
118134-30-8	Spiroxamine	5	488	6862	0	6622	3.5	5.00E-04	2.77E-02	4.33E-02	2.50E-02	5.00E-02	5.00E-02	2.68E+00
		4	229	2594	0	2354	9.25	5.00E-04	1.37E-02	6.62E-02	1.00E-02	1.00E-02	2.63E-02	2.68E+00
119446-68-3	Difenoconazole	5	1086	11177	69	11077	0.28	5.00E-04	3.60E-02	2.54E-02	2.50E-02	1.00E-01	1.00E-01	1.00E-01
		5	1086	11177	69	11077	0.28	5.00E-04	3.60E-02	2.54E-02	2.50E-02	1.00E-01	1.00E-01	1.00E-01
1194-65-6	Dichlobenil	9	3173	44074	3662	39830	1.32	5.00E-04	1.68E-02	3.82E-02	1.25E-02	2.50E-02	2.50E-02	6.40E+00
		9	3173	44074	3662	39830	1.32	5.00E-04	1.68E-02	3.82E-02	1.25E-02	2.50E-02	2.50E-02	6.40E+00

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
120-32-1	Chlorophene	7	51	51	0	51	0	2.50E-01	2.50E-01	0.00E+00	2.50E-01	2.50E-01	2.50E-01	2.50E-01
		7	51	51	0	51	0	2.50E-01	2.50E-01	0.00E+00	2.50E-01	2.50E-01	2.50E-01	2.50E-01
120-36-5	Dichlorprop	12	2733	35564	485	33793	3.62	2.50E-04	1.25E-02	6.32E-02	1.00E-02	2.00E-02	2.50E-02	9.50E+00
		12	2733	35563	485	33792	3.62	2.50E-04	1.25E-02	6.32E-02	1.00E-02	2.00E-02	2.50E-02	9.50E+00
120-83-2	2,4-Dichlorophenol	9	2836	41122	1264	39264	1.44	2.50E-03	4.24E+00	1.26E+02	2.50E-02	5.00E-02	1.00E-01	1.00E+04
		9	2835	41065	1207	39264	1.45	2.50E-03	7.72E-01	8.55E+01	2.50E-02	5.00E-02	1.00E-01	1.00E+04
120923-37-7	Amidosulfuron	5	956	8275	0	8195	0.97	1.00E-03	3.82E-02	1.75E-02	5.00E-02	5.00E-02	5.00E-02	2.70E-01
		5	956	8275	0	8195	0.97	1.00E-03	3.82E-02	1.75E-02	5.00E-02	5.00E-02	5.00E-02	2.70E-01
121-14-2	2,4-Dinitrotoluene	4	297	4420	97	4145	4.03	1.25E-02	1.71E-01	1.75E+00	2.50E-02	1.25E-01	3.00E-01	1.00E+02
		4	278	4361	38	4145	4.08	1.25E-02	1.19E-01	1.71E+00	2.50E-02	1.25E-01	1.30E-01	1.00E+02
121552-61-2	Cyprodinil	5	1736	17718	0	17401	1.79	2.50E-03	1.82E-02	1.39E-02	2.00E-02	2.50E-02	4.00E-02	6.14E-01
		5	1736	17716	0	17399	1.79	2.50E-03	1.82E-02	1.38E-02	2.00E-02	2.50E-02	4.00E-02	6.14E-01
121-73-3	1-Cloro-4-nitrobenzene	6	1437	12612	55	12547	0.08	5.00E-05	2.40E-01	3.56E+00	1.50E-01	5.00E-01	5.00E-01	2.00E+02
		6	1437	12612	55	12547	0.08	5.00E-05	2.40E-01	3.56E+00	1.50E-01	5.00E-01	5.00E-01	2.00E+02
121-75-5	Malathion	11	5496	78368	6933	70726	0.9	1.00E-04	8.89E-03	6.76E-02	5.00E-03	2.00E-02	2.50E-02	1.71E+01
		7	320	1338	0	629	52.99	1.00E-04	2.91E-02	5.05E-01	3.00E-03	4.00E-02	4.61E-02	1.71E+01
122-14-5	Fenitrothion	13	3551	49811	2698	46868	0.49	2.50E-04	8.51E-03	1.34E-02	5.00E-03	2.00E-02	2.25E-02	2.00E+00
		11	2338	30037	1502	28290	0.82	2.50E-04	3.88E-03	1.25E-02	5.00E-03	5.00E-03	5.00E-03	2.00E+00
122-39-4	Diphenylamine	5	609	4245	102	4138	0.12	1.00E-02	4.77E-02	1.53E+00	1.00E-02	5.00E-02	5.00E-02	1.00E+02
		5	609	4245	102	4138	0.12	1.00E-02	4.77E-02	1.53E+00	1.00E-02	5.00E-02	5.00E-02	1.00E+02
122931-48-0	Rimsulfuron	6	834	7192	1	7170	0.29	1.00E-03	3.57E-01	1.18E+01	2.50E-02	2.50E-02	2.50E-02	7.96E+02
		6	234	3063	0	3042	0.69	1.00E-03	6.32E-01	1.80E+01	1.00E-02	1.00E-02	1.00E-02	7.96E+02
123-91-1	1,4-Dioxane	4	54	118	0	1	99.15	3.90E-02	7.01E-01	4.19E-01	6.40E-01	1.25E+00	1.55E+00	2.24E+00

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
		4	54	118	0	1	99.15	3.90E-02	7.01E-01	4.19E-01	6.40E-01	1.25E+00	1.55E+00	2.24E+00
124-48-1	Dibromochloromethane	10	1444	15201	0	15076	0.82	2.50E-03	1.83E-01	1.65E-01	1.00E-01	5.00E-01	5.00E-01	2.50E+00
		10	1444	15200	0	15075	0.82	2.50E-03	1.83E-01	1.64E-01	1.00E-01	5.00E-01	5.00E-01	2.40E+00
126535-15-7	Triflusulfuron-methyl	4	148	2751	0	2712	1.42	1.00E-03	2.78E-02	2.22E-02	1.00E-02	5.00E-02	5.00E-02	2.56E-01
		4	148	2751	0	2712	1.42	1.00E-03	2.78E-02	2.22E-02	1.00E-02	5.00E-02	5.00E-02	2.56E-01
126-71-6	Triisobutyl phosphate	8	301	2962	635	986	45.27	5.00E-03	3.13E-01	1.59E+00	6.00E-02	2.50E-01	6.30E-01	4.00E+01
		8	301	2962	635	986	45.27	5.00E-03	3.13E-01	1.59E+00	6.00E-02	2.50E-01	6.30E-01	4.00E+01
126-73-8	Tributyl phosphate	13	2405	31004	818	26354	12.36	1.40E-03	2.11E-01	9.19E-01	5.00E-02	5.00E-01	5.00E-01	3.30E+01
		13	2132	25084	199	21053	15.28	1.40E-03	7.86E-02	8.00E-01	5.00E-02	5.00E-02	1.00E-01	3.30E+01
126833-17-8	Fenhexamid	4	743	8365	0	8091	3.28	2.50E-03	2.46E-02	1.11E-01	2.50E-02	2.50E-02	2.50E-02	9.03E+00
		4	743	8365	0	8091	3.28	2.50E-03	2.46E-02	1.11E-01	2.50E-02	2.50E-02	2.50E-02	9.03E+00
128639-02-1	Carfentrazone-ethyl	4	243	3642	0	3636	0.16	5.00E-03	2.42E-02	1.94E-02	1.25E-02	5.00E-02	5.00E-02	5.40E-02
		4	243	3642	0	3636	0.16	5.00E-03	2.42E-02	1.94E-02	1.25E-02	5.00E-02	5.00E-02	5.40E-02
129-00-0	Pyrene	14	1983	30085	269	19618	33.9	1.00E-05	5.66E-01	1.21E+01	5.00E-03	2.30E-02	4.70E-02	1.10E+03
		13	1329	13980	116	3666	72.95	1.00E-05	1.18E+00	1.77E+01	8.20E-03	4.30E-02	9.00E-02	1.10E+03
131-11-3	Dimethyl phthalate	6	1027	16765	192	16529	0.26	5.00E-03	3.48E-01	1.07E+00	2.00E-01	5.00E-01	5.00E-01	1.00E+02
		6	1027	16765	192	16529	0.26	5.00E-03	3.48E-01	1.07E+00	2.00E-01	5.00E-01	5.00E-01	1.00E+02
131341-86-1	Fludioxonil	5	1492	14094	0	13803	2.06	2.50E-03	2.10E-02	7.51E-02	2.00E-02	2.50E-02	5.00E-02	8.82E+00
		5	1492	14094	0	13803	2.06	2.50E-03	2.10E-02	7.51E-02	2.00E-02	2.50E-02	5.00E-02	8.82E+00
131860-33-8	Azoxystrobin	8	2102	21361	210	19779	6.42	1.00E-03	1.40E-02	3.53E-02	1.00E-02	2.50E-02	4.00E-02	1.90E+00
		8	2102	21356	210	19774	6.42	1.00E-03	1.39E-02	3.46E-02	1.00E-02	2.50E-02	4.00E-02	1.90E+00

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
131983-72-7	Triticonazole	4	191	3267	0	3263	0.12	1.00E-03	2.49E-02	2.16E-02	1.00E-02	5.00E-02	5.00E-02	3.91E-01
		4	191	3267	0	3263	0.12	1.00E-03	2.49E-02	2.16E-02	1.00E-02	5.00E-02	5.00E-02	3.91E-01
1330-20-7	Xylene	15	5323	124321	683	122350	1.04	5.00E-04	4.19E-01	1.22E+00	2.50E-01	1.00E+00	1.00E+00	1.00E+02
		15	5323	124321	683	122350	1.04	5.00E-04	4.19E-01	1.22E+00	2.50E-01	1.00E+00	1.00E+00	1.00E+02
133-06-2	Captan	5	1640	23136	210	22918	0.03	2.50E-03	2.99E-02	5.15E-02	2.00E-02	2.50E-02	1.25E-01	2.50E-01
		5	1640	23136	210	22918	0.03	2.50E-03	2.99E-02	5.15E-02	2.00E-02	2.50E-02	1.25E-01	2.50E-01
133-07-3	Folpet	5	1887	18252	467	17721	0.35	5.00E-03	2.05E-02	1.87E-01	1.00E-02	2.50E-02	5.00E-02	2.50E+01
		5	1858	18097	313	17720	0.35	5.00E-03	1.72E-02	1.75E-02	1.00E-02	2.50E-02	5.00E-02	8.80E-01
1330-78-5	Tricresyl Phosphate	7	53	105	0	84	20	8.50E-05	2.60E-03	7.71E-03	1.15E-04	9.10E-03	1.38E-02	5.40E-02
		7	53	105	0	84	20	8.50E-05	2.60E-03	7.71E-03	1.15E-04	9.10E-03	1.38E-02	5.40E-02
1336-36-3	PCB-sum (Polychlorinated biphenyls)	10	705	8064	148	7539	4.68	2.50E-04	5.00E-03	4.60E-02	3.50E-03	1.65E-02	1.65E-02	4.00E+00
		10	630	7086	143	6566	5.32	2.50E-04	2.95E-03	1.15E-02	2.50E-03	4.00E-03	4.00E-03	8.30E-01
133855-98-8	Epoxiconazole	7	2385	26476	909	25211	1.34	1.25E-03	1.84E-02	2.64E-02	1.00E-02	5.00E-02	5.00E-02	1.40E+00
		7	2378	26355	909	25090	1.35	1.25E-03	1.74E-02	2.13E-02	1.00E-02	5.00E-02	5.00E-02	1.40E+00
134-62-3	Diethyltoluamide (DEET)	9	234	6473	104	1791	70.72	7.60E-04	4.34E-02	4.89E-01	1.61E-02	8.80E-02	1.40E-01	3.90E+01
		9	234	6473	104	1791	70.72	7.60E-04	4.34E-02	4.89E-01	1.61E-02	8.80E-02	1.40E-01	3.90E+01
13674-84-5	Tris(1-chloro-2-propyl) phosphate (TCPP)	8	398	4413	5	1168	73.42	1.00E-02	2.63E-01	4.74E-01	1.40E-01	6.10E-01	9.00E-01	1.76E+01
		8	398	4413	5	1168	73.42	1.00E-02	2.63E-01	4.74E-01	1.40E-01	6.10E-01	9.00E-01	1.76E+01
13674-87-8	Tris(1,3-dichloropropyl) phosphate (TDCPP)	7	383	3791	0	1425	62.41	4.00E-04	4.89E-02	6.22E-02	3.00E-02	1.00E-01	1.30E-01	1.69E+00

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
		7	383	3791	0	1425	62.41	4.00E-04	4.89E-02	6.22E-02	3.00E-02	1.00E-01	1.30E-01	1.69E+00
13684-56-5	Desmedipham	4	1221	12484	728	11690	0.53	2.50E-03	3.42E-02	5.39E-02	1.00E-02	1.50E-01	1.50E-01	1.50E+00
		4	1019	10605	728	9811	0.62	2.50E-03	1.35E-02	2.04E-02	1.00E-02	5.00E-02	5.00E-02	1.10E+00
13684-63-4	Phenmedipham	6	2242	20614	823	19727	0.31	1.00E-03	1.22E-01	1.40E+01	2.50E-02	5.00E-02	5.00E-02	2.01E+03
		6	2242	20614	823	19727	0.31	1.00E-03	1.22E-01	1.40E+01	2.50E-02	5.00E-02	5.00E-02	2.01E+03
136-85-6	5-Methyl-1H-benzotriazole	8	82	312	0	12	96.15	5.00E-03	1.08E-01	7.71E-02	9.85E-02	2.10E-01	2.60E-01	4.90E-01
		8	82	312	0	12	96.15	5.00E-03	1.08E-01	7.71E-02	9.85E-02	2.10E-01	2.60E-01	4.90E-01
138261-41-3	Imidacloprid	7	4549	64458	3241	52949	12.83	5.00E-04	8.93E-02	3.35E+00	1.00E-02	3.00E-02	7.00E-02	4.50E+02
		5	2435	22900	1423	13209	36.1	5.00E-04	2.16E-01	5.61E+00	5.00E-03	9.00E-02	2.50E-01	4.50E+02
139-13-9	Nitrilotriacetic acid	4	850	12951	21	4782	62.91	2.50E-02	2.84E+00	1.36E+01	1.00E+00	4.04E+00	7.62E+00	6.20E+02
		4	850	12951	21	4782	62.91	2.50E-02	2.84E+00	1.36E+01	1.00E+00	4.04E+00	7.62E+00	6.20E+02
139-40-2	Propazine	13	4461	57749	2997	54416	0.58	2.50E-04	1.66E-02	2.43E-01	1.00E-02	2.50E-02	2.50E-02	1.25E+01
		13	4461	57724	2997	54391	0.58	2.50E-04	1.16E-02	2.23E-02	1.00E-02	2.50E-02	2.50E-02	1.30E+00
141517-21-7	Trifloxystrobin	4	631	7359	8	7332	0.26	1.00E-03	2.51E-02	1.95E-02	2.50E-02	5.00E-02	5.00E-02	1.20E+00
		4	631	7359	8	7332	0.26	1.00E-03	2.51E-02	1.95E-02	2.50E-02	5.00E-02	5.00E-02	1.20E+00
141776-32-1	Sulfosulfuron	4	316	4269	0	4217	1.22	1.00E-03	2.68E-02	1.70E-02	2.50E-02	5.00E-02	5.00E-02	5.00E-02
		4	316	4269	0	4217	1.22	1.00E-03	2.68E-02	1.70E-02	2.50E-02	5.00E-02	5.00E-02	5.00E-02
142-28-9	1,3-Dichloropropane	8	699	6585	0	6581	0.06	2.50E-03	3.67E+00	4.74E+00	2.50E-01	1.00E+01	1.00E+01	1.00E+01
		8	336	4220	0	4216	0.09	2.50E-03	1.25E-01	1.19E-01	5.00E-02	2.50E-01	2.50E-01	2.30E+00
142459-58-3	Flufenacet	7	2944	27879	518	26089	4.56	1.50E-03	4.58E-01	9.77E+00	1.25E-02	5.00E-02	5.00E-02	1.09E+03
		7	2804	24639	518	22849	5.16	1.50E-03	4.23E-01	1.04E+01	1.00E-02	2.50E-02	2.50E-02	1.09E+03
143390-89-0	Kresoxim-methyl	5	1306	13688	1	13651	0.26	5.00E-04	1.24E-02	1.23E-02	5.00E-03	2.50E-02	5.00E-02	2.30E-01
		5	1306	13688	1	13651	0.26	5.00E-04	1.24E-02	1.23E-02	5.00E-03	2.50E-02	5.00E-02	2.30E-01

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
144550-36-7	Iodosulfuron	5	714	7255	81	7169	0.07	1.00E-03	2.83E-02	1.16E-02	3.50E-02	3.50E-02	3.50E-02	1.38E-01
		5	650	6922	81	6836	0.07	1.00E-03	2.73E-02	1.08E-02	3.50E-02	3.50E-02	3.50E-02	1.38E-01
145701-23-1	Florasulam	4	229	2337	0	2328	0.39	2.00E-03	3.17E-02	2.07E-02	5.00E-02	5.00E-02	5.00E-02	5.70E-02
		n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
1461-25-2	Tetrabutyltin	10	2334	23078	643	21809	2.71	5.00E-08	9.75E-03	3.15E-02	3.42E-03	2.50E-02	2.50E-02	9.00E-01
		10	2334	23026	591	21809	2.72	5.00E-08	8.38E-03	9.79E-03	3.08E-03	2.50E-02	2.50E-02	6.15E-02
14797-65-0	Nitrite (NO2)	8	6757	72700	14292	2916	76.33	1.00E-02	4.68E+01	2.54E+02	1.77E+01	8.83E+01	1.45E+02	3.75E+04
		8	6711	71905	14066	2347	77.17	1.00E-02	4.71E+01	2.55E+02	1.80E+01	8.90E+01	1.46E+02	3.75E+04
14816-18-3	Phoxim	4	2408	31910	578	31188	0.45	7.50E-05	2.65E-02	4.08E-02	2.50E-02	5.00E-02	5.00E-02	5.00E+00
		n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
150-68-5	Monuron	4	1134	10187	156	9998	0.32	2.50E-03	1.85E-02	1.11E-02	1.25E-02	2.50E-02	5.00E-02	1.26E-01
		n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
152019-73-3	Metolachlor OA	10	322	2614	50	1674	34.05	5.00E-04	1.85E-02	3.00E-02	7.50E-03	4.50E-02	6.30E-02	3.70E-01
		10	322	2614	50	1674	34.05	5.00E-04	1.85E-02	3.00E-02	7.50E-03	4.50E-02	6.30E-02	3.70E-01
15299-99-7	Napropamide	5	892	9927	214	9648	0.65	2.50E-03	1.44E-02	1.63E-02	1.00E-02	2.50E-02	2.50E-02	1.10E+00
		5	892	9927	214	9648	0.65	2.50E-03	1.44E-02	1.63E-02	1.00E-02	2.50E-02	2.50E-02	1.10E+00
15307-86-5	Diclofenac	14	732	11063	252	2412	75.92	2.50E-04	1.37E-01	2.40E-01	5.40E-02	3.50E-01	5.70E-01	7.10E+00
		14	732	11063	252	2412	75.92	2.50E-04	1.37E-01	2.40E-01	5.40E-02	3.50E-01	5.70E-01	7.10E+00
153719-23-4	Thiamethoxam	7	543	5062	1595	3185	5.57	1.00E-03	1.33E-02	6.51E-02	1.00E-02	1.50E-02	2.50E-02	3.18E+00
		7	543	5062	1595	3185	5.57	1.00E-03	1.33E-02	6.51E-02	1.00E-02	1.50E-02	2.50E-02	3.18E+00
15545-48-9	Chlorotoluron	15	5587	73567	4520	59969	12.34	2.50E-05	3.31E-02	3.33E-01	1.00E-02	5.00E-02	6.30E-02	4.98E+01
		15	5587	73215	4195	59942	12.4	2.50E-05	2.83E-02	2.41E-01	1.00E-02	5.00E-02	5.70E-02	4.98E+01
1563-66-2	Carbofuran	8	2311	27395	206	26601	2.15	1.00E-04	2.07E-02	2.94E-01	1.00E-02	2.50E-02	2.50E-02	3.10E+01
		7	1943	21792	116	21088	2.7	1.00E-04	1.85E-02	3.30E-01	7.50E-03	1.25E-02	1.25E-02	3.10E+01

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
15687-27-1	Ibuprofen	15	707	9367	183	4466	50.37	2.50E-04	5.16E-02	1.66E-01	2.00E-02	1.09E-01	1.70E-01	1.00E+01
		15	707	9367	183	4466	50.37	2.50E-04	5.16E-02	1.66E-01	2.00E-02	1.09E-01	1.70E-01	1.00E+01
15950-66-0	2,3,4-Trichlorphenol	4	786	9277	0	9277	0	1.00E-03	8.02E-02	1.05E-01	2.50E-02	2.50E-01	2.50E-01	5.00E-01
		4	786	9277	0	9277	0	1.00E-03	8.02E-02	1.05E-01	2.50E-02	2.50E-01	2.50E-01	5.00E-01
1610-18-0	Prometon	4	1727	22469	0	22460	0.04	1.25E-03	1.04E-02	5.60E-03	1.00E-02	2.00E-02	2.00E-02	5.00E-02
		4	1727	22469	0	22460	0.04	1.25E-03	1.04E-02	5.60E-03	1.00E-02	2.00E-02	2.00E-02	5.00E-02
1634-04-4	Methyl-tert-butyl ether (MTBE)	7	1937	32631	720	28266	11.17	1.08E-03	1.14E+00	1.89E+00	2.50E-01	5.00E+00	5.00E+00	6.79E+01
		7	1937	32631	720	28266	11.17	1.08E-03	1.14E+00	1.89E+00	2.50E-01	5.00E+00	5.00E+00	6.79E+01
1646-88-4	Aldicarb sulfone	4	1733	15420	2924	12372	0.8	2.50E-03	2.07E-02	2.93E-02	1.00E-02	5.00E-02	5.00E-02	1.80E+00
		4	1733	15420	2924	12372	0.8	2.50E-03	2.07E-02	2.93E-02	1.00E-02	5.00E-02	5.00E-02	1.80E+00
16752-77-5	Methomyl	6	2943	37193	3190	33729	0.74	5.00E-04	1.70E-02	5.30E-02	1.00E-02	5.00E-02	5.00E-02	5.53E+00
		6	2764	33412	2975	30163	0.82	5.00E-04	1.21E-02	3.72E-02	1.00E-02	2.50E-02	2.50E-02	5.53E+00
16887-00-6	Chloride	7	720	20070	65	521	97.08	1.25E-04	2.07E+04	4.47E+05	1.50E+01	1.26E+02	7.10E+03	1.79E+07
		7	720	20070	65	521	97.08	1.25E-04	2.07E+04	4.47E+05	1.50E+01	1.26E+02	7.10E+03	1.79E+07
1689-84-5	Bromoxynil	4	2410	31836	200	31476	0.5	2.50E-03	1.48E-02	5.76E-02	1.25E-02	2.50E-02	2.50E-02	1.00E+01
		4	2410	31836	200	31476	0.5	2.50E-03	1.48E-02	5.76E-02	1.25E-02	2.50E-02	2.50E-02	1.00E+01
16984-48-8	Fluoride	14	3084	35044	435	11158	66.92	6.25E-07	1.98E+02	2.05E+03	1.25E+02	3.40E+02	4.80E+02	2.60E+05
		14	3084	35044	435	11158	66.92	6.25E-07	1.98E+02	2.05E+03	1.25E+02	3.40E+02	4.80E+02	2.60E+05
1698-60-8	Chloridazon	16	5496	74955	4314	67614	4.04	1.80E-04	7.40E-02	1.42E+00	1.50E-02	5.00E-02	2.50E-01	2.25E+02
		16	5496	74955	4314	67614	4.04	1.80E-04	7.40E-02	1.42E+00	1.50E-02	5.00E-02	2.50E-01	2.25E+02
1702-17-6	Clopyralid	10	3456	40592	776	39197	1.52	1.25E-03	3.14E-02	1.31E-01	2.50E-02	5.00E-02	5.00E-02	2.50E+01
		10	3456	40592	776	39197	1.52	1.25E-03	3.14E-02	1.31E-01	2.50E-02	5.00E-02	5.00E-02	2.50E+01
17040-19-6	Demeton-S-methylsulfon	4	1251	16478	4	16471	0.02	5.00E-03	2.86E-02	1.36E-02	2.50E-02	5.00E-02	5.00E-02	2.50E-01

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
		4	1251	16477	4	16470	0.02	5.00E-03	2.86E-02	1.35E-02	2.50E-02	5.00E-02	5.00E-02	5.00E-02
171118-09-5	Metolachlor ethanesulfonic acid (ESA)	10	353	3587	96	1948	43.02	5.00E-04	4.14E-02	5.82E-02	2.50E-02	1.05E-01	1.49E-01	7.86E-01
		10	353	3587	96	1948	43.02	5.00E-04	4.14E-02	5.82E-02	2.50E-02	1.05E-01	1.49E-01	7.86E-01
17254-80-7	Chloridazon methyl-desphenyl	9	258	2320	44	1060	52.41	2.50E-03	9.05E-02	1.49E-01	3.00E-02	2.50E-01	3.09E-01	3.69E+00
		9	258	2320	44	1060	52.41	2.50E-03	9.05E-02	1.49E-01	3.00E-02	2.50E-01	3.09E-01	3.69E+00
173159-57-4	Foramsulfuron	4	148	2875	73	2794	0.28	5.00E-04	2.83E-02	2.01E-02	2.50E-02	5.00E-02	5.00E-02	7.00E-02
		n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
1746-81-2	Monolinuron	8	2546	25786	285	25400	0.39	5.00E-03	1.80E-02	2.55E-02	1.25E-02	2.50E-02	2.50E-02	1.70E+00
		7	2507	25680	180	25399	0.39	5.00E-03	1.71E-02	2.07E-02	1.25E-02	2.50E-02	2.50E-02	1.70E+00
175013-18-0	Pyraclostrobine	4	1227	13988	0	13918	0.5	2.50E-03	2.42E-02	1.48E-02	2.50E-02	5.00E-02	5.00E-02	1.00E+00
		4	1227	13988	0	13918	0.5	2.50E-03	2.42E-02	1.48E-02	2.50E-02	5.00E-02	5.00E-02	1.00E+00
18691-97-9	Methabenzthiazuron	8	2702	27570	173	27129	0.97	1.00E-03	2.01E-02	1.55E-02	2.00E-02	2.50E-02	2.50E-02	9.10E-01
		8	2533	26506	173	26065	1.01	1.00E-03	1.89E-02	1.45E-02	2.00E-02	2.50E-02	2.50E-02	9.10E-01
188425-85-6	Boscalid	4	734	8902	0	7125	19.96	1.00E-03	2.65E-02	1.05E-01	1.00E-02	2.50E-02	7.19E-02	6.60E+00
		4	734	8902	0	7125	19.96	1.00E-03	2.65E-02	1.05E-01	1.00E-02	2.50E-02	7.19E-02	6.60E+00
1897-45-6	Chlorothalonil	5	2516	26620	3117	23082	1.58	5.00E-04	9.97E-03	9.53E-02	1.00E-02	2.00E-02	2.50E-02	1.50E+01
		5	2516	26620	3117	23082	1.58	5.00E-04	9.97E-03	9.53E-02	1.00E-02	2.00E-02	2.50E-02	1.50E+01
1918-00-9	Dicamba	9	4298	55927	2183	52614	2.02	7.50E-04	2.55E-02	1.58E-01	1.25E-02	5.00E-02	5.00E-02	2.50E+01
		9	4298	55924	2182	52612	2.02	7.50E-04	2.46E-02	5.19E-02	1.25E-02	5.00E-02	5.00E-02	5.44E+00
19666-30-9	Oxadiazon	5	3769	48512	116	45402	6.17	1.00E-03	2.93E-01	4.52E+00	1.00E-02	2.50E-02	2.50E-02	2.70E+02
		5	3769	48301	116	45191	6.2	1.00E-03	2.34E-01	4.39E+00	1.00E-02	2.50E-02	2.50E-02	2.70E+02

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
1982-47-4	Chloroxuron	5	2218	22747	295	22430	0.1	1.00E-03	2.72E-02	4.14E-01	1.00E-02	2.50E-02	2.50E-02	1.25E+01
		5	2218	22722	295	22405	0.1	1.00E-03	1.34E-02	9.27E-03	1.00E-02	2.50E-02	2.50E-02	1.32E-01
19937-59-8	Metoxuron	7	3445	35336	4040	30945	0.99	1.00E-03	2.27E-02	3.32E-01	1.00E-02	2.50E-02	2.50E-02	1.25E+01
		7	3445	35306	4036	30919	0.99	1.00E-03	1.38E-02	1.49E-02	1.00E-02	2.50E-02	2.50E-02	1.00E+00
2008-58-4	2,6-Dichlorobenzamide	6	1377	15178	149	14499	3.49	5.00E-06	1.23E-02	1.56E-02	1.00E-02	2.50E-02	3.11E-02	3.00E-01
		6	1377	15178	149	14499	3.49	5.00E-06	1.23E-02	1.56E-02	1.00E-02	2.50E-02	3.11E-02	3.00E-01
2032-65-7	Methiocarb	7	2377	22542	2878	19293	1.65	1.00E-03	1.18E-02	1.50E-02	1.00E-02	2.50E-02	2.50E-02	9.60E-01
		5	498	2654	0	2283	13.98	1.00E-03	5.18E-03	3.12E-02	1.00E-03	8.00E-03	1.40E-02	9.60E-01
208-96-8	Acenaphthylene	12	1591	27526	104	26350	3.89	2.00E-05	7.34E-02	9.51E-01	5.00E-03	2.50E-02	5.00E-02	1.17E+02
		12	1567	27169	104	25993	3.95	2.00E-05	2.19E-02	8.44E-01	5.00E-03	2.50E-02	5.00E-02	1.17E+02
21087-64-9	Metribuzin	11	3267	47107	318	46122	1.42	6.10E-05	1.82E-02	1.99E-01	1.25E-02	2.50E-02	2.50E-02	3.59E+01
		11	3267	47103	318	46118	1.42	6.10E-05	1.81E-02	1.99E-01	1.25E-02	2.50E-02	2.50E-02	3.59E+01
210880-92-5	Clothianidin	4	264	3699	161	3440	2.65	2.50E-03	1.24E-02	1.08E-02	1.00E-02	2.50E-02	2.50E-02	2.66E-01
		4	264	3699	161	3440	2.65	2.50E-03	1.24E-02	1.08E-02	1.00E-02	2.50E-02	2.50E-02	2.66E-01
2163-68-0	2-Hydroxyatrazine	6	1431	20856	0	19076	8.53	5.00E-06	3.29E-02	4.49E-02	2.50E-02	5.00E-02	1.00E-01	9.00E-01
		5	357	1811	0	31	98.29	5.00E-06	4.77E-02	4.56E-02	2.70E-02	1.00E-01	1.00E-01	9.00E-01
#2164-08-1	Lenacil	4	2907	28630	147	28264	0.76	2.50E-03	3.52E-02	5.68E-01	2.50E-02	5.00E-02	5.00E-02	4.90E+01
		4	2907	28630	147	28264	0.76	2.50E-03	3.52E-02	5.68E-01	2.50E-02	5.00E-02	5.00E-02	4.90E+01
21725-46-2	Cyanazine	10	3940	55033	2207	52660	0.3	2.50E-04	2.72E-02	3.48E-01	1.00E-02	2.50E-02	2.50E-02	1.00E+01
		10	3932	54974	2207	52601	0.3	2.50E-04	1.81E-02	2.06E-01	1.00E-02	2.50E-02	2.50E-02	7.50E+00
218-01-9	Chrysene	14	1973	31690	288	23151	26.04	2.00E-04	1.97E-01	3.60E+00	2.50E-03	1.10E-02	2.50E-02	3.90E+02
		14	989	9751	41	1459	84.62	2.00E-04	6.12E-01	6.47E+00	7.00E-03	3.70E-02	1.00E-01	3.90E+02

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
2212-67-1	Molinate	4	2557	23889	0	23793	0.4	1.20E-05	2.25E-02	3.73E-01	1.00E-02	5.00E-02	5.00E-02	4.60E+01
		4	2557	23887	0	23791	0.4	1.20E-05	2.21E-02	3.71E-01	1.00E-02	5.00E-02	5.00E-02	4.60E+01
22204-53-1	Naproxen	13	502	4957	53	2715	44.16	2.50E-04	9.22E-02	2.63E+00	1.25E-02	6.00E-02	1.00E-01	1.36E+02
		13	502	4957	53	2715	44.16	2.50E-04	9.22E-02	2.63E+00	1.25E-02	6.00E-02	1.00E-01	1.36E+02
23103-98-2	Pirimicarb	9	1686	21679	529	20540	2.81	2.50E-04	1.14E-02	7.91E-02	5.00E-03	2.50E-02	2.50E-02	6.15E+00
		9	1686	21676	529	20537	2.81	2.50E-04	1.14E-02	7.89E-02	5.00E-03	2.50E-02	2.50E-02	6.15E+00
23135-22-0	Oxamyl	5	879	7127	117	6990	0.28	2.50E-03	3.56E-02	1.77E-02	5.00E-02	5.00E-02	5.00E-02	9.30E-02
		5	879	7127	117	6990	0.28	2.50E-03	3.56E-02	1.77E-02	5.00E-02	5.00E-02	5.00E-02	9.30E-02
2385-85-5	Mirex	5	325	2358	267	2053	1.61	5.00E-04	4.40E-03	5.51E-03	2.50E-03	5.00E-03	2.50E-02	4.00E-02
		n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
23950-58-5	Propyzamide	8	4226	64486	1812	58789	6.02	5.00E-04	3.03E-02	4.18E+00	1.00E-02	2.50E-02	2.50E-02	1.06E+03
		8	4226	64486	1812	58789	6.02	5.00E-04	3.03E-02	4.18E+00	1.00E-02	2.50E-02	2.50E-02	1.06E+03
24017-47-8	Triazophos	6	1548	15350	479	14715	1.02	5.00E-04	2.62E-02	1.87E-02	2.50E-02	5.00E-02	5.00E-02	2.03E-01
		n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
24579-73-5	Propamocarb	4	164	2877	0	2805	2.5	1.00E-03	2.75E-02	2.14E-02	1.00E-02	5.00E-02	5.00E-02	1.80E-01
		4	164	2877	0	2805	2.5	1.00E-03	2.75E-02	2.14E-02	1.00E-02	5.00E-02	5.00E-02	1.80E-01
25057-89-0	Bentazone	20	6560	79284	2258	63387	17.2	5.00E-06	2.31E-02	1.99E-01	1.00E-02	3.00E-02	5.90E-02	3.00E+01
		20	6560	79284	2258	63387	17.2	5.00E-06	2.31E-02	1.99E-01	1.00E-02	3.00E-02	5.90E-02	3.00E+01
25812-30-0	Gemfibrozil	12	364	2632	70	2438	4.71	2.50E-04	1.41E-02	4.32E-02	1.25E-02	1.25E-02	1.25E-02	1.14E+00
		12	364	2632	70	2438	4.71	2.50E-04	1.41E-02	4.32E-02	1.25E-02	1.25E-02	1.25E-02	1.14E+00
26225-79-6	Ethofumesate	11	5642	79714	3062	72774	4.86	1.30E-05	4.23E-02	1.15E+00	1.25E-02	2.50E-02	6.00E-02	2.84E+02
		11	5642	79714	3062	72774	4.86	1.30E-05	4.23E-02	1.15E+00	1.25E-02	2.50E-02	6.00E-02	2.84E+02
26259-45-0	Secbumeton	4	2193	34896	210	34669	0.05	6.25E-04	1.85E-02	2.67E-01	1.00E-02	2.00E-02	2.50E-02	1.00E+01
		4	2193	34869	210	34642	0.05	6.25E-04	1.14E-02	6.80E-03	1.00E-02	2.00E-02	2.50E-02	7.80E-02

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
2642-71-9	Azinphos-ethyl	8	3346	40821	3172	37387	0.64	1.25E-03	1.66E-02	1.18E-02	2.00E-02	2.50E-02	2.50E-02	1.40E+00
		6	116	262	0	0	100	7.00E-03	2.59E-02	9.16E-02	2.00E-02	3.00E-02	5.00E-02	1.40E+00
29122-68-7	Atenolol	12	371	4150	6	2537	38.72	2.00E-03	2.38E-02	5.63E-02	1.25E-02	4.60E-02	6.40E-02	2.04E+00
		12	371	4150	6	2537	38.72	2.00E-03	2.38E-02	5.63E-02	1.25E-02	4.60E-02	6.40E-02	2.04E+00
29232-93-7	Pirimiphos-methyl	5	2101	22004	1287	20693	0.11	5.00E-04	1.15E-02	9.79E-03	1.00E-02	2.00E-02	2.50E-02	1.00E+00
		4	925	8240	363	7853	0.29	5.00E-04	4.93E-03	1.11E-02	5.00E-03	5.00E-03	5.00E-03	1.00E+00
298-04-4	Disulfoton	4	749	9052	107	8939	0.07	1.00E-03	1.47E-02	1.54E-02	1.00E-02	2.50E-02	5.00E-02	1.00E-01
		n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
298-46-4	Carbamazepine	15	2290	26624	842	8262	65.81	5.00E-04	6.20E-01	3.51E+00	5.10E-02	3.80E-01	6.80E-01	8.00E+01
		15	2290	26624	842	8262	65.81	5.00E-04	6.20E-01	3.51E+00	5.10E-02	3.80E-01	6.80E-01	8.00E+01
301-12-2	Oxydemeton-methyl	4	1365	10707	72	10627	0.07	5.00E-03	4.08E-02	1.83E-02	5.00E-02	5.00E-02	5.00E-02	8.45E-01
		n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
30125-63-4	Desethylterbuthylazine	15	5446	147284	962	139970	4.31	5.00E-06	3.82E-02	1.23E+00	1.00E-02	2.50E-02	2.50E-02	2.16E+02
		15	5446	147220	962	139906	4.31	5.00E-06	3.47E-02	1.22E+00	1.00E-02	2.50E-02	2.50E-02	2.16E+02
302-17-0	Chloral hydrate	4	171	1473	38	1433	0.14	5.00E-02	5.53E-01	3.84E-01	5.00E-01	5.00E-01	5.00E-01	3.81E+00
		4	171	1473	38	1433	0.14	5.00E-02	5.53E-01	3.84E-01	5.00E-01	5.00E-01	5.00E-01	3.81E+00
3060-89-7	Metobromuron	4	1923	21152	0	21028	0.59	1.25E-03	1.85E-02	8.59E-02	1.25E-02	2.50E-02	2.50E-02	8.00E+00
		4	1923	21152	0	21028	0.59	1.25E-03	1.85E-02	8.59E-02	1.25E-02	2.50E-02	2.50E-02	8.00E+00
307-24-4	Perfluorohexanoic acid (PFHxA)	8	386	3848	13	2278	40.46	2.00E-04	1.76E-02	5.18E-02	5.00E-03	2.80E-02	6.50E-02	8.92E-01
		8	386	3848	13	2278	40.46	2.00E-04	1.76E-02	5.18E-02	5.00E-03	2.80E-02	6.50E-02	8.92E-01
314-40-9	Bromacil	7	4524	66058	1866	63674	0.78	2.50E-04	2.28E-02	5.88E-02	2.50E-02	5.00E-02	5.00E-02	1.00E+01
		5	1510	17640	784	16338	2.94	2.50E-04	8.98E-03	2.66E-02	1.00E-02	1.00E-02	1.00E-02	2.00E+00

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
32809-16-8	Procymidone	5	1771	16440	8	15989	2.69	3.70E-05	4.36E-02	6.99E-01	2.00E-02	2.50E-02	2.50E-02	7.50E+01
		5	1771	16440	8	15989	2.69	3.70E-05	4.36E-02	6.99E-01	2.00E-02	2.50E-02	2.50E-02	7.50E+01
330-55-2	Linuron	17	7429	139811	7156	129551	2.22	2.50E-05	8.93E+00	1.34E+02	1.00E-02	2.50E-02	2.50E-02	4.84E+03
		16	7390	138718	6326	129288	2.24	2.50E-05	1.35E-02	2.24E-01	1.00E-02	2.50E-02	2.50E-02	5.60E+01
333-41-5	Diazinon	19	4978	57845	7287	49338	2.11	1.10E-05	5.83E+01	4.12E+02	1.00E-02	2.50E-02	4.00E-02	8.10E+03
		18	4041	42235	4442	36573	2.89	1.10E-05	1.14E+00	5.26E+01	6.50E-03	1.00E-02	1.00E-02	7.56E+03
335-67-1	Perfluorooctanoic acid (PFOA)	14	951	8890	45	5216	40.82	1.00E-06	5.30E-02	3.13E-01	1.10E-02	6.70E-02	1.40E-01	1.20E+01
		14	950	8889	45	5215	40.83	1.00E-06	5.24E-02	3.09E-01	1.10E-02	6.62E-02	1.40E-01	1.20E+01
3380-34-5	Triclosan	10	686	5430	88	3044	42.32	2.50E-04	1.46E-01	1.68E+00	1.15E-02	4.00E-02	4.66E-02	2.80E+01
		10	589	4234	88	1848	54.27	2.50E-04	1.76E-01	1.91E+00	5.40E-03	3.50E-02	5.20E-02	2.80E+01
3397-62-4	Desisopropyldesethylatrazine	4	546	7592	97	7486	0.12	5.00E-03	2.38E-02	1.58E-02	2.50E-02	5.00E-02	5.00E-02	4.90E-01
		n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
3424-82-6	DDE, o,p'	12	2185	37990	424	37370	0.52	2.50E-04	5.18E-01	1.60E+01	2.50E-03	5.00E-03	6.25E-03	5.00E+02
		12	2041	36587	421	35970	0.54	2.50E-04	4.33E-03	6.52E-02	2.50E-03	5.00E-03	5.00E-03	2.50E+00
34256-82-1	Acetochlor	4	2345	35952	205	34170	4.39	5.00E-04	1.27E-02	5.70E-02	8.75E-03	2.50E-02	2.50E-02	7.70E+00
		4	2153	31430	0	29853	5.02	5.00E-04	1.10E-02	6.07E-02	5.00E-03	1.25E-02	1.25E-02	7.70E+00
35367-38-5	Diflubenzuron	4	415	4725	116	4607	0.04	2.50E-03	1.87E-02	8.24E-03	2.50E-02	2.50E-02	2.50E-02	7.80E-02
		n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
35554-44-0	Imazalil	6	919	7197	3	7188	0.08	4.99E-04	2.53E-02	4.22E-02	1.00E-02	7.50E-02	7.50E-02	2.95E+00
		6	919	7197	3	7188	0.08	4.99E-04	2.53E-02	4.22E-02	1.00E-02	7.50E-02	7.50E-02	2.95E+00
36734-19-7	Iprodione	7	1852	17387	169	16971	1.42	5.00E-04	2.01E-02	3.16E-02	2.00E-02	2.50E-02	5.00E-02	2.71E+00
		7	1852	17386	169	16970	1.42	5.00E-04	2.00E-02	3.11E-02	2.00E-02	2.50E-02	5.00E-02	2.71E+00
37350-58-6	Metoprolol	12	445	7338	41	925	86.84	1.00E-03	1.80E-01	2.53E-01	9.00E-02	4.50E-01	6.50E-01	3.40E+00

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
		12	445	7338	41	925	86.84	1.00E-03	1.80E-01	2.53E-01	9.00E-02	4.50E-01	6.50E-01	3.40E+00
375-73-5	Perfluorobutane sulfonic acid	8	349	3714	0	2163	41.76	1.50E-04	2.26E-02	1.31E-01	5.00E-03	2.99E-02	5.73E-02	4.33E+00
		8	349	3714	0	2163	41.76	1.50E-04	2.26E-02	1.31E-01	5.00E-03	2.99E-02	5.73E-02	4.33E+00
40487-42-1	Pendimethalin	11	5363	77467	2046	74811	0.79	5.00E-06	1.40E-02	2.97E-02	1.00E-02	2.50E-02	2.50E-02	4.30E+00
		11	4275	54325	1806	51909	1.12	5.00E-06	8.99E-03	3.40E-02	1.00E-02	1.25E-02	1.25E-02	4.30E+00
41394-05-2	Metamitron	11	5617	80722	4570	74389	2.18	2.50E-04	2.95E-02	3.50E-01	1.25E-02	5.00E-02	5.00E-02	6.90E+01
		11	5617	80719	4570	74386	2.18	2.50E-04	2.93E-02	3.48E-01	1.25E-02	5.00E-02	5.00E-02	6.90E+01
41859-67-0	Bezafibrate	13	485	5927	87	2968	48.46	2.50E-04	5.32E-02	4.23E-01	2.50E-02	9.70E-02	1.50E-01	2.12E+01
		13	485	5927	87	2968	48.46	2.50E-04	5.32E-02	4.23E-01	2.50E-02	9.70E-02	1.50E-01	2.12E+01
43121-43-3	Triadimefon	6	1658	19398	790	18599	0.05	2.50E-03	2.59E-02	3.11E-01	1.00E-02	5.00E-02	5.00E-02	2.50E+01
		6	1658	19395	790	18596	0.05	2.50E-03	2.20E-02	1.54E-02	1.00E-02	5.00E-02	5.00E-02	7.50E-02
439-14-5	Diazepam	4	407	3565	24	3499	1.18	3.50E-04	1.03E-02	4.24E-02	1.00E-02	1.25E-02	1.25E-02	2.40E+00
		4	407	3565	24	3499	1.18	3.50E-04	1.03E-02	4.24E-02	1.00E-02	1.25E-02	1.25E-02	2.40E+00
50-00-0	Formaldehyde	4	807	9040	3	8597	4.87	2.50E-02	3.48E+00	1.03E+01	2.50E+00	2.50E+00	1.00E+01	3.40E+02
		4	777	8707	3	8264	5.05	2.50E-02	2.25E+00	6.63E+00	2.50E+00	2.50E+00	2.50E+00	3.40E+02
50-28-2	17-beta-Estradiol	6	230	1170	4	1127	3.33	5.00E-06	5.15E-04	8.39E-04	5.00E-04	5.00E-04	5.00E-04	1.50E-02
		6	81	254	4	211	15.35	5.00E-06	5.04E-04	1.73E-03	5.00E-06	1.00E-03	1.94E-03	1.50E-02
50471-44-8	Vinclozolin	6	1235	12684	220	12407	0.45	1.00E-03	1.73E-02	8.81E-03	1.50E-02	2.50E-02	2.50E-02	1.70E-01
		6	1235	12684	220	12407	0.45	1.00E-03	1.73E-02	8.81E-03	1.50E-02	2.50E-02	2.50E-02	1.70E-01
51218-45-2	Metolachlor	17	6948	95345	2006	82133	11.75	1.10E-05	1.02E-01	8.47E+00	1.00E-02	2.50E-02	5.00E-02	1.74E+03
		17	6948	95335	2006	82123	11.75	1.10E-05	1.02E-01	8.47E+00	1.00E-02	2.50E-02	5.00E-02	1.74E+03
51235-04-2	Hexazinone	10	3647	53819	807	51983	1.91	2.50E-04	1.65E-02	1.70E-02	1.25E-02	2.50E-02	5.00E-02	1.17E+00
		10	3528	51106	804	49273	2.01	2.50E-04	1.47E-02	1.54E-02	1.25E-02	2.50E-02	2.50E-02	1.17E+00
525-66-6	Propranolol	4	299	4069	9	3529	13.05	1.50E-04	1.26E-02	1.10E-02	1.25E-02	1.50E-02	2.00E-02	3.90E-01

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
		4	299	4069	9	3529	13.05	1.50E-04	1.26E-02	1.10E-02	1.25E-02	1.50E-02	2.00E-02	3.90E-01
52645-53-1	Permethrin	7	2431	29730	1580	28035	0.39	2.50E-04	2.16E+00	2.03E+01	1.25E-02	2.50E-02	2.50E-02	1.95E+02
		4	120	461	324	22	24.95	2.50E-04	1.10E-02	8.47E-02	1.50E-03	1.00E-02	2.00E-02	1.40E+00
52-68-6	Trichlorfon	7	2184	30613	351	30236	0.08	5.00E-04	2.99E-02	5.16E-02	2.50E-02	5.00E-02	5.00E-02	5.00E+00
		n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
52888-80-9	Prosulfocarb	6	1622	16871	0	16688	1.08	5.00E-06	2.30E-02	6.81E-02	2.00E-02	5.00E-02	5.00E-02	5.80E+00
		6	1622	16871	0	16688	1.08	5.00E-06	2.30E-02	6.81E-02	2.00E-02	5.00E-02	5.00E-02	5.80E+00
52918-63-5	Deltamethrin	7	2766	28842	2077	26559	0.71	3.00E-05	1.79E-02	6.44E-02	1.00E-02	5.00E-02	5.00E-02	1.00E+01
		n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
53112-28-0	Pyrimethanil	4	1723	16391	0	15998	2.4	2.50E-03	1.88E-02	4.08E-02	2.00E-02	2.50E-02	5.00E-02	2.70E+00
		4	1723	16390	0	15997	2.4	2.50E-03	1.87E-02	3.72E-02	2.00E-02	2.50E-02	5.00E-02	2.70E+00
53-16-7	Estrone	11	239	784	28	695	7.78	1.00E-04	4.03E-03	7.63E-03	2.50E-03	2.50E-03	2.50E-02	9.90E-02
		11	238	762	6	695	8.01	1.00E-04	3.43E-03	6.84E-03	2.50E-03	2.50E-03	5.00E-03	9.90E-02
53-19-0	DDD, o,p'	13	3948	57826	3048	54368	0.71	1.00E-04	3.42E-01	1.30E+01	2.50E-03	5.00E-03	1.00E-02	5.00E+02
		8	1049	14534	774	13350	2.82	1.00E-04	7.57E-03	2.59E-01	5.00E-04	5.00E-04	5.00E-04	2.74E+01
534-52-1	Dinitro-o-cresol (DNOC)	4	1677	15967	0	15392	3.6	2.50E-04	1.86E-02	2.81E-02	1.25E-02	2.50E-02	4.00E-02	1.58E+00
		4	1677	15967	0	15392	3.6	2.50E-04	1.86E-02	2.81E-02	1.25E-02	2.50E-02	4.00E-02	1.58E+00
53-70-3	Dibenz(a,h)anthracene	14	1915	30090	248	28033	6.01	1.50E-05	3.64E-02	4.94E-01	2.50E-03	5.00E-03	5.00E-03	3.00E+01
		11	738	9717	125	7783	18.62	1.50E-05	8.41E-02	8.55E-01	5.00E-04	1.50E-03	7.02E-03	3.00E+01
540-59-0	1,2-Dichloroethene	11	2145	85646	225	84540	1.03	2.50E-04	2.80E+00	6.04E+00	2.50E-01	1.25E+01	2.00E+01	2.50E+01
		11	2036	76432	225	75326	1.15	2.50E-04	8.87E-01	1.61E+00	1.25E-01	5.00E+00	5.00E+00	1.33E+01
541-73-1	1,3-Dichlorobenzene	12	2679	44404	225	44015	0.37	2.50E-04	2.57E-01	4.42E-01	1.25E-01	5.00E-01	1.00E+00	1.92E+01

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
		12	2653	43318	201	42953	0.38	2.50E-04	1.99E-01	2.54E-01	1.25E-01	5.00E-01	5.00E-01	1.92E+01
542-75-6	1,3-Dichloropropene	9	2028	30886	83	30784	0.06	2.50E-03	1.24E+00	5.23E+00	5.00E-01	1.00E+00	1.50E+00	5.00E+01
		9	1986	29634	83	29532	0.06	2.50E-03	5.63E-01	4.30E-01	5.00E-01	1.00E+00	1.00E+00	2.20E+00
55179-31-2	Bitertanol	4	924	9575	0	9553	0.23	5.00E-03	2.27E-02	1.71E-02	2.50E-02	2.50E-02	2.50E-02	1.60E+00
		4	924	9575	0	9553	0.23	5.00E-03	2.27E-02	1.71E-02	2.50E-02	2.50E-02	2.50E-02	1.60E+00
55219-65-3	Triadimenol	4	1393	11385	0	11293	0.81	5.00E-04	3.64E-02	1.79E-02	5.00E-02	5.00E-02	5.00E-02	6.45E-01
		4	1393	11385	0	11293	0.81	5.00E-04	3.64E-02	1.79E-02	5.00E-02	5.00E-02	5.00E-02	6.45E-01
55335-06-3	Triclopyr	4	1283	10331	133	9828	3.58	1.00E-03	1.78E-02	2.37E-01	1.00E-02	2.50E-02	2.50E-02	2.41E+01
		4	1283	10331	133	9828	3.58	1.00E-03	1.78E-02	2.37E-01	1.00E-02	2.50E-02	2.50E-02	2.41E+01
55-38-9	Fenthion	10	3406	39462	3632	35584	0.62	1.00E-04	1.49E-02	6.62E-02	1.00E-02	2.50E-02	2.50E-02	1.00E+01
		5	104	246	0	0	100	1.00E-04	1.59E-02	1.23E-02	1.00E-02	3.00E-02	5.00E-02	8.00E-02
5598-13-0	Chlorpyriphos methyl	9	3766	56096	1132	54832	0.24	5.00E-04	9.17E-03	6.01E-02	5.00E-03	2.00E-02	2.50E-02	1.00E+01
		6	138	1090	269	689	12.11	5.00E-04	3.32E-03	1.74E-02	5.00E-04	1.00E-02	2.00E-02	4.80E-01
563-12-2	Ethion	6	2227	21404	1118	20179	0.5	2.50E-03	4.97E-02	4.46E-01	1.00E-02	1.00E-02	2.50E-02	5.00E+00
		4	46	107	0	0	100	6.00E-03	1.87E-02	1.05E-02	2.00E-02	2.00E-02	2.00E-02	9.00E-02
56-38-2	Parathion	13	6286	138866	6422	131210	0.89	5.00E-06	1.04E-02	1.69E-01	1.00E-02	2.50E-02	2.50E-02	6.10E+01
		8	1007	8189	0	6955	15.07	5.00E-06	1.01E-02	6.76E-01	1.00E-05	5.00E-03	5.00E-03	6.10E+01
56-55-3	Benzo(a)anthracene	16	4315	60446	8070	36585	26.12	3.00E-06	1.41E-01	2.14E+00	2.50E-03	1.50E-02	2.80E-02	2.60E+02
		13	2170	15793	0	2	99.99	3.00E-06	3.41E-01	4.13E+00	7.00E-03	3.00E-02	5.30E-02	2.60E+02
56-72-4	Coumaphos	6	1329	15312	237	15045	0.2	1.50E-03	2.02E-02	1.06E-02	2.50E-02	2.50E-02	2.50E-02	1.00E-01
		n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
57018-04-9	Tolclofos-methyl	5	564	4703	3305	944	9.65	2.50E-03	1.89E-02	1.08E-01	5.00E-03	2.50E-02	5.00E-02	5.70E+00
		5	564	4703	3305	944	9.65	2.50E-03	1.89E-02	1.08E-01	5.00E-03	2.50E-02	5.00E-02	5.70E+00

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
57-12-5	Cyanide (as total CN)	14	2283	17908	2781	10953	23.31	1.75E-07	3.04E+00	1.83E+01	2.15E+00	5.00E+00	7.50E+00	1.63E+03
		14	2283	17908	2781	10953	23.31	1.75E-07	3.04E+00	1.83E+01	2.15E+00	5.00E+00	7.50E+00	1.63E+03
57-63-6	17-alpha-Ethinylestradiol	4	48	180	7	169	2.22	5.00E-06	1.29E-04	2.81E-04	5.00E-06	5.00E-04	5.50E-04	1.25E-03
		n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
57-68-1	Sulfamethazine	11	439	3798	48	3633	3.08	3.00E-04	1.41E-02	2.21E-02	1.25E-02	2.50E-02	2.50E-02	8.40E-01
		11	439	3798	48	3633	3.08	3.00E-04	1.41E-02	2.21E-02	1.25E-02	2.50E-02	2.50E-02	8.40E-01
57-74-9	Chlordane	6	1729	45286	10	45239	0.08	2.50E-04	1.61E-02	2.46E-01	5.00E-03	1.00E-02	2.50E-02	3.16E+01
		n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
57837-19-1	Metalaxyl	11	4913	72962	3228	67544	3	2.50E-04	1.80E-02	2.35E-01	1.00E-02	2.50E-02	2.50E-02	4.40E+01
		11	4913	72962	3228	67544	3	2.50E-04	1.80E-02	2.35E-01	1.00E-02	2.50E-02	2.50E-02	4.40E+01
58-08-2	Caffeine	11	306	3923	573	544	71.53	2.00E-03	1.83E-01	2.70E-01	1.30E-01	3.30E-01	5.00E-01	6.80E+00
		11	306	3923	573	544	71.53	2.00E-03	1.83E-01	2.70E-01	1.30E-01	3.30E-01	5.00E-01	6.80E+00
58-73-1	Diphenhydramine	7	52	53	52	0	1.89	9.50E-04	1.10E-03	1.11E-03	9.50E-04	9.50E-04	9.50E-04	9.00E-03
		7	52	53	52	0	1.89	9.50E-04	1.10E-03	1.11E-03	9.50E-04	9.50E-04	9.50E-04	9.00E-03
58955-93-4	10,11-Dihydro-10,11-dihydroxycarbamazepine	7	141	1425	0	599	57.96	1.00E-02	1.79E-01	4.24E-01	4.00E-02	6.10E-01	8.18E-01	1.11E+01
		7	141	1425	0	599	57.96	1.00E-02	1.79E-01	4.24E-01	4.00E-02	6.10E-01	8.18E-01	1.11E+01
5915-41-3	Terbuthylazine	19	5585	74228	446	63212	14.24	5.00E-06	7.83E-02	3.98E+00	1.00E-02	2.50E-02	6.60E-02	9.28E+02
		19	5585	74200	446	63184	14.25	5.00E-06	7.81E-02	3.98E+00	1.00E-02	2.50E-02	6.51E-02	9.28E+02
59-50-7	Chlorocresol (3-Methyl-4-chlorophenol)	9	1932	25664	642	24764	1.01	1.25E-03	5.90E+00	1.21E+02	2.50E-02	1.25E-01	2.50E-01	2.50E+03

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
		9	1931	25602	582	24762	1.01	1.25E-03	4.93E-02	7.60E-02	2.50E-02	1.25E-01	2.50E-01	1.75E+00
60-00-4	Edetic acid (EDTA)	6	1102	15827	1	3715	76.52	1.25E-02	5.47E+00	1.45E+01	2.70E+00	1.10E+01	1.70E+01	7.40E+02
		6	1102	15827	1	3715	76.52	1.25E-02	5.47E+00	1.45E+01	2.70E+00	1.10E+01	1.70E+01	7.40E+02
60168-88-9	Fenarimol	5	2048	20210	550	19612	0.24	5.00E-04	2.04E-02	1.35E-02	2.00E-02	5.00E-02	5.00E-02	1.60E-01
		n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
60207-90-1	Propiconazole	15	4051	52413	2321	48363	3.3	2.50E-04	2.72E-02	3.75E-01	2.00E-02	5.00E-02	5.00E-02	7.70E+01
		15	4051	52413	2321	48363	3.3	2.50E-04	2.72E-02	3.75E-01	2.00E-02	5.00E-02	5.00E-02	7.70E+01
60-51-5	Dimethoate	16	5105	73632	5341	67207	1.47	2.50E-05	3.46E-02	4.83E+00	1.00E-02	2.50E-02	5.00E-02	1.31E+03
		15	3983	49791	3946	44761	2.18	2.50E-05	3.82E-02	5.87E+00	1.00E-02	1.00E-02	1.00E-02	1.31E+03
608-27-5	2,3-Dichloroaniline	4	1430	12653	104	12539	0.08	5.00E-03	3.66E-02	3.83E-02	2.50E-02	5.00E-02	5.00E-02	1.43E+00
		4	1430	12653	104	12539	0.08	5.00E-03	3.66E-02	3.83E-02	2.50E-02	5.00E-02	5.00E-02	1.43E+00
6190-65-4	Desethylatrazine	19	6492	92740	4555	67736	22.05	2.50E-04	2.71E-02	3.47E-01	1.00E-02	5.00E-02	8.10E-02	6.00E+01
		19	6490	92703	4551	67703	22.06	2.50E-04	2.46E-02	2.79E-01	1.00E-02	5.00E-02	8.00E-02	6.00E+01
62-53-3	Aniline	5	254	3309	467	2508	10.09	1.00E-02	2.92E-01	2.01E+00	1.00E-01	5.00E-01	5.00E-01	1.00E+02
		5	254	3309	467	2508	10.09	1.00E-02	2.92E-01	2.01E+00	1.00E-01	5.00E-01	5.00E-01	1.00E+02
630-20-6	1,1,1,2-Tetrachloroethane	6	1074	10552	0	10546	0.06	1.00E-02	5.22E-01	9.34E-01	5.00E-02	2.50E+00	2.50E+00	2.50E+00
		6	1074	10552	0	10546	0.06	1.00E-02	5.22E-01	9.34E-01	5.00E-02	2.50E+00	2.50E+00	2.50E+00
63-25-2	Carbaryl	5	1931	22120	2519	19395	0.93	5.00E-04	1.16E-02	3.28E-02	1.00E-02	2.50E-02	2.50E-02	3.17E+00
		5	1513	18771	1178	17387	1.1	5.00E-04	7.60E-03	3.09E-02	1.00E-02	1.00E-02	1.00E-02	3.17E+00
66230-04-4	Esfenvalerate	4	1152	8661	1460	7155	0.53	5.00E-05	2.24E-02	1.40E-02	2.00E-02	5.00E-02	5.00E-02	2.50E-01
		n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
66246-88-6	Penconazole	5	1547	14037	0	13650	2.76	1.25E-03	2.07E-02	2.70E-02	2.50E-02	2.50E-02	5.00E-02	2.50E+00

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
		5	1547	14037	0	13650	2.76	1.25E-03	2.07E-02	2.70E-02	2.50E-02	2.50E-02	5.00E-02	2.50E+00
668-34-8	Triphenyltin	10	1515	11440	990	10329	1.06	5.00E-05	5.32E-03	6.06E-03	3.50E-03	1.70E-02	1.70E-02	1.40E-01
		9	154	171	50	0	70.76	5.00E-05	5.66E-03	1.46E-02	2.00E-03	1.35E-02	1.85E-02	1.40E-01
67129-08-2	Metazachlor	15	6536	86817	3943	75388	8.62	5.00E-04	3.25E-02	3.51E+00	1.25E-02	2.50E-02	2.80E-02	1.03E+03
		15	6536	86791	3924	75381	8.63	5.00E-04	3.21E-02	3.51E+00	1.25E-02	2.50E-02	2.80E-02	1.03E+03
67306-00-7	Fenpropidin	5	1353	13880	88	13787	0.04	5.00E-04	1.99E-02	1.07E-02	2.50E-02	2.50E-02	2.50E-02	5.00E-02
		n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
67564-91-4	Fenpropimorph	7	3011	47753	3405	43931	0.87	5.00E-04	1.54E-02	2.71E-01	1.00E-02	2.50E-02	2.50E-02	1.80E+01
		7	2702	38675	2869	35389	1.08	5.00E-04	1.26E-02	3.02E-01	5.00E-03	1.25E-02	1.25E-02	1.80E+01
67-72-1	Hexachloroethane	7	1225	11166	273	10889	0.04	5.00E-03	1.28E-01	9.68E-01	5.00E-02	2.50E-01	2.50E-01	1.00E+02
		6	1208	11141	248	10889	0.04	5.00E-03	1.20E-01	9.51E-01	5.00E-02	2.50E-01	2.50E-01	1.00E+02
67747-09-5	Prochloraz	7	2742	32674	1596	30466	1.87	5.00E-04	2.11E-02	4.36E-02	1.50E-02	3.50E-02	5.00E-02	4.80E+00
		7	2742	32673	1595	30466	1.87	5.00E-04	2.10E-02	4.22E-02	1.50E-02	3.50E-02	5.00E-02	4.80E+00
68359-37-5	Cyfluthrin	5	1489	14579	975	13265	2.33	2.50E-04	2.03E-02	8.64E-02	1.00E-02	2.50E-02	1.00E-01	1.00E+01
		n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
69377-81-7	Fluroxypyr	7	3787	45762	1973	42168	3.54	2.00E-03	2.84E-02	9.95E-01	2.00E-02	2.50E-02	5.00E-02	2.09E+02
		7	3787	45761	1973	42167	3.54	2.00E-03	2.79E-02	9.88E-01	2.00E-02	2.50E-02	5.00E-02	2.09E+02
709-98-8	Propanil	6	2320	25786	263	25517	0.02	1.00E-03	2.02E-02	2.33E-02	1.50E-02	5.00E-02	5.00E-02	2.00E+00
		5	2281	25712	190	25516	0.02	1.00E-03	1.96E-02	1.98E-02	1.50E-02	5.00E-02	5.00E-02	2.00E+00
71-55-6	1,1,1-Trichloroethane	14	3324	48291	1979	45799	1.06	5.00E-04	1.64E-01	4.02E-01	1.25E-01	2.50E-01	5.00E-01	5.00E+01
		14	3324	48291	1979	45799	1.06	5.00E-04	1.64E-01	4.02E-01	1.25E-01	2.50E-01	5.00E-01	5.00E+01
723-46-6	Sulfamethoxazole	14	1023	11684	61	4016	65.11	5.00E-04	1.09E+00	4.96E+00	2.50E-02	2.00E-01	1.17E+00	7.80E+01
		14	1023	11680	61	4012	65.13	5.00E-04	1.09E+00	4.96E+00	2.50E-02	2.00E-01	1.21E+00	7.80E+01

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
72-43-5	Methoxychlor	9	3164	49393	186	49150	0.12	8.60E-05	1.14E-02	8.45E-03	1.00E-02	2.50E-02	2.50E-02	1.50E-01
		5	174	4202	10	4135	1.36	8.60E-05	5.76E-04	3.38E-03	2.50E-04	5.00E-04	5.00E-04	1.40E-01
7286-69-3	Sebuthylazine	4	1386	17779	2657	15087	0.2	2.50E-04	9.04E-03	9.31E-03	5.00E-03	2.00E-02	2.50E-02	5.80E-01
		4	1042	14307	1099	13173	0.24	2.50E-04	6.04E-03	7.44E-03	5.00E-03	1.00E-02	1.00E-02	5.80E-01
7287-19-6	Prometryn	10	4517	57985	1542	56263	0.31	2.50E-04	1.48E-02	2.08E-02	1.00E-02	2.50E-02	2.50E-02	2.01E+00
		10	4517	57985	1542	56263	0.31	2.50E-04	1.48E-02	2.08E-02	1.00E-02	2.50E-02	2.50E-02	2.01E+00
731-27-1	Tolylfluanid	6	2134	25240	2183	22993	0.25	2.50E-03	2.00E-02	3.55E-02	1.50E-02	5.00E-02	5.00E-02	5.00E+00
		6	2134	25239	2183	22992	0.25	2.50E-03	1.98E-02	1.66E-02	1.50E-02	5.00E-02	5.00E-02	2.50E-01
738-70-5	Trimethoprim	4	352	4613	30	3391	25.84	5.00E-04	2.09E-02	5.52E-02	1.25E-02	4.00E-02	6.74E-02	2.70E+00
		4	352	4613	30	3391	25.84	5.00E-04	2.09E-02	5.52E-02	1.25E-02	4.00E-02	6.74E-02	2.70E+00
74223-64-6	Metsulfuron-methyl	6	904	9806	3	9771	0.33	1.00E-03	3.15E-02	1.80E-02	2.50E-02	5.00E-02	5.00E-02	1.09E-01
		5	196	2707	0	2675	1.18	1.00E-03	8.11E-03	4.48E-03	1.00E-02	1.00E-02	1.00E-02	1.09E-01
74-95-3	Dibromomethane	7	710	5795	343	5447	0.09	5.00E-03	1.55E-01	1.65E-01	1.50E-01	2.50E-01	2.50E-01	1.10E+01
		7	710	5795	343	5447	0.09	5.00E-03	1.55E-01	1.65E-01	1.50E-01	2.50E-01	2.50E-01	1.10E+01
75-01-4	Vinylchloride	11	1699	32632	154	32339	0.43	1.56E-02	2.51E+00	1.00E+01	2.50E-01	1.25E+00	5.00E+00	5.00E+01
		9	281	2635	125	2371	5.28	1.56E-02	1.41E-01	1.77E+00	2.50E-02	5.00E-02	1.00E-01	5.00E+01
75-25-2	Bromoform	10	1493	15778	0	15597	1.15	2.50E-03	2.46E-01	1.84E-01	2.50E-01	5.00E-01	5.00E-01	3.10E+00
		10	1493	15778	0	15597	1.15	2.50E-03	2.46E-01	1.84E-01	2.50E-01	5.00E-01	5.00E-01	3.10E+00
75-27-4	Dichlorobromomethane	10	1671	24724	68	24561	0.38	6.25E-04	1.59E-01	1.45E-01	1.25E-01	2.50E-01	5.00E-01	2.50E+00
		10	1671	24724	68	24561	0.38	6.25E-04	1.59E-01	1.45E-01	1.25E-01	2.50E-01	5.00E-01	2.50E+00
75-34-3	1,1-Dichloroethane	13	1971	35367	375	34807	0.52	2.50E-03	1.60E+00	2.71E+00	2.50E-01	5.00E+00	1.00E+01	1.51E+01
		13	1971	35364	375	34804	0.52	2.50E-03	1.60E+00	2.71E+00	2.50E-01	5.00E+00	1.00E+01	1.51E+01

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
75-35-4	1,1-Dichloroethylene	14	2073	35945	383	35398	0.46	6.25E-04	5.26E-01	7.45E-01	2.50E-01	2.50E+00	2.50E+00	5.70E+00
		14	2073	35945	383	35398	0.46	6.25E-04	5.26E-01	7.45E-01	2.50E-01	2.50E+00	2.50E+00	5.70E+00
76-03-9	Trichloroacetic acid	4	61	823	0	444	46.05	5.00E-06	7.27E-02	1.07E-01	5.00E-02	1.80E-01	2.40E-01	1.20E+00
		4	40	625	0	246	60.64	5.00E-06	7.91E-02	1.21E-01	1.80E-02	2.10E-01	2.80E-01	1.20E+00
7664-41-7	Ammonia	5	553	4706	640	1040	64.3	5.00E-02	9.70E+01	4.55E+02	1.50E+01	2.10E+02	3.76E+02	1.70E+04
		5	553	4706	640	1040	64.3	5.00E-02	9.70E+01	4.55E+02	1.50E+01	2.10E+02	3.76E+02	1.70E+04
76674-21-0	Flutriafol	4	1367	22277	133	22113	0.14	1.00E-03	3.55E-02	1.91E-02	5.00E-02	5.00E-02	5.00E-02	1.10E-01
		4	1367	22277	133	22113	0.14	1.00E-03	3.55E-02	1.91E-02	5.00E-02	5.00E-02	5.00E-02	1.10E-01
7786-34-7	Mevinphos	9	2900	30042	4232	25493	1.06	5.00E-05	1.30E-02	9.88E-03	1.00E-02	2.00E-02	2.50E-02	2.50E-01
		5	152	337	0	20	94.07	5.00E-05	1.03E-02	5.99E-03	1.00E-02	1.00E-02	2.00E-02	7.50E-02
78-51-3	Tris(2-butoxyethyl) phosphate (TBEP)	7	356	3210	0	2424	24.49	5.65E-04	7.55E-02	3.46E-01	2.50E-02	1.00E-01	1.95E-01	1.60E+01
		7	356	3210	0	2424	24.49	5.65E-04	7.55E-02	3.46E-01	2.50E-02	1.00E-01	1.95E-01	1.60E+01
78587-05-0	Hexythiazox	5	926	7124	0	7116	0.11	5.00E-03	2.50E-02	1.30E-02	2.50E-02	5.00E-02	5.00E-02	5.00E-02
		5	926	7124	0	7116	0.11	5.00E-03	2.50E-02	1.30E-02	2.50E-02	5.00E-02	5.00E-02	5.00E-02
78-87-5	1,2-Dichloropropane	11	1680	19620	108	19292	1.12	2.50E-03	1.62E+00	3.27E+00	2.50E-01	1.00E+01	1.00E+01	1.00E+01
		11	1680	19620	108	19292	1.12	2.50E-03	1.62E+00	3.27E+00	2.50E-01	1.00E+01	1.00E+01	1.00E+01
79-00-5	1,1,2-Trichloroethane	14	4863	61290	2771	58304	0.35	5.00E-04	4.53E-01	6.56E-01	2.50E-01	1.25E+00	2.50E+00	1.70E+01
		14	4863	61288	2771	58302	0.35	5.00E-04	4.53E-01	6.53E-01	2.50E-01	1.25E+00	2.50E+00	1.70E+01
79-11-8	Chloroacetic acid	4	764	4152	34	4114	0.1	2.50E-03	4.13E+00	1.61E+01	1.25E-02	5.00E+00	1.00E+01	1.00E+02
		n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
79241-46-6	Fluazifop-P-butyl	4	662	4796	0	4795	0.02	5.00E-03	2.31E-02	4.91E-03	2.50E-02	2.50E-02	2.50E-02	1.10E-01

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
		4	662	4796	0	4795	0.02	5.00E-03	2.31E-02	4.91E-03	2.50E-02	2.50E-02	2.50E-02	1.10E-01
79277-27-3	Thifensulfuron methyl	5	998	9873	0	9841	0.32	5.00E-03	3.69E-02	2.24E-02	5.00E-02	5.00E-02	5.00E-02	1.04E+00
		5	998	9873	0	9841	0.32	5.00E-03	3.69E-02	2.24E-02	5.00E-02	5.00E-02	5.00E-02	1.04E+00
79-34-5	1,1,2,2-Tetrachloroethane	12	1860	21070	274	20729	0.32	5.00E-03	7.02E-01	9.19E-01	2.50E-01	2.50E+00	2.50E+00	1.10E+01
		12	1860	21070	274	20729	0.32	5.00E-03	7.02E-01	9.19E-01	2.50E-01	2.50E+00	2.50E+00	1.10E+01
79622-59-6	Fluazinam	4	157	3234	0	3233	0.03	2.50E-03	1.50E-02	1.32E-02	1.00E-02	2.50E-02	2.50E-02	5.86E-01
		4	157	3234	0	3233	0.03	2.50E-03	1.50E-02	1.32E-02	1.00E-02	2.50E-02	2.50E-02	5.86E-01
80-05-7	Bisphenol A	15	1825	18610	552	12108	31.97	5.00E-06	2.99E+00	1.56E+02	2.90E-02	2.50E-01	3.15E-01	2.00E+04
		15	1814	17198	180	11068	34.6	5.00E-06	2.92E+00	1.62E+02	2.50E-02	1.20E-01	2.25E-01	2.00E+04
80-09-1	Bisphenol S	7	52	55	0	52	5.45	5.00E-02	5.85E-02	3.80E-02	5.00E-02	5.00E-02	7.70E-02	2.70E-01
		7	52	55	0	52	5.45	5.00E-02	5.85E-02	3.80E-02	5.00E-02	5.00E-02	7.70E-02	2.70E-01
8065-48-3	Demeton	4	912	8007	107	7900	0	2.50E-03	4.09E-02	1.82E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02
		4	912	8007	107	7900	0	2.50E-03	4.09E-02	1.82E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02
81-15-2	Musk xylene	4	909	10745	1	10668	0.71	2.50E-04	1.25E-01	2.00E-01	1.00E-02	5.00E-01	5.00E-01	5.00E-01
		4	909	10745	1	10668	0.71	2.50E-04	1.25E-01	2.00E-01	1.00E-02	5.00E-01	5.00E-01	5.00E-01
82097-50-5	Triasulfuron	4	831	6580	0	6577	0.05	5.00E-03	3.76E-02	1.66E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02
		n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
82558-50-7	Isoxaben	4	1051	10602	0	10568	0.32	2.50E-03	2.49E-02	1.94E-02	2.00E-02	5.00E-02	5.00E-02	1.40E+00
		4	1051	10602	0	10568	0.32	2.50E-03	2.49E-02	1.94E-02	2.00E-02	5.00E-02	5.00E-02	1.40E+00
82-68-8	Quintozene	4	1189	9889	147	9738	0.04	1.25E-03	6.72E-03	6.86E-03	2.50E-03	1.25E-02	2.50E-02	2.50E-02
		4	1189	9889	147	9738	0.04	1.25E-03	6.72E-03	6.86E-03	2.50E-03	1.25E-02	2.50E-02	2.50E-02
83121-18-0	Teflubenzuron	4	822	6970	0	6961	0.13	2.50E-03	2.15E-02	6.83E-03	2.50E-02	2.50E-02	2.50E-02	5.00E-02

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
		n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
83164-33-4	Diflufenican	8	3723	47162	815	42197	8.8	5.00E-04	2.47E-01	3.57E+00	1.25E-02	2.50E-02	2.60E-02	1.50E+02
		7	1395	7902	204	3548	52.52	5.00E-04	1.16E+00	8.31E+00	5.00E-03	5.40E-02	1.00E-01	1.50E+02
83-32-9	Acenaphthene	14	3225	35165	252	31362	10.1	1.00E-06	2.06E-01	7.77E+00	5.00E-03	1.25E-02	2.50E-02	9.80E+02
		14	3216	34829	227	31051	10.2	1.00E-06	1.71E-01	7.80E+00	5.00E-03	1.25E-02	2.50E-02	9.80E+02
834-12-8	Ametryn	7	4682	46654	511	46050	0.2	6.25E-04	2.69E-02	6.16E-01	1.00E-02	2.50E-02	2.50E-02	2.75E+01
		7	4682	46628	511	46024	0.2	6.25E-04	1.26E-02	8.96E-03	1.00E-02	2.50E-02	2.50E-02	1.00E-01
84-66-2	Diethyl phthalate	8	1177	13018	474	10657	14.5	5.00E-03	3.40E-01	8.80E-01	2.00E-01	5.00E-01	5.00E-01	1.21E+01
		8	1177	13018	474	10657	14.5	5.00E-03	3.40E-01	8.80E-01	2.00E-01	5.00E-01	5.00E-01	1.21E+01
84-74-2	Di-n-butylphthalate	10	1948	26077	600	19148	24.27	2.50E-03	3.39E-01	1.73E+00	2.00E-01	5.00E-01	5.00E-01	2.06E+02
		10	1948	26077	600	19148	24.27	2.50E-03	3.39E-01	1.73E+00	2.00E-01	5.00E-01	5.00E-01	2.06E+02
85-01-8	Phenanthrene	15	4373	57360	602	33928	39.8	2.00E-06	2.50E-01	4.97E+00	5.00E-03	2.10E-02	5.00E-02	9.00E+02
		15	4217	55898	516	32552	40.84	2.00E-06	1.29E-01	4.91E+00	5.00E-03	1.90E-02	3.00E-02	9.00E+02
85509-19-9	Flusilazole	6	2841	38304	124	37894	0.75	5.00E-04	2.07E-02	3.05E-02	2.50E-02	5.00E-02	5.00E-02	5.00E+00
		5	2840	38301	123	37892	0.75	5.00E-04	2.05E-02	1.64E-02	2.50E-02	5.00E-02	5.00E-02	1.18E+00
85-68-7	Butylbenzyl phthalate	8	1291	15442	372	13659	9.14	2.50E-05	2.82E-01	1.15E+00	5.00E-02	5.00E-01	5.00E-01	1.00E+02
		8	1288	15342	372	13559	9.2	2.50E-05	2.28E-01	9.46E-01	5.00E-02	5.00E-01	5.00E-01	1.00E+02
86-50-0	Azinphos-methyl	9	2585	25451	1053	24039	1.41	5.00E-04	6.65E-02	3.25E+00	2.00E-02	2.50E-02	2.50E-02	5.02E+02
		7	1206	9493	948	8186	3.78	5.00E-04	1.40E-01	5.32E+00	5.00E-03	5.00E-03	5.00E-03	5.02E+02
86-73-7	Fluorene	14	3427	37131	216	32362	12.26	3.00E-06	9.21E-02	2.51E+00	5.00E-03	1.00E-02	1.25E-02	2.90E+02
		14	3427	36876	216	32107	12.35	3.00E-06	7.89E-02	2.52E+00	5.00E-03	1.00E-02	1.00E-02	2.90E+02
87-65-0	2,6-Dichlorophenol	4	1320	12452	0	12414	0.31	1.25E-03	2.29E-02	1.40E-02	2.50E-02	5.00E-02	5.00E-02	4.00E-01

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
		4	1320	12452	0	12414	0.31	1.25E-03	2.29E-02	1.40E-02	2.50E-02	5.00E-02	5.00E-02	4.00E-01
87674-68-8	Dimethenamid	6	3613	45645	784	42646	4.85	5.00E-04	2.14E-02	1.14E-01	2.00E-02	2.50E-02	2.50E-02	1.54E+01
		6	3613	45640	784	42641	4.85	5.00E-04	2.11E-02	1.07E-01	2.00E-02	2.50E-02	2.50E-02	1.54E+01
88-06-2	2,4,6-Trichlorophenol	9	4150	47444	1039	45247	2.44	6.25E-04	5.08E-02	6.36E-02	5.00E-02	1.25E-01	1.25E-01	2.02E+00
		9	4131	47202	1039	45005	2.45	6.25E-04	4.85E-02	5.50E-02	5.00E-02	1.25E-01	1.25E-01	2.02E+00
882-09-7	Clofibric acid (Clofibrate)	10	372	5370	193	5038	2.59	1.50E-04	1.40E-02	2.24E-02	1.25E-02	1.50E-02	2.50E-02	1.50E+00
		10	372	5370	193	5038	2.59	1.50E-04	1.40E-02	2.24E-02	1.25E-02	1.50E-02	2.50E-02	1.50E+00
88-72-2	o-Nitrotoluene	5	251	1564	16	1533	0.96	5.00E-03	1.55E-01	1.21E-01	2.50E-01	2.50E-01	2.50E-01	1.10E+00
		5	251	1564	16	1533	0.96	5.00E-03	1.55E-01	1.21E-01	2.50E-01	2.50E-01	2.50E-01	1.10E+00
88-73-3	1-Cloro-2-nitrobenzene	6	1344	12142	54	12071	0.14	5.00E-05	2.29E-01	3.15E+00	1.50E-01	5.00E-01	5.00E-01	2.00E+02
		6	1344	12142	54	12071	0.14	5.00E-05	2.29E-01	3.15E+00	1.50E-01	5.00E-01	5.00E-01	2.00E+02
88-85-7	Dinoseb	6	1731	15084	0	15048	0.24	2.50E-03	1.54E-02	1.71E-02	1.25E-02	2.50E-02	2.50E-02	1.47E+00
		6	1731	15084	0	15048	0.24	2.50E-03	1.54E-02	1.71E-02	1.25E-02	2.50E-02	2.50E-02	1.47E+00
89-59-8	4-Chloro-2-nitrotoluene	5	581	5404	38	5347	0.35	5.00E-05	2.24E-01	3.65E-01	2.50E-01	2.50E-01	5.00E-01	2.70E+00
		5	565	5284	38	5227	0.36	5.00E-05	1.73E-01	1.27E-01	2.50E-01	2.50E-01	2.50E-01	2.70E+00
89-63-4	4-Chloro-2-nitroaniline	4	755	7356	0	7356	0	5.00E-03	4.46E-02	5.97E-02	2.50E-02	5.00E-02	1.00E-01	1.50E+00
		4	755	7352	0	7352	0	5.00E-03	4.38E-02	4.92E-02	2.50E-02	5.00E-02	1.00E-01	5.00E-01
90-12-0	1-Methylnaphthalene	4	650	5247	0	4900	6.61	2.50E-04	2.66E-02	2.91E-01	5.00E-03	1.00E-02	1.00E-02	1.30E+01
		4	650	5247	0	4900	6.61	2.50E-04	2.66E-02	2.91E-01	5.00E-03	1.00E-02	1.00E-02	1.30E+01

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
90-13-1	1-Chloronaphthalene	4	403	4244	38	4155	1.2	2.50E-03	2.93E-01	8.10E-01	2.50E-01	2.50E-01	2.50E-01	5.00E+00
		n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
90717-03-6	Quinmerac	5	1952	22615	156	20142	10.25	1.00E-03	2.02E-02	6.38E-02	1.25E-02	2.50E-02	3.40E-02	4.40E+00
		5	1952	22615	156	20142	10.25	1.00E-03	2.02E-02	6.38E-02	1.25E-02	2.50E-02	3.40E-02	4.40E+00
91465-08-6	lambda-Cyhalothrin	6	2064	21729	670	20929	0.6	2.50E-05	1.80E-02	9.70E-02	1.00E-02	5.00E-02	5.00E-02	1.00E+01
		4	54	228	98	0	57.02	2.50E-05	6.85E-03	1.39E-02	2.00E-03	1.00E-02	5.00E-02	5.00E-02
919-86-8	Demeton-S-methyl	5	2035	19583	221	19265	0.5	1.25E-03	2.30E-02	1.69E-02	2.50E-02	5.00E-02	5.00E-02	2.50E-01
		5	2035	19582	221	19264	0.5	1.25E-03	2.30E-02	1.68E-02	2.50E-02	5.00E-02	5.00E-02	1.00E-01
92-52-4	Biphenyl	8	2690	35323	956	33905	1.31	1.00E-06	4.90E-02	3.91E-01	1.00E-02	5.00E-02	5.00E-02	5.00E+01
		8	2610	35062	696	33904	1.32	1.00E-06	3.87E-02	2.68E-01	1.00E-02	5.00E-02	5.00E-02	1.10E+01
933-75-5	2,3,6-Trichlorphenol	4	786	9276	0	9276	0	1.00E-03	8.02E-02	1.05E-01	2.50E-02	2.50E-01	2.50E-01	5.00E-01
		4	579	6909	0	6909	0	1.00E-03	2.82E-02	1.33E-02	2.50E-02	5.00E-02	5.00E-02	5.00E-02
933-78-8	2,3,5-Trichlorphenol	4	675	5712	0	5708	0.07	1.00E-03	6.35E-02	9.88E-02	2.50E-02	1.25E-01	1.25E-01	5.00E-01
		4	473	4643	0	4639	0.09	1.00E-03	2.98E-02	1.64E-02	2.50E-02	5.00E-02	5.00E-02	2.70E-01
93-65-2	Mecoprop	20	4581	43784	1681	37811	9.8	5.00E-06	2.29E-02	2.19E-01	1.00E-02	2.50E-02	4.00E-02	2.80E+01
		20	4581	43784	1681	37811	9.8	5.00E-06	2.29E-02	2.19E-01	1.00E-02	2.50E-02	4.00E-02	2.80E+01
93-72-1	Fenoprop	6	323	4005	114	3790	2.52	6.25E-04	1.35E-02	1.17E-02	1.25E-02	2.50E-02	2.50E-02	1.00E-01
		6	323	4005	114	3790	2.52	6.25E-04	1.35E-02	1.17E-02	1.25E-02	2.50E-02	2.50E-02	1.00E-01
93-76-5	2,4,5-Trichlorophenoxyacetic acid	9	3509	33643	609	32860	0.52	1.00E-03	1.27E-02	2.20E-02	1.00E-02	2.50E-02	2.50E-02	1.74E+00
		9	3509	33642	608	32860	0.52	1.00E-03	1.27E-02	2.20E-02	1.00E-02	2.50E-02	2.50E-02	1.74E+00

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
94361-06-5	Cyproconazole	5	1987	21499	512	20617	1.72	2.50E-03	1.88E-02	5.18E-02	1.00E-02	2.50E-02	2.50E-02	5.00E+00
		5	1987	21497	512	20615	1.72	2.50E-03	1.84E-02	1.94E-02	1.00E-02	2.50E-02	2.50E-02	1.88E+00
94-74-6	2-Methyl-4-chlorophenoxyacetic acid (MCPA)	23	7093	113396	2803	97417	11.62	5.00E-06	5.02E-01	3.17E+01	1.00E-02	2.50E-02	5.12E-02	2.50E+03
		23	7076	113264	2692	97396	11.63	5.00E-06	3.09E-02	1.24E+00	1.00E-02	2.50E-02	5.00E-02	3.84E+02
94-75-7	2,4-Dichlorophenoxyacetic acid (2,4-D)	20	6198	73856	3333	63010	10.17	2.50E-05	2.83E+00	7.17E+01	1.00E-02	2.50E-02	4.00E-02	5.85E+03
		20	6196	73594	3332	62749	10.21	2.50E-05	1.72E-02	1.31E-01	1.00E-02	2.50E-02	3.70E-02	2.49E+01
94-81-5	4-(4-Chloro-o-tolyloxy) butyric acid	8	3918	39801	2327	37125	0.88	6.25E-04	1.87E-02	5.26E-02	1.00E-02	2.50E-02	2.50E-02	1.73E+00
		8	3918	39801	2327	37125	0.88	6.25E-04	1.87E-02	5.26E-02	1.00E-02	2.50E-02	2.50E-02	1.73E+00
94-82-6	4-(2,4-Dichlorophenoxy)butyric acid (2,4-DB)	6	2133	20586	458	19980	0.72	1.00E-03	1.30E-02	1.03E-02	1.25E-02	2.00E-02	2.50E-02	6.76E-01
		6	2133	20586	458	19980	0.72	1.00E-03	1.30E-02	1.03E-02	1.25E-02	2.00E-02	2.50E-02	6.76E-01
950-37-8	Methidathion	5	1306	11747	98	11640	0.08	2.50E-03	1.60E-02	2.03E-02	2.00E-02	2.50E-02	2.50E-02	2.00E+00
		n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
95-14-7	1H-Benzotriazole	9	175	1920	0	66	96.56	2.50E-03	6.35E-01	1.08E+00	2.70E-01	1.70E+00	2.80E+00	1.20E+01
		9	175	1920	0	66	96.56	2.50E-03	6.35E-01	1.08E+00	2.70E-01	1.70E+00	2.80E+00	1.20E+01
95-49-8	2-Chlorotoluene	10	1689	18907	142	18672	0.49	2.50E-03	5.95E-01	1.31E+00	2.50E-01	5.00E-01	5.00E+00	5.00E+00
		10	1469	17392	142	17157	0.53	2.50E-03	2.12E-01	1.52E-01	2.50E-01	5.00E-01	5.00E-01	2.10E+00
95-50-1	1,2-Dichlorobenzene	12	3546	44438	226	44027	0.42	5.00E-04	2.53E-01	4.23E-01	1.25E-01	5.00E-01	1.00E+00	5.00E+00

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
		12	3520	42427	200	42042	0.44	5.00E-04	1.73E-01	1.55E-01	1.25E-01	2.50E-01	5.00E-01	4.98E+00
95-51-2	2-Chloroaniline	4	1104	9205	38	9161	0.07	5.00E-03	4.49E-02	7.26E-02	2.50E-02	1.00E-01	2.50E-01	1.50E+00
		4	1060	8505	38	8461	0.07	5.00E-03	2.70E-02	2.21E-02	2.50E-02	5.00E-02	5.00E-02	9.40E-01
95-57-8	2-Chlorophenol	9	2933	31836	1357	29572	2.85	2.50E-03	5.02E-02	6.16E-02	5.00E-02	5.00E-02	1.00E-01	1.85E+00
		9	2933	31836	1357	29572	2.85	2.50E-03	5.02E-02	6.16E-02	5.00E-02	5.00E-02	1.00E-01	1.85E+00
95-63-6	1,2,4-Trimethylbenzene	9	983	10149	0	10041	1.06	2.50E-03	4.44E-01	5.40E-01	5.00E-01	1.00E+00	1.00E+00	1.20E+01
		9	946	9701	0	9593	1.11	2.50E-03	3.49E-01	3.18E-01	2.50E-01	5.00E-01	1.00E+00	1.20E+01
95-76-1	3,4-Dichloroaniline	9	1516	13348	38	13222	0.66	5.00E-03	3.48E-02	4.93E-02	2.50E-02	5.00E-02	1.50E-01	1.04E+00
		7	542	3979	0	3891	2.21	5.00E-03	8.63E-03	2.33E-02	5.00E-03	1.00E-02	2.00E-02	1.04E+00
95-85-2	2-Amino-4-chlorophenol	4	618	4036	38	3997	0.02	5.00E-03	6.68E-01	3.91E-01	1.00E+00	1.00E+00	1.00E+00	1.00E+00
		4	618	4036	38	3997	0.02	5.00E-03	6.68E-01	3.91E-01	1.00E+00	1.00E+00	1.00E+00	1.00E+00
95-94-3	1,2,4,5-Tetrachlorobenzene	5	1708	15435	38	15388	0.06	5.00E-04	1.12E-01	3.82E-01	2.50E-02	5.00E-01	5.00E-01	5.00E+00
		4	133	1010	0	1001	0.89	5.00E-04	1.60E-03	9.18E-03	1.00E-03	1.00E-03	1.00E-03	1.30E-01
95-95-4	2,4,5-Trichlorophenol	7	3535	45114	361	44676	0.17	6.25E-04	4.81E-02	2.42E-01	2.50E-02	6.50E-02	1.25E-01	5.00E+01
		7	3221	41222	361	40784	0.19	6.25E-04	3.29E-02	2.14E-02	2.50E-02	6.50E-02	6.50E-02	4.98E-01
96-12-8	1,2-Dibromo-3-chloropropane	5	119	1455	0	1453	0.14	2.50E-02	1.91E-01	2.54E-01	5.00E-02	6.50E-01	6.50E-01	2.00E+00
		5	119	1455	0	1453	0.14	2.50E-02	1.91E-01	2.54E-01	5.00E-02	6.50E-01	6.50E-01	2.00E+00
96-18-4	1,2,3-Trichloropropane	8	654	4357	1	4346	0.23	2.50E-03	1.34E+00	1.21E+00	2.50E+00	2.50E+00	2.50E+00	2.50E+00
		8	654	4357	1	4346	0.23	2.50E-03	1.34E+00	1.21E+00	2.50E+00	2.50E+00	2.50E+00	2.50E+00

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
96525-23-4	Flurtamone	10	3033	32412	51	31928	1.34	1.00E-03	1.92E-02	2.79E-01	1.50E-02	2.50E-02	2.50E-02	5.00E+01
		10	3033	32412	51	31928	1.34	1.00E-03	1.92E-02	2.79E-01	1.50E-02	2.50E-02	2.50E-02	5.00E+01
97-00-7	1-Chloro-2,4-dinitrobenzene	5	785	7277	50	7208	0.26	2.50E-04	2.70E-01	6.47E-01	2.50E-01	5.00E-01	5.00E-01	5.00E+01
		5	775	7216	50	7147	0.26	2.50E-04	2.46E-01	2.02E-01	2.50E-01	5.00E-01	5.00E-01	1.30E+00
98-82-8	Isopropylbenzene	9	2652	33055	107	32861	0.26	5.00E-03	3.15E-01	3.52E-01	2.50E-01	5.00E-01	1.00E+00	4.70E+00
		9	2367	30262	107	30068	0.29	5.00E-03	2.28E-01	1.24E-01	2.50E-01	2.50E-01	5.00E-01	4.70E+00
98-87-3	alpha,alpha-Dichlorotoluene	4	336	2659	38	2621	0	2.50E-02	2.09E+00	2.43E+00	2.50E-02	5.00E+00	5.00E+00	5.00E+00
		n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
98-95-3	Nitrobenzene	5	997	11809	119	11468	1.88	5.00E-03	3.39E-01	9.43E+00	5.00E-02	2.50E-01	2.50E-01	1.01E+03
		4	838	8727	0	8505	2.54	5.00E-03	2.02E-01	1.09E+01	5.00E-02	1.00E-01	1.00E-01	1.01E+03
99-87-6	p-Cymene	4	732	6475	0	6471	0.06	3.25E-02	3.46E-01	2.74E-01	2.50E-01	1.00E+00	1.00E+00	4.00E+00
		4	732	6475	0	6471	0.06	3.25E-02	3.46E-01	2.74E-01	2.50E-01	1.00E+00	1.00E+00	4.00E+00

Table II-2. Summary monitoring data - inland whole water for metals/metalloids.

For each substance, two scenarios are presented. Top/shaded: Sc2 (all monitoring records; non-quantified records are set as half LOD/Q); Bottom/white: Sc2-PNEC QC (quantified records plus non-quantified samples excluding those for which ½LOD/Q > PNEC). Substances are sorted by CAS number; concentrations in µg/L.

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
18540-29-9	Chromium 6+	4	473	2541	83	2074	15.11	2.50E-01	1.05E+01	6.36E+00	1.50E+01	1.50E+01	1.50E+01	3.76E+01
		4	107	415	12	19	92.53	2.50E-01	2.29E+00	3.07E+00	1.25E+00	5.00E+00	6.00E+00	3.76E+01
7439-95-4	Magnesium	6	453	7839	0	14	99.82	5.08E-04	2.53E+03	1.47E+04	5.35E+00	5.74E+03	1.00E+04	3.48E+05
		6	453	7839	0	14	99.82	5.08E-04	2.53E+03	1.47E+04	5.35E+00	5.74E+03	1.00E+04	3.48E+05
7440-22-4	Silver	9	1134	13196	554	11477	8.83	1.25E-02	4.50E-01	6.50E-01	1.25E-01	1.25E+00	2.50E+00	2.50E+00
		7	169	1424	0	259	81.81	1.25E-02	2.21E-01	2.51E-01	1.00E-01	5.00E-01	7.50E-01	1.90E+00
7440-23-5	Sodium	5	380	9824	0	0	100.00	3.00E-03	2.66E+04	2.51E+05	9.30E+00	3.80E+03	4.20E+04	8.97E+06
		5	380	9824	0	0	100.00	3.00E-03	2.66E+04	2.51E+05	9.30E+00	3.80E+03	4.20E+04	8.97E+06
7440-24-6	Strontium	4	251	3804	0	227	94.03	1.50E-02	1.51E+02	2.67E+02	5.00E+01	4.50E+02	5.20E+02	3.03E+03
		4	251	3804	0	227	94.03	1.50E-02	1.51E+02	2.67E+02	5.00E+01	4.50E+02	5.20E+02	3.03E+03
7440-28-0	Thallium	7	730	11282	24	8815	21.65	2.50E-03	4.23E-01	9.39E-01	7.00E-02	1.25E+00	2.50E+00	1.80E+01
		7	297	6139	0	3696	39.79	2.50E-03	1.01E-01	7.02E-01	5.00E-02	5.00E-02	1.20E-01	1.80E+01
7440-31-5	Tin	9	1132	12807	965	9764	16.23	1.25E-02	3.16E+00	7.10E+00	5.00E-01	5.00E+00	2.50E+01	2.24E+02
		8	781	7348	184	5086	28.28	1.25E-02	5.93E-01	4.46E+00	3.83E-01	5.00E-01	7.00E-01	2.24E+02
7440-32-6	Titanium	6	704	7465	0	3494	53.19	1.00E-06	6.45E+00	1.36E+01	2.50E+00	1.50E+01	2.50E+01	3.26E+02
		6	704	7324	0	3353	54.22	1.00E-06	6.10E+00	1.35E+01	2.50E+00	1.30E+01	2.23E+01	3.26E+02
7440-36-0	Antimony	11	1148	14566	262	12162	14.71	7.50E-02	9.60E-01	1.47E+01	2.50E-01	1.50E+00	2.50E+00	1.00E+03
		11	1148	14560	262	12156	14.71	7.50E-02	9.57E-01	1.47E+01	2.50E-01	1.50E+00	2.50E+00	1.00E+03
7440-41-7	Beryllium	9	778	11835	49	9503	19.29	2.50E-03	4.32E-01	9.93E-01	9.00E-02	1.25E+00	2.50E+00	1.03E+01
		7	310	6881	49	4549	33.18	2.50E-03	1.42E-01	8.84E-01	2.50E-02	1.20E-01	2.40E-01	1.03E+01
7440-61-1	Uranium	5	595	8844	0	3155	64.33	1.00E-02	4.13E+01	2.47E+02	6.60E-01	2.50E+00	1.00E+02	1.40E+04
		5	386	7293	0	1604	78.01	1.00E-02	2.47E+01	2.24E+02	5.13E-01	2.00E+00	4.30E+00	1.40E+04
7440-70-2	Calcium	6	523	8412	0	68	99.19	5.00E-04	5.14E+03	1.95E+04	1.89E+01	4.87E+03	4.60E+04	2.11E+05
		6	523	8412	0	68	99.19	5.00E-04	5.14E+03	1.95E+04	1.89E+01	4.87E+03	4.60E+04	2.11E+05

Table II-3. Summary monitoring data - inland water (dissolved fraction).

For each substance, two scenarios are presented. Top/shaded: Sc2 (all monitoring records; non-quantified records are set as half LOD/Q); Bottom/white: Sc2-PNEC QC (quantified records plus non-quantified samples excluding those for which ½LOD/Q > PNEC). Substances are sorted by CAS number; concentrations in µg/L.

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
7429-90-5	Aluminium	9	1591	16194	0	9447	41.7	5.70E-01	89.22	190.91	50.00	168.00	278.35	9442.0
		9	944	8886	0	2139	75.9	5.70E-01	105.77	255.61	32.00	260.00	395.72	9442.0
7439-89-6	Iron	9	755	18089	154	1812	89.1	1.00E-05	332.81	633.16	115.00	870.00	1420.00	28000.0
		9	755	18089	154	1812	89.1	1.00E-05	332.81	633.16	115.00	870.00	1420.00	28000.0
7439-96-5	Manganese	10	605	15979	246	1677	88.0	2.55E-06	44.34	68.89	21.00	110.00	168.10	1740.0
		10	605	15979	246	1677	88.0	2.55E-06	44.34	68.89	21.00	110.00	168.10	1740.0
7439-98-7	Molybdenum	5	182	2204	0	1350	38.7	1.00E-05	1.87	14.76	0.01	2.01	5.67	600.0
		5	182	2203	0	1349	38.8	1.00E-05	1.60	7.44	0.01	2.01	5.49	130.0
7440-38-2	Arsenic	20	5137	54605	124	33598	38.2	5.00E-03	2.80	11.32	1.99	5.00	10.00	767.0
		20	5124	54544	124	33537	38.3	5.00E-03	2.75	11.05	1.94	5.00	10.00	767.0
7440-39-3	Barium	5	60	855	2	0	99.8	2.50E-02	47.88	19.73	47.00	72.90	84.00	120.0
		5	60	855	2	0	99.8	2.50E-02	47.88	19.73	47.00	72.90	84.00	120.0
7440-42-8	Boron	5	3104	22538	30	15043	33.1	5.00E-01	86.25	222.01	50.00	150.00	250.00	10520.0
		4	3035	22307	10	14832	33.5	5.00E-01	84.56	222.52	50.00	150.00	221.63	10520.0
7440-47-3	Chromium	21	5447	62964	884	50511	18.4	1.25E-02	14.64	289.28	1.00	5.00	10.00	9909.6
		21	5113	56425	884	43972	20.5	1.25E-02	15.46	305.57	0.70	2.50	2.50	9909.6
7440-48-4	Cobalt	7	1013	13919	3	8106	41.7	2.50E-03	7.71	10.81	0.50	25.00	25.00	50.0
		7	511	7832	3	2019	74.2	2.50E-03	0.31	1.29	0.13	0.52	0.83	40.0
7440-50-8	Copper	24	7251	104254	331	55457	46.5	1.00E-02	11.12	152.46	1.97	8.74	30.00	10000.0

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
		24	7009	97036	330	48240	49.9	1.00E-02	9.13	157.78	1.70	5.00	6.00	10000.0
7440-62-2	Vanadium	8	380	7794	0	2368	69.6	1.00E-02	1.43	2.12	0.58	5.00	5.00	40.0
		8	357	6639	0	1213	81.7	1.00E-02	0.79	1.48	0.50	1.40	2.30	40.0
7440-66-6	Zinc	22	7010	87895	484	43010	50.5	1.00E-02	18.27	157.51	6.00	50.00	50.00	34200.0
		22	6626	77371	484	32486	57.4	1.00E-02	15.95	167.64	5.00	28.00	48.50	34200.0
7782-49-2	Selenium	7	3286	25422	51	21890	13.7	5.00E-04	8.21	39.03	0.50	5.40	12.50	250.0
		7	913	4509	30	998	77.2	5.00E-04	1.62	3.87	1.05	3.50	5.11	154.6

Table II-4. Summary monitoring data - coastal and transitional waters (whole fraction).

For each substance, two scenarios are presented. Top/shaded: Sc2 (all monitoring records; non-quantified records are set as half LOD/Q); Bottom/white: Sc2-PNEC QC (quantified records plus non-quantified samples excluding those for which ½LOD/Q > PNEC). Substances are sorted by CAS number; concentrations in µg/L.

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
108-88-3	Toluene	4	37	885	161	614	12.4	2.50E-03	0.06	0.53	0.01	0.05	0.05	13.0
		4	37	885	161	614	12.4	2.50E-03	0.06	0.53	0.01	0.05	0.05	13.0
129-00-0	Pyrene	10	218	1942	276	1006	34.0	3.50E-06	0.14	1.98	0.00	0.05	0.08	47.0
		10	161	1612	276	676	40.9	3.50E-06	0.16	2.18	0.00	0.05	0.08	47.0
218-01-9	Chrysene	7	149	1897	344	1240	16.5	4.00E-04	0.02	0.02	0.00	0.05	0.05	0.4
		7	149	1897	344	1240	16.5	4.00E-04	0.02	0.02	0.00	0.05	0.05	0.4
330-55-2	Linuron	4	33	1044	142	856	4.4	2.50E-04	0.00	0.01	0.00	0.01	0.01	0.2
		4	33	1044	142	856	4.4	2.50E-04	0.00	0.01	0.00	0.01	0.01	0.2
56-55-3	Benzo(a)anthracene	10	221	2066	356	1256	22.0	5.00E-07	0.01	0.02	0.00	0.05	0.05	0.2
		10	221	2066	356	1256	22.0	5.00E-07	0.01	0.02	0.00	0.05	0.05	0.2
85-01-8	Phenanthrene	10	225	2176	227	1079	40.0	1.85E-05	0.02	0.07	0.00	0.05	0.05	3.1
		10	225	2176	227	1079	40.0	1.85E-05	0.02	0.07	0.00	0.05	0.05	3.1

Table II-5. Summary monitoring data - coastal and transitional waters (dissolved fraction).

For each substance, two scenarios are presented. Top/shaded: Sc2 (all monitoring records; non-quantified records are set as half LOD/Q); Bottom/white: Sc2-PNEC QC (quantified records plus non-quantified samples excluding those for which ½LOD/Q > PNEC). Substances are sorted by CAS number; concentrations in µg/L.

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
7440-47-3	Chromium	7	71	475	12	378	17.9	1.00E-01	0.89	2.12	0.50	1.00	1.75	29.0
		6	51	370	12	273	23.0	1.00E-01	0.59	1.13	0.50	0.53	0.70	13.6
7440-50-8	Copper	6	69	462	0	171	63.0	1.00E-01	1.48	1.12	1.25	2.50	3.08	8.1
		6	68	461	0	170	63.1	1.00E-01	1.47	1.09	1.25	2.50	3.08	8.1
7440-66-6	Zinc	6	74	466	0	84	82.0	1.00E-01	4.67	5.04	2.73	12.25	15.00	33.6
		5	60	391	0	9	97.7	1.00E-01	4.29	5.18	2.12	11.80	15.25	33.6

Table II-6. Summary monitoring data - sediments.

For each substance, two scenarios are presented. Top/shaded: Sc2 (all monitoring records; non-quantified records set as half LOD/Q); Bottom/white: Sc2-PNEC QC (quantified records plus non-quantified samples excluding those for which ½LOD/Q > PNEC). Substances are sorted by CAS number, concentrations in µg/kg. The data contains only inland water sediments (rivers; lakes). The records for transitional and coastal water were excluded because they were few. In addition to the outlier procedure applied, some additional non-realistic high concentrations were excluded (as 1kg/kg dd).

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
1002-53-5	Dibutyltin (dichloride)	9	1604	1927	47	1583	15.4	5.00E-04	7.9	12.7	2.0	19.5	19.5	300.8
		9	1081	1306	47	962	22.7	5.00E-04	3.1	12.6	1.0	3.9	8.6	300.8
1163-19-5	Decabromodiphenyl ether (BDE-209)	9	1867	2519	0	1945	22.8	5.00E-08	114.5	457.3	12.5	250.0	250.0	5000.0
		9	1867	2519	0	1945	22.8	5.00E-08	114.5	457.3	12.5	250.0	250.0	5000.0
1461-25-2	Tetrabutyltin	10	1507	1837	71	1693	4.0	1.25E-03	11.8	130.8	2.0	17.1	17.1	5000.0
		10	142	144	71	0	50.7	1.25E-03	49.5	208.0	2.2	79.8	175.5	1800.0
207122-16-5	Heptabromodiphenyl ether (BDE-183)	9	254	300	0	293	2.3	5.00E-05	0.1	0.1	0.1	0.1	0.1	0.3
		9	254	300	0	293	2.3	5.00E-05	0.1	0.1	0.1	0.1	0.1	0.3
53-19-0	DDD, o,p'	11	1777	2132	80	1943	5.1	1.25E-03	5.9	5.9	2.5	12.5	12.5	25.0
		11	522	679	80	490	16.1	1.25E-03	0.6	1.4	0.5	0.5	1.8	19.0
56-55-3	Benzo(a)anthracene	10	2462	3365	30	589	81.6	5.00E-03	323.3	1216.7	87.1	698.8	1212.4	57511.0
		10	2462	3365	30	589	81.6	5.00E-03	323.3	1216.7	87.1	698.8	1212.4	57511.0
668-34-8	Triphenyltin	9	1276	1481	62	1390	2.0	1.25E-03	5.1	8.2	1.7	16.9	16.9	121.7
		9	1276	1481	62	1390	2.0	1.25E-03	5.1	8.2	1.7	16.9	16.9	121.7
7440-38-2	Arsenic	11	1890	2542	0	112	95.6	1.54E+00	9290.5	13802.5	5700.0	20300.0	28680.0	288300.0
		11	1890	2542	0	112	95.6	1.54E+00	9290.5	13802.5	5700.0	20300.0	28680.0	288300.0

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
7440-47-3	Chromium	12	1921	2574	0	7	99.7	5.20E+00	33770.9	36781.7	28432.5	62100.0	77540.0	609000.0
		12	1921	2574	0	7	99.7	5.20E+00	33770.9	36781.7	28432.5	62100.0	77540.0	609000.0
7440-50-8	Copper	12	2401	3884	0	183	95.3	4.19E+00	22977.8	35930.4	14000.0	45000.0	75085.0	583000.0
		12	2401	3884	0	183	95.3	4.19E+00	22977.8	35930.4	14000.0	45000.0	75085.0	583000.0
7440-66-6	Zinc	11	1896	2531	0	3	99.9	1.00E+00	102599.8	116851.4	70200.0	224000.0	315950.0	898000.0
		11	1896	2531	0	3	99.9	1.00E+00	102599.8	116851.4	70200.0	224000.0	315950.0	898000.0
78763-54-9	Monobutyltin	9	1242	1459	39	1181	16.4	1.25E-03	19.8	26.1	27.9	33.2	33.2	671.0
		9	387	442	39	164	54.1	1.25E-03	12.2	41.3	1.0	32.7	66.2	671.0
85-01-8	Phenanthrene	9	2436	3328	9	823	75.0	1.30E-02	292.8	929.3	91.0	650.3	1050.0	30318.0
		9	2436	3328	9	823	75.0	1.30E-02	292.8	929.3	91.0	650.3	1050.0	30318.0

Table II-7. Summary monitoring data - biota: fish.

For each substance, two scenarios are presented. Top/shaded: Sc2 (all monitoring records; non-quantified records set as half LOD/Q); Bottom/white: Sc2-PNEC QC (quantified records plus non-quantified samples excluding those for which ½LOD/Q > PNEC). Substances are sorted by CAS number, concentrations in µg/kg. The data contains only coastal and transitional waters. Data given in dry weight have been converted to wet weight. In addition to the outlier procedure applied, some additional non-realistic high concentrations were excluded.

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
7440-47-3	Chromium	6	84	1955	471	964	26.6	2.70E-01	326.2	9055.0	39.0	300.0	416.0	400400.0
		6	84	1955	471	964	26.6	2.70E-01	326.2	9055.0	39.0	300.0	416.0	400400.0

Table II-8. Summary monitoring data - biota: mollusc.

For each substance, two scenarios are presented. Top/shaded: Sc2 (all monitoring records; non-quantified records set as half LOD/Q); Bottom/white: Sc2-PNEC QC (quantified records plus non-quantified samples excluding those for which ½LOD/Q > PNEC). Substances are sorted by CAS number, concentrations in µg/kg. The data contains only coastal and transitional waters. Data given in dry weight have been converted to wet weight. In addition to the outlier procedure applied, some additional non-realistic high concentrations were excluded.

CAS	Substance	Countries	Sites	Samples	< LOD	< LOQ	% quantified	Min	Mean	SD	Median	P90	P95	Max
129-00-0	Pyrene	12	655	2491	4	76	96.8	5.18E-06	8.2	18.1	3.1	18.1	34.9	347.3
		12	626	2449	4	34	98.4	5.18E-06	8.3	18.2	3.1	18.6	35.1	347.3
218-01-9	Chrysene	11	336	1483	7	158	88.9	5.00E-02	6.9	16.8	2.3	16.5	32.0	324.7
		11	302	1427	1	108	92.4	5.00E-02	7.0	17.1	2.3	17.1	32.6	324.7
53-70-3	Dibenzo(a,h)anthracene	11	517	1697	74	892	43.1	1.00E-03	5.2	42.6	0.3	1.4	5.0	864.0
		11	419	1440	56	653	50.8	1.00E-03	5.4	45.6	0.2	1.2	3.0	864.0
56-55-3	Benzo(a)anthracene	12	749	2675	11	386	85.2	1.24E-03	4.2	11.4	1.2	8.7	17.0	198.0
		12	697	2565	1	286	88.8	1.24E-03	4.2	11.6	1.1	9.2	18.0	198.0
7440-38-2	Arsenic	13	603	2924	0	34	98.8	1.82E-02	2162.5	1274.1	1960.0	3423.8	4180.0	20000.0
		13	603	2924	0	34	98.8	1.82E-02	2162.5	1274.1	1960.0	3423.8	4180.0	20000.0
7440-47-3	Chromium	14	744	3410	1	81	97.6	1.82E-01	406.9	1020.3	224.9	648.1	962.9	21753.3
		14	744	3410	1	81	97.6	1.82E-01	406.9	1020.3	224.9	648.1	962.9	21753.3
85-01-8	Phenanthrene	12	668	2684	1	148	94.4	7.65E-02	34.2	273.7	3.4	11.5	18.2	6462.4
		12	643	2618	1	82	96.8	7.65E-02	35.0	277.1	3.3	11.7	18.6	6462.4

Annex III: Summary of PNECs

<u>Note:</u> The PNEC/EQS values reported as selected in Annex III, are values chosen for the sake of STE exercise (following the criteria mentioned in section 2.3.2.), and they are not to be intended as reference values for any other purpose.

Table III-1. List of PNEC/EQS$_{fw,eco}$

The values stated under the column "Selected PNEC/EQS$_{fw,eco}$" were used in the STE.

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
100-00-5	1-Chloro-4-nitrobenzene	EQS	BE	3	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	FI	15	RBSP-ECOSTAT, UBA (2014)		
		EQS	IT	1	RBSP-ECOSTAT, UBA (2014)	1	
		EQS	NL	19	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	FR	2.8	INERIS, 2013		
		PNEC	CZ	2	RBSP-ECOSTAT, UBA (2014)		
		PNEC	-	2	Von der Ohe, 2011		
1002-53-5	Dibutyltin	EQS	AT	0.01	RBSP database WRc, 2012	0.01	**DE:** 78763-54-9: Monobutyltin. PNEC sed 1.17 µg/kg dw. Review of data needed. PNEC aquatic?
		EQS	BE	0.08	RBSP database WRc, 2012		
		EQS	SI	0.02	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	0.13	NL SPECIFIC POLLUTANTS		
100-41-4	Ethylbenzene	EQS	CZ	1	RBSP-ECOSTAT, UBA (2014)	1	
		EQS	LU	2	RBSP-ECOSTAT, UBA (2014)		
		EQS	BE	5	RBSP-ECOSTAT, UBA (2014)		
		EQS	AT	10	RBSP-ECOSTAT, UBA (2014)		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
		EQS	DE	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	LV	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	DK	20	RBSP-ECOSTAT, UBA (2014)		
		EQS	ES	30	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	65	NL SPECIFIC POLLUTANTS		
		EQS	FR	100	INERIS, 2014		
		PNEC	ECHA	100	ECHA DOSSIER		
		PNEC	-	100	Von der Ohe, 2011		
100-42-5	Styrene	EQS	SK	0.63	RBSP-ECOSTAT, UBA (2014)	0.63	
		EQS	NL	570	RBSP-ECOSTAT, UBA (2014)		
		PNEC	ECHA	28	ECHA DOSSIER		
		PNEC	-	40	Verbruggen, 2008		
1007-28-9	6-Desisopropylatrazine	EQS	DK	0.01	RBSP-ECOSTAT, UBA (2014)	0.01	**DE:** EQS for Atrazine exists, EQS for metabolite needed? Proposed EQS should be reviewed
		PNEC	-	3.7	COMMPS database		
101200-48-0	Tribenuron-methyl	EQS	FI	0.1	RBSP-ECOSTAT, UBA (2014)	0.1	**DE:** Lemna gibba, 14 d NOEC Biomasse = 1 µg/l (UBA ICS database)
		EQS	SE	0.1	RBSP database WRc, 2012		
101205-02-1	Cycloxydim	PNEC	-	2150	JRC derivation (EFSA-dataset)	2150	
101-21-3	Chlorpropham	EQS	NL	4	NL Specific Pollutants	4	
		EQS	FR	4	INERIS, 2014		
1014-69-3	Desmetryn	pEQS	DE	0.025	UBA (DE) Communication		**DE:** Short-term PNEC, 25 µg/L, AF1000, pEQS rounded = 0.03 µg/L.
		PNEC_st	FR	0.025	ECOTOX database, US-EPA	0.025	
		PNEC_st	-	0.025	Von der Ohe, 2011		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
10265-92-6	Methamidophos	EQS	NL	0.016	RBSP-ECOSTAT, UBA (2014)	0.016	
		EQS	DE	0.1	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	0.1	RBSP-ECOSTAT, UBA (2014)		
		EQS	BE	0.3	RBSP-ECOSTAT, UBA (2014)		
		EQS	IT	0.5	RBSP-ECOSTAT, UBA (2014)		
		EQS	FR	2.6	INERIS, 2012		
		PNEC	-	2.6	Von der Ohe, 2011		
102851-06-9	Tau-fluvalinate	PNEC	-	0.0021	JRC derivation (EFSA-dataset)	0.0021	**ADAMA:** PNEC: 0.021µg/L, AF10. Available database justifies a reduction in the AF from 50 to 10
1031-07-8	Endosulfan sulfate	PNEC	INERIS	0.005	CIRCA data sheet, Dir. 2008/105/EC	0.005	
		PNEC	-	0.005	Von der Ohe, 2011		
103-65-1	n-Propylbenzene	PNEC	ECHA	35	ECHA DOSSIER	35	Value from isopropylbenzene (CAS98-82-8) since both substances are included under the same entry in Regulation EC 1272/2008
103-90-2	Acetaminophen (Paracetamol)	PNEC	-	136	JRC derivation (ECOTOX US EPA)	136	
104-35-8	4-Nonylphenol mono-ethoxylate (NP1EO)	EQS	DK	0.05	RBSP-ECOSTAT, UBA (2014)	0.05	**NL:** Concordance with the order of magnitude
104-51-8	n-Butylbenzene	PNEC	-	3.3	Quality standard for water Japan	3.3	https://www.env.go.jp/en/chemi/chemicals/profile_erac/profile7/pf2-08.pdf
10605-21-7	Carbendazim	EQS	FR	0.15	INERIS, 2013	0.15	
		EQS	UK	0.15	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	0.15	UBA, DE		https://webetox.uba.de/webETOX/public/basics/literatur.do?id=24234
		EQS	CH	0.34	Swiss ECOTOX Centre		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
		EQS	NL	0.6	NL Specific Pollutants		
106-43-4	4-Chlorotoluene	EQS	DE	1	RBSP-ECOSTAT, UBA (2014)	1	
		EQS	IT	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	BE	3	RBSP-ECOSTAT, UBA (2014)		
		EQS	FR	32	INERIS, 2011		
		EQS	NL	310	RBSP-ECOSTAT, UBA (2014)		
		PNEC	ECHA	32	ECHA DOSSIER		
		PNEC	-	32	Von der Ohe, 2011		
106-46-7	1,4-Dichlorobenzene	EQS	BG	1	RBSP database WRc, 2012	1	
		PNEC	CZ	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	IT	2	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	LU	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	FR	20	INERIS, 2014		
		EQS	BE	20	RBSP-ECOSTAT, UBA (2014)		
		EQS	FI	20	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	250	RBSP-ECOSTAT, UBA (2014)		
		PNEC	ECHA	20	ECHA DOSSIER		
		PNEC	-	20	Von der Ohe, 2011		
		PNEC	-	20	EU RAR 2004		
106-47-8	4-Chloroaniline	EQS	DE	0.05	RBSP-ECOSTAT, UBA (2014)	0.05	
		EQS	LU	0.05	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	0.05	RBSP-ECOSTAT, UBA (2014)		
		EQS	FR	1	INERIS, 2011		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
		EQS	BE	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	IT	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	0.22	NL Specific Pollutants		
		PNEC	-	1	Von der Ohe, 2011		
106-48-9	4-Chlorophenol	EQS	IT	2	RBSP-ECOSTAT, UBA (2014)	2	
		PNEC	CZ	3.2	RBSP-ECOSTAT, UBA (2014)		
		EQS	FR	4	INERIS, 2011		
		EQS	DE	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	16	RBSP-ECOSTAT, UBA (2014)		
		EQS	BE	20	RBSP-ECOSTAT, UBA (2014)		
1066-51-9	Aminomethylphosphonic acid (AMPA)	PNEC	-	540	Substance factsheet (2015)	540	Substance ranking high during the last prioritisation exercise. WFD compliant, updated in the AMPA working group under the SG-R (2015)
106-89-8	Epichlorhydrin (1-Chloro-2,3-epoxypropane)	EQS	NL	0.65	RBSP-ECOSTAT, UBA (2014)	0.65	
		EQS	FR	1.3	INERIS, 2012		
		EQS	BE	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	SI	12	RBSP-ECOSTAT, UBA (2014)		
		PNEC	ECHA	10.6	ECHA DOSSIER		
		PNEC	-	1.3	Von der Ohe, 2011		
106-93-4	1,2-Dibromoethane	EQS	DK	0.002	RBSP-ECOSTAT, UBA (2014)	0.002	
		EQS	NL	0.003	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	2	RBSP-ECOSTAT, UBA (2014)		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
		EQS	RO	2	RBSP-ECOSTAT, UBA (2014)		
		EQS	BE	50	RBSP-ECOSTAT, UBA (2014)		
		PNEC	ECHA	58.1	ECHA DOSSIER		
1071-83-6	Glyphosate	PNEC	-	56	Substance factsheet (2015)	56	Substance ranking high during the last prioritisation exercise. WFD compliant, updated in the Glyphosate working group under the SG-R (2015)
107534-96-3	Tebuconazole	PNEC		0.578	UBA (DE) Communication	0.578	**DE:** RAC 0.578 µg/l, AF10 using UBA ICS data; https://webetox.uba.de/webETOX/public/basics/literatur.do?id=2645
		EQS	FR	1	INERIS, 2013		
		EQS	CH	1.2	Swiss ECOTOX Centre		
		PNEC	DK	1	EU_REPO_2013		
108-41-8	3-Chlorotoluene	EQS	IT	1	RBSP-ECOSTAT, UBA (2014)	1	
		EQS	BE	3	RBSP-ECOSTAT, UBA (2014)		
		EQS	FR	8	INERIS, 2011		
		EQS	DE	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	310	RBSP-ECOSTAT, UBA (2014)		
108-42-9	3-Chloroaniline	EQS	NL	0.41	RBSP-ECOSTAT, UBA (2014)	0.41	
		EQS	RO	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	FR	1.3	INERIS, 2011		
		EQS	IT	2	RBSP-ECOSTAT, UBA (2014)		
		PNEC	-	1.3	Von der Ohe, 2011		
		PNEC	ECHA	2.94	ECHA DOSSIER		
108-43-0	3-Chlorophenol	EQS	IT	2	RBSP-ECOSTAT, UBA (2014)	2	

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
		EQS	FR	4	INERIS, 2011		
		EQS	NL	4	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	BE	20	RBSP-ECOSTAT, UBA (2014)		
		PNEC	CZ	3.47	RBSP-ECOSTAT, UBA (2014)		
1085-98-9	Dichlofluanid	PNEC		0.26	Substance factsheet (2015)	0.26	Substance ranking high during the last prioritisation exercise. Updated in the Dichlofluanid working group under the SG-R (2015)
108-60-1	Dichloroisopropyl ether (Propane, 2,2'-oxybis 1-chloro-)	EQS	DE	10	RBSP-ECOSTAT, UBA (2014)	10	
		EQS	NL	10	RBSP-ECOSTAT, UBA (2014)		
108-67-8	1,3,5-Trimethylbenzene	EQS	SE	2	RBSP-ECOSTAT, UBA (2014)	2	
		PNEC	ECHA	101	ECHA DOSSIER		
108-88-3	Toluene	PNEC		74	Substance factsheet (2015)	74	Substance ranking high during the last prioritisation exercise
108-90-7	Chlorobenzene	EQS	CZ	1	RBSP-ECOSTAT, UBA (2014)	1	
		EQS	DE	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	IE	1.5	RBSP-ECOSTAT, UBA (2014)		
		EQS	IT	3	RBSP-ECOSTAT, UBA (2014)		
		EQS	BE	6	RBSP-ECOSTAT, UBA (2014)		
		EQS	FI	9.3	RBSP-ECOSTAT, UBA (2014)		
		EQS	ES	20	RBSP-ECOSTAT, UBA (2014)		
		EQS	FR	32	INERIS, 2014		
		EQS	NL	690	RBSP-ECOSTAT, UBA (2014)		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
		PNEC	ECHA	32	ECHA DOSSIER		
		PNEC		32	Von der Ohe, 2011		
108-95-2	Phenol	EQS	EE	1	RBSP-ECOSTAT, UBA (2014)	1	
		EQS	LT	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	IE	1.5	RBSP-ECOSTAT, UBA (2014)		
		EQS	CZ	3	RBSP-ECOSTAT, UBA (2014)		
		EQS	SI	7.7	RBSP-ECOSTAT, UBA (2014)		
		EQS	UK	7.7	RBSP-ECOSTAT, UBA (2014)		
		EQS	DK	7.7	RBSP-ECOSTAT, UBA (2014)		
		PNEC	ECHA	7.7	ECHA DOSSIER		
		PNEC	FR	7.7	EU RAR 2006 (final report, revised edition)		
		PNEC	-	7.7	Von der Ohe, 2011		
110488-70-5	Dimethomorph	EQS	FR	5.6	INERIS, 2014	5.6	**DE:** Lowest 60d *O. mykiss* (ELS) = 56 µg/L; Datasheet for DE pEQS= 22 ug/L needs to be updated
1113-02-6	Omethoate	PNEC		0.00084	Substance factsheet (2015)	0.00084	Substance ranking high during the last prioritisation exercise. Updated in the Omethoate working group under the SG-R (2015). **Cheminova A/S:** Proposed PNEC value: 0.01 µg/L. A proposal for an updated omethoate PNEC value is taking into account relevant new studies, including a new chronic Daphnia study (details under comment no. 91 in the List of comments).
111988-49-9	Thiacloprid	EQS	CH	0.01	Swiss ECOTOX Centre	0.01	**NL:** Value WFD compliant for compounds that are not RBSP but relevant for water quality policy
		PNEC	-	0.01	RIVM (NL)		**DE:** Proposed RAC 0,004 µg/l, based on NOEC aquatic Insects 0,013 µg/l AF=3
		RAC		0.004	UBA (DE)		
		PNEC	-	0.05	Watch list report		
		PNEC	UK	0.05	EU_REPO_2008		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
111991-09-4	Nicosulfuron	EQS	CH	0.035	Swiss ECOTOX Centre		**Du Pont:** Currently there is a Task Force (all data to be used from several companies) established for the resubmission of the active substance nicosulfuron for Annex I renewal (EU reregistration, to be submitted in July 2016). Using the complete set of studies now available it is proposed that the appropriate value for the PNEC based on the lowest end point of yield frond number, frond area is 0.172 µg /L. If however the higher tier microcosm study is included in the derivation of the EQS then a PNEC of 0.67 µg /L is proposed.
		EQS	FR	0.035	INERIS, 2014		
		EQS	DE	0.0087	UBA, DE	0.0087	**DE:** AA-EQS derived by Wenzel 2014 [UBA-FB 002062 and TEXTE 47/2015]; https://webetox.uba.de/webETOX/public/basics/literatur.do?id=24229
114-26-1	Propoxur	EQS	NL	0.01	NL Specific Pollutants	0.01	**DE:** PNEC 0.01 µg/L, NL Specific Pollutants - review of PNEC needed
115-86-6	Triphenyl phosphate (TPT)	EQS	DK	0.74	RBSP-ECOSTAT, UBA (2014)	3.7	
		PNEC	ECHA	3.7	ECHA DOSSIER		
		EQS	DE	3.7	UBA, DE		**DE:** AA-EQS derived by Wenzel 2014 UBA-FB 002062 and TEXTE 47/2015; https://webetox.uba.de/webETOX/public/basics/literatur.do?id=24358.
115-96-8	Tris(2-chloroethyl)phosphate (TCEP)	QN-V	DE	4	ETOX database(UBA, DE)	4	**DE:** QN-V, Aquatic life annual average, Jahnel, 2004. https://webetox.uba.de/webETOX/public/basics/literatur.do?id=2207
		PNEC	-	65	DRAFT RAR		https://webetox.uba.de/webETOX/public/basics/literatur.do?id=6648
116-06-3	Aldicarb	PNEC_st	FR	0.08	Pesticide Ecotoxicity Database, US-EPA	0.08	PNEC short-term based on Chironomus
116-29-0	Tetradifon	PNEC	-	0.11	JRC derivation (ECOTOX US EPA-dataset)	0.11	
1163-19-5	Decabromodiphenyl ether (BDE-209)	PNEC	Japan	0.046	Profiles of the initial ERA Japan	0.046	https://www.env.go.jp/en/chemi/chemicals/profile_erac/profile5/pf2-04.pdf

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
117428-22-5	Picoxystrobin	PNEC	-	0.8	ETOX database(UBA, DE)	0.8	**DE:** PNEC based on data in UBA ICS internal database. PNEC fw Daphnia magna NOEC 8 µg/L AF10; Lowest acute 4-d LC50, *O. mykiss* = 60 µg/L
117-84-0	Di-n-octyl phthalate	PNEC	-	19.793	JRC derivation (ECOTOX US EPA-dataset)	19.793	**DE:** PNEC is above the aqueous solubility of this substance is 0.02 mg/L (25°C)
118134-30-8	Spiroxamine	PNEC	-	0.02	JRC derivation (EFSA dossier)	0.02	
119446-68-3	Difenoconazole	EQS	FR	0.6	INERIS, 2013	0.6	**DE:** Lowest NOEC-FLC *Pimephales promelas* = 3,6 µg/L.
1194-65-6	Dichlobenil	PNEC	-	0.63	RIVM, NL	0.63	**NL:** Where NL PNEC is added, this refers to officially set indicative value. Secondary poisoning and human fish comsumption were not addressed. Most likely not critical.
		PNEC	ECHA	1.9	ECHA DOSSIER		
120-32-1	Chlorophene	pPNEC		0.59	NORMAN factsheet	0.59	
120-36-5	Dichlorprop	EQS	CZ	0.1	RBSP-ECOSTAT, UBA (2014)	0.1	
		EQS	DE	0.1	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	0.1	RBSP-ECOSTAT, UBA (2014)		
		EQS	FR	1.6	INERIS, 2012		
		EQS	SE	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	BE	20	RBSP-ECOSTAT, UBA (2014)		
		PNEC		1.3	Von der Ohe, 2011		
120-83-2	2,4-Dichlorophenol	EQS	NL	0.54	RBSP-ECOSTAT, UBA (2014)	0.54	
		EQS	IT	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	AT	2	RBSP-ECOSTAT, UBA (2014)		
		EQS	CZ	5	RBSP-ECOSTAT, UBA (2014)		
		EQS	FR	10	INERIS, 2012		
		EQS	DE	10	RBSP-ECOSTAT, UBA (2014)		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
		EQS	RO	10	RBSP-ECOSTAT, UBA (2014)		
		PNEC	UK	20	RBSP-ECOSTAT, UBA (2014)		
		EQS	BE	20	RBSP-ECOSTAT, UBA (2014)		
120923-37-7	Amidosulfuron	PNEC	-	0.18	Swedish Chemicals Agency, 2008	0.18	
121-14-2	2,4-Dinitrotoluene	PNEC	INERIS	2	EU RAR 2008 (Final report)	2	
		PNEC	-	2	Von der Ohe, 2011		
		PNEC	-	2	ETOX UBA, DE		
121552-61-2	Cyprodinil	EQS	FR	0.03	INERIS, 2014		
		EQS	NL	0.16	RIVM, 2016	0.16	
		EQS	CH	0.43	Swiss ECOTOX Centre		
		PNEC	-	1.15	EFSA 2006 Opinion of Scientific Panel		
		PNEC	-	1.2	Von der Ohe, 2011		
121-73-3	1-Cloro-4-nitrobenzene	EQS	NL	0.55	RBSP-ECOSTAT, UBA (2014)	0.55	
		EQS	DE	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	IT	1	RBSP-ECOSTAT, UBA (2014)		
		PNEC	CZ	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	BE	3	RBSP-ECOSTAT, UBA (2014)		
		EQS	FR	3.2	INERIS, 2012		
		PNEC	-	3.2	Von der Ohe, 2011		
121-75-5	Malathion	EQS	RO	0.0002	RBSP-ECOSTAT, UBA (2014)	0.0002	**Cheminova A/S:** A proposed PNEC value is 0.006 µg/L, taking into account relevant FMC/Cheminova GLP studies. It shall be mentioned that the data behind the selected current value in the JRC report could not be taken into account since we do not have the source of this information. (details under comment no. 93 in the List of comments)

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
							DE: PNEC 0.0002 µg/L need to be checked/should be reviewed
		EQS	BE	0.0008	RBSP-ECOSTAT, UBA (2014)		
		EQS	FR	0.006	INERIS, 2011		
		EQS	UK	0.01	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	0.013	NL Specific Pollutants		
		EQS	CZ	0.01	RBSP-ECOSTAT, UBA (2014)		
		EQS	IT	0.01	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	0.02	RBSP-ECOSTAT, UBA (2014)		
		PNEC		0.006	Von der Ohe, 2011		
122-14-5	Fenitrothion	EQS	BE	0.0009	RBSP-ECOSTAT, UBA (2014)		**DE:** PNEC value need to be checked, tenfold lower compared to other values
		EQS	LU	0.001	RBSP-ECOSTAT, UBA (2014)		
		EQS	FR	0.0087	INERIS, 2014		
		EQS	DE	0.009	RBSP-ECOSTAT, UBA (2014)	0.009	
		EQS	NL	0.009	NL Specific Pollutants		
		EQS	CZ	0.01	RBSP-ECOSTAT, UBA (2014)		
		EQS	IT	0.01	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	0.02	RBSP-ECOSTAT, UBA (2014)		
		EQS	UK	0.01	RBSP-ECOSTAT, UBA (2014)		
		PNEC		0.0087	Von der Ohe, 2011		
122-39-4	Diphenylamine	EQS	SK	1.6	RBSP-ECOSTAT, UBA (2014)	1.6	
122931-48-0	Rimsulfuron	EQS	FR	0.009	INERIS, 2014		**DuPont:** proposed EQS=PNEC =0.1 µg/L
		PNEC	JRC	0.012	JRC	0.012	
123-91-1	1,4-Dioxane	PNEC	ECHA	10000	ECHA DOSSIER	10000	
124-48-1	Dibromochloromethane	PNEC	Japan	0.63	Profiles of the initial ERA (Japan)	0.63	https://www.env.go.jp/en/chemi/chemicals/profile_erac/profile7/pf1-05.pdf

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
126535-15-7	Triflusulfuron-methyl	EQS	NL	0.13	RIVM, 2016	0.13	**NL:** Lowest endpoint 1.3 µg/L for macrophyte
		PNEC	-	110	JRC derivation based on EFSA dossier		
126-71-6	Triisobutyl phosphate	PNEC	ECHA	11	ECHA DOSSIER	11	
		EQS	DE	11	RIVM, 2005		https://webetox.uba.de/webETOX/public/basics/literatur.do?id=2207.
126-73-8	Tributyl phosphate	EQS	NL	66	NL Specific Pollutants		
		EQS	FR	82	INERIS, 2013		
		EQS	BE	40	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	DK	82	RBSP-ECOSTAT, UBA (2014)		
		EQS	LU	0.1	RBSP-ECOSTAT, UBA (2014)	0.1	**DE:** Derivation LU EQS=0.1 ug/L should be checked. ECHA Website PNEC Freshwater 35 - 82 µg/L
		PNEC	ECHA	82	ECHA DOSSIER		
		PNEC		82	Von der Ohe, 2011		
126833-17-8	Fenhexamid	PNEC		1.01	JRC derivation (ECOTOX US EPA database)	1	
127-18-4	Tetrachloroethene	EQS	CZ	10	RBSP-ECOSTAT, UBA (2014)	10	
		EQS	DK	10	RBSP-ECOSTAT, UBA (2014)		
		PNEC	ECHA	51	ECHA DOSSIER		
		PNEC	INERIS	51	EU RAR 2005 (final draft)		
		PNEC		10	Von der Ohe, 2011		
128639-02-1	Carfentrazone-ethyl	PNEC	ETOX	0.092	UBA (DE)	0.092	PNEC derived for the purpose of the prioritisation exercise only. Personal communication Dieter Schudoma (UBA): PNEC fw, *L. gibba* NOEC 0.92 µg/l AF10
129-00-0	Pyrene	EQS	BE	0.04	RBSP-ECOSTAT, UBA (2014)		**DE:** PNEC 0.0023 µg/L should be reviewed

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
		EQS	CZ	0.024	RBSP-ECOSTAT, UBA (2014)		
		EQS	DK	0.0046	RBSP-ECOSTAT, UBA (2014)		
		PNEC		0.023	Verbruggen et al. 2008		
		EQS	DE	0.0023	UBA, DE	0.0023	**DE:** MAC-EQS=0.023 µg/L; https://webetox.uba.de/webETOX/public/basics/literatur.do?id=6668
131-11-3	Dimethyl phthalate	PNEC	ECHA	192	ECHA DOSSIER	192	
131341-86-1	Fludioxonil	PNEC		0.5	JRC	0.5	JRC derivation based on EFSA report, updated with additional study for algae (Hoberg 1992 CGA 173506/02438 and supplement CGA 173605/6950, reported by Mick Hamer, Syngenta) leading to three trophic levels: AF 10
131860-33-8	Azoxystrobin	EQS	CH	0.2	Swiss ECOTOX Centre	0.2	
		EQS	FR	0.95	INERIS, 2014		
131983-72-7	Triticonazole	PNEC	BASF	1	Proposed PNEC received from BASF on 2015/07	1	
1330-20-7	Xylene (mixed isomers)	EQS	FR	1.3	INERIS, 2014		
	p-Xylene 106-42-3	EQS	AT	10	RBSP-ECOSTAT, UBA (2014)		
	o-Xylene 95-47-6	EQS	BE	4	RBSP-ECOSTAT, UBA (2014)		
	m-Xylene 108-38-3	EQS	DK	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	ES	30	RBSP-ECOSTAT, UBA (2014)		
		EQS	IE	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	IT	5	RBSP-ECOSTAT, UBA (2014)		
		EQS	LU	2	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	2.4	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	33	RBSP-ECOSTAT, UBA (2014)		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
		EQS	SK	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	SI	185	RBSP-ECOSTAT, UBA (2014)		
		EQS	UK	30	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	17.2	NL	17.2	http://www.rivm.nl/Documenten_en_publicaties/Wetenschappelijk/Rapporten/2015/januari/Environmental_risk_limits_for_xylenes_Update_of_the_2009_report
		PNEC	ECHA	327	ECHA DOSSIER		**CEFIC:** The value from REACH should be taken instead
133-06-2	Captan	EQS	NL	0.34	NL Specific Pollutants	0.34	
		PNEC	INERIS	1.65	RED, US-EPA 2004		**ADAMA:** Endpoint and AF should consider the entire and updated data basis submitted under Reg. 1107/2009 in 2016
133-07-3	Folpet	PNEC	INERIS	0.0881	Pesticide Ecotoxicity Database, US-EPA	0.0881	
							ADAMA: Endpoint and AF should consider the entire and updated data basis submitted under Reg. 1107/2009 in 2016
1330-78-5	Tricresyl Phosphate	PNEC	ECHA	1	ECHA DOSSIER		
		EQS	NL	0.033	RIVM, 2005	0.033	**NL:** PNEC from registration dossiers are only containing direct toxicity. RIVM derived an EQS for TCP 0f 0.033 µg/L
1336-36-3	PCB-sum (Polychlorinated biphenyls)	EQS	CZ	0.007		0.007	
		EQS	SK	0.01			
		EQS	EE	0.5			
133855-98-8	Epoxiconazole	EQS	FR	0.18	INERIS, 2014	0.18	
		EQS	CZ	0.4	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	0.2	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	0.19	RIVM, 2016		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
134-62-3	Diethyltoluamide (DEET)	EQS	CH	41	Swiss ECOTOX Centre	41	
		pEQS	DE	71.3	UBA, DE		**DE:** https://webetox.uba.de/webETOX/public/basics/literatur.do?id=2645
13674-84-5	Tris(1-chloro-2-propyl) phosphate (TCPP)	EQS	DK	640	RBSP-ECOSTAT, UBA (2014)	640	
13674-87-8	Tris(1,3-dichloropropyl) phosphate (TDCPP)	PNEC	ECHA	10	ECHA DOSSIER	10	
138261-41-3	Imidacloprid	EQS	NL	0.0083	NL Specific Pollutants	0.0083	**NL:** SSD method is preferred over deterministic method in EQS setting. We propose to use 0.0083 instead of 0.0024 µg/L
		EQS	CH	0.013	Swiss ECOTOX Centre		
		EQS	FR	0.2	INERIS, 2013		
		PNEC		0.009	JRC Watch list		**Bayer Cropscience:** Proposed PNEC of 0.128 µg/L based on mesocosm study.
		QSfw eco	ETOX	0.0024	ETOX, UBA		**DE:** DE AA-EQS=0.0024 ug/L. Value is lower than EFSA conclusion RAC = 0,009 µg/L.
13684-56-5	Desmedipham	EQS	SK	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	0.13		0.13	
13684-63-4	Phenmedipham	PNEC		113	JRC derivation (ECOTOX US EPA database)	113	
136-85-6	5-Methyl-1H-benzotriazole	PNEC	LfU Bayern	150	ETOX database	150	
139-13-9	Nitrilotriacetic acid	EQS	AT	50	RBSP-ECOSTAT, UBA (2014)	5	
		EQS	CZ	5	RBSP-ECOSTAT, UBA (2014)		
		EQS	CH	190	Swiss ECOTOX Centre		
		PNEC	INERIS	5	ECOTOX US EPA		
		PNEC	ECHA	690	ECHA DOSSIER		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
139-40-2	Propazine	EQS	BG	0.25	RBSP-ECOSTAT, UBA (2014)	0.25	
		PNEC	CZ	11	RBSP-ECOSTAT, UBA (2014)		
141517-21-7	Trifloxystrobin	PNEC		0.57	JRC derivation (ECOTOX US EPA database)		
		EQS	NL	0.27	RIVM, 2016	0.27	https://rvs.rivm.nl/zoeksysteem/stof/detail/1294
141776-32-1	Sulfosulfuron	EQS	SE	0.05	RBSP-ECOSTAT, UBA (2014)	0.05	
142-28-9	1,3-Dichloropropane			2	Japan quality standard for water	2	
142459-58-3	Flufenacet	PNEC	JRC	0.00245	JRC derivation (ECOTOX US EPA database)		
		EQS	DE	0.04	UBA	0.04	
		EQS	NL	0.137	RIVM		
143390-89-0	Kresoxim-methyl	PNEC	JRC	0.81	JRC derivation based on EFSA dossier		
		EQS	NL	0.63	RIVM, 2016	0.63	
144550-36-7	Iodosulfuron	PNEC	ETOX	0.04	UBA (DE) PNEC fw *L. gibba* NOEC 0.4 µg/l AF10	0.04	PNEC derived for the purpose of the prioritisation exercise only. Personal communication Dieter Schudoma (UBA)
145701-23-1	Florasulam	PNEC	JRC	0.0126	EFSA conclusions	0.0126	
1461-25-2	Tetrabutyltin	EQS	BE	0.12	RBSP-ECOSTAT		
		EQS	RO	0.001	RBSP-ECOSTAT		
		EQS	NL	1.6	RBSP-ECOSTAT		
		EQS	DE	0.14	DE RBSP-ECOSTAT OGewV	0.14	https://webetox.uba.de/webETOX/public/basics/literatur.do?id=24362
14797-65-0	Nitrite (NO2)	EQS	AT	10-300	RBSP-ECOSTAT, UBA (2014)		**DE:** PNEC 6 µg/l need to be reviewed
		EQS	CYP	9.8	RBSP-ECOSTAT, UBA (2014)		
		EQS	LU	300	RBSP-ECOSTAT, UBA (2014)		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
		PNEC	FR	6	ECOTOX database, US-EPA	6	
14816-18-3	Phoxim	EQS	FR	1	INERIS, 2012	0.008	
		EQS	BE	0.02	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	0.008	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	0.082	RBSP-ECOSTAT, UBA (2014)		
		PNEC		0.0005	Von der Ohe, 2011		
150-68-5	Monuron	PNEC		0.0065	JRC derivation (ECOTOX US EPA database)	0.0065	
152019-73-3	Metolachlor OA	PNEC		0.2		0.2	
15299-99-7	Napropamide	EQS	CH	5.12	Swiss ECOTOX Centre	5.1	
		PNEC	FR	5.12	DAR, EFSA 2006		
		PNEC		5.1	Von der Ohe, 2011		
15307-86-5	Diclofenac	PNEC		0.05	Substance factsheet (2015)	0.05	Substance ranking high during the last prioritisation exercise
153719-23-4	Thiamethoxam	EQS	CH	1	Swiss ECOTOX Centre		JRC Watch list report
		PNEC		0.14	JRC derivation from EU_REPO_2012		**DE:** Proposed RAC 0,043 µg/L, based on estimated HC5- EC10 for aquatic Insects 0,13 µg/L , AF=3 .
		EQS	NL	0.14	RIVM (2016)	0.14	
15545-48-9	Chlorotoluron	EQS	NL	0.4	NL Specific Pollutants		**ADAMA:** The EQS should be 10.6 µg/L based on SSD with 8 algal species and an AF of 3. Complete data set was submitted in April 2015 under Reg. 1107/2009.
		EQS	CH	0.6	Swiss ECOTOX Centre		
		EQS	FR	0.1	INERIS, 2013	0.1	
		EQS	CZ	0.4	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	0.4	RBSP-ECOSTAT, UBA (2014)		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
		EQS	LU	0.4	RBSP-ECOSTAT, UBA (2014)		
		EQS	SI	0.8	RBSP-ECOSTAT, UBA (2014)		
1563-66-2	Carbofuran	PNEC	FR	0.016	DAR, EFSA 2005	0.016	
15687-27-1	Ibuprofen	PNEC		0.3		0.3	**CH:** Oekotoxzentrum / Swiss Centre for Applied Ecotoxicology Most sensitive: based on Ji et al. 2013 21d reproduction endpoint PNEC= NOEC / AF = 0.1 µg /L / 10 = 10 ng/L Medium sensitive: Using our old SSD Approach from 2011 which includes the Han et al. 2010 90 d endpoint for mortality: PNEC = HC5/ AF = 1.2 microgramm /L / 4 = 300 ng/L Less sensitive: Using the from industry agreed Flippin et al.2007 endpoint: PNEC = NOEC / AF = 10 µg /L / 10 = 1000 ng/L
15950-66-0	2,3,4-Trichlorphenol	EQS	DE	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	LU	0.1	RBSP-ECOSTAT, UBA (2014)		
		PNEC	FR	0.6	British Columbia		
		EQS	NL	0.54	RIVM (2016)	0.54	
1610-18-0	Prometon	PNEC		1	JRC derivation (ECOTOX US EPA database)	1	
1634-04-4	Methyl-tert-butyl ether (MTBE)	EQS	DK	10	RBSP-ECOSTAT, UBA (2014)		
		PNEC	ECHA	5100	ECHA DOSSIER		**CEFIC:** the value from REACH should be chosen instead
		PNEC	FR	2600	EU RAR 2002 (final)	2600	http://echa.europa.eu/documents/10162/5602401f-1d75-4931-aa77-abd37d436dc9
		PNEC		2600	Von der Ohe, 2011		
1646-88-4	Aldicarb sulfone	PNEC		0.66	JRC derivation (ECOTOX US EPA database)	0.66	
16752-77-5	Methomyl	PNEC	FR	0.04	Pesticide Ecotoxicity Database, US-EPA	0.04	
		PNEC	JRC	0.16	JRC derivation from EFSA dossier		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
16887-00-6	Chloride	MPC	RIVM (NL)	94000	RIVM report 711701075/2008	94000	
1689-84-5	Bromoxynil	EQS	DE	0.5	RBSP-ECOSTAT, UBA (2014)	0.5	
		PNEC	INERIS	2.45	DG-SANCO 2004		
		PNEC		2.5	Von der Ohe, 2011		
16984-48-8	Fluoride	EQS	AT	1000	RBSP-ECOSTAT, UBA (2014)		
		EQS	BE	900	RBSP database WRc, 2012		
		EQS	CZ	800	RBSP-ECOSTAT, UBA (2014)		
		EQS	ES	1700	RBSP-ECOSTAT, UBA (2014)		
		EQS	IE	500	RBSP-ECOSTAT, UBA (2014)	500	
		EQS	NL	1500	RBSP-ECOSTAT, UBA (2014)		
		EQS	PL	1500	RBSP-ECOSTAT, UBA (2014)		
		EQS	SI	680	RBSP-ECOSTAT, UBA (2014)		
		PNEC	FR	400	EU RAR 2001 (final report)		
1698-60-8	Chloridazon	EQS	NL	27	NL Specific Pollutants		**BASF:** PNEC 10 µg/L, proposed based on lowest NOEC L. gibba 100 µg/L and 3 trophic levels, AF 10. Personal communication Anastasia Del Signore **NL:** Agree with BASF comment
		EQS	CH	10	Swiss ECOTOX Centre		
		EQS	FR	10	INERIS, 2012	10	
		EQS	BE	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	0.1	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	0.1	RBSP-ECOSTAT, UBA (2014)		
		EQS	SE	10	RBSP-ECOSTAT, UBA (2014)		
1702-17-6	Clopyralid	EQS	SK	70	RBSP-ECOSTAT, UBA (2014)	70	

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
17040-19-6	Demeton-S-methylsulfon	EQS	DE	0.1	RBSP-ECOSTAT, UBA (2014)	0.1	
171118-09-5	Metolachlor ethanesulfonic acid (ESA)			0.2	Chosen as equal to lowest QS for Metolachlor as RBSP (JRC)	0.2	
17254-80-7	Chloridazon methyl-desphenyl	EQS	CH	37	Swiss ECOTOX Centre	37	
173159-57-4	Foramsulfuron	PNEC	ETOX	0.036	UBA (DE) PNEC fw *L. gibba* NOEC 0.36 µg/l AF10	0.036	PNEC derived for the purpose of the prioritisation exercise only. Personal communication Dieter Schudoma (UBA)
1746-81-2	Monolinuron	EQS	NL	0.15	NL Specific Pollutants		
		EQS	FR	1	INERIS, 2012		
		EQS	BE	0.3	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	0.1	RBSP-ECOSTAT, UBA (2014)	0.1	
		EQS	RO	0.1	RBSP-ECOSTAT, UBA (2014)		
		PNEC		1	Von der Ohe, 2011		
175013-18-0	Pyraclostrobine	PNEC		0.24	PNEC proposed 0.24 µg/l BASF communication received 2015/07	0.24	
18691-97-9	Methabenzthiazuron	EQS	NL	1.8	NL Specific Pollutants		
		EQS	FR	0.033	INERIS, 2014	0.033	
		EQS	DE	2	RBSP-ECOSTAT, UBA (2014)		
188425-85-6	Boscalid	EQS	CH	11.6	Swiss ECOTOX Centre	11.6	
		EQS	FR	11.6	INERIS, 2014		
1897-45-6	Chlorothalonil	PNEC		0.06	Substance factsheet (2015)	0.06	Substance ranking high during the last prioritisation exercise. WFD compliant, updated in the Chlorothalonil Working Group under the SG-R (2015).

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
1918-00-9	Dicamba	EQS	CH	11	Swiss ECOTOX Centre		
		EQS	FR	0.5	INERIS, 2013	0.5	
19666-30-9	Oxadiazon	EQS	FR	0.088	INERIS, 2014	0.088	
		EQS		0.088	JRC Watch list report		
1982-47-4	Chloroxuron	PNEC_ st		0.0024	Von der Ohe, 2011	0.27	**DE:** Short-term PNEC. Values need to be reviewed before a final decision is made. Only acute data available. Proposed EQS to protect aquatic life is 0.27 µg/L (using AF 1000). Calculated bioconcentration factors of up to 485 and the log P value of 3.84 indicate that bioaccumulation and therefore a secondary intoxication is relevant.
19937-59-8	Metoxuron	PNEC_ st	FR	0.064	Agritox	0.064	
2008-58-4	2,6-Dichlorobenzamide	EQS	DK	78	RBSP-ECOSTAT, UBA (2014)	78	
2032-65-7	Methiocarb	EQS	UK	0.01	RBSP-ECOSTAT, UBA (2014)		
		PNEC	FR	0.01	EFSA 2006		
		EQS	NL	0.002	RIVM (2016)	0.002	
208-96-8	Acenaphthylene	EQS	BE	4	RBSP-ECOSTAT, UBA (2014)		
		EQS	DK	1.3	RBSP-ECOSTAT, UBA (2014)	1.3	
		EQS	RO	2.8	RBSP database WRc, 2012		
		PNEC	CZ	0.01	RBSP-ECOSTAT, UBA (2014)		
		PNEC	FR	1.3	EU RAR 2007 (draft)		
		PNEC		1.3	Von der Ohe, 2011		
21087-64-9	Metribuzin	EQS	CH	0.058	Swiss ECOTOX Centre		
		EQS	DE	0.2	RBSP-ECOSTAT, UBA (2014)		
		EQS	SE	0.08	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	0.12	RIVM (2016)	0.12	
210880-92-5	Clothianidin	PNEC		0.13	EU_REPO_2007	0.13	**DE**: Proposed RAC = 0,007 , AF = 3, NOEC aquatic insects 0,02 µg/L

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
2163-68-0	2-Hydroxyatrazine	EQS	JDS3	0.002	ECOSTAT 2013	0.002	**DE:** JDS3 (source?) PNEC need to be reviewed. Value not plausible. 2-Hydroxyatrazine is a metabolite Atrazine, which is regulated.
		EQS	DK	0.01	RBSP-ECOSTAT, UBA (2014)		
2164-08-1	Lenacil	QN-V	ETOX	1	ETOX database UBA	0.65	**DE:** PNEC derived for the purpose of the prioritisation exercise only. Proposed RAC 0,65 µg/L
21725-46-2	Cyanazine	EQS	SE	1	RBSP-ECOSTAT, UBA (2014)	1	
		PNEC	INERIS	0.012	Pesticide Ecotoxicity Database, US-EPA		
218-01-9	Chrysene	EQS	NL	0.0012	NL Specific Pollutants	0.0012	**DE:** 0.0012 µg/l Derivation? other value in RBSP (NL) http://wetten.overheid.nl/BWBR0027502/2015-11-19 PNEC should be reviewed **NL:** The value of NL EQS of 0.0029 µg/l (reported earlier) is for total concentration. Original value is 0.0012 µg/l
		EQS	BE	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	CZ	0.1	RBSP-ECOSTAT, UBA (2014)		
		EQS	DK	0.014	RBSP-ECOSTAT, UBA (2014)		
		PNEC		0.07	Verbruggen et al. 2008		
2212-67-1	Molinate	PNEC	INERIS	3.8	DG-SANCO 2000	3.8	
		PNEC		3.8	Von der Ohe, 2011		
22204-53-1	Naproxen	EQS	CH	1.7	Swiss ECOTOX Centre	1.7	
2303-17-5	Triallate	PNEC		0.41	Substance factsheet (2015)	0.41	Substance ranking high during the last prioritisation exercise. WFD compliant, updated in the Triallate working group under the SG-R (2015).
23103-98-2	Pirimicarb	EQS	NL	0.09	NL Specific Pollutants	0.09	
		EQS	CH	0.09	Swiss ECOTOX Centre		
		EQS	DE	0.09	RBSP-ECOSTAT, UBA (2014)		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
		EQS	SE	0.09	RBSP-ECOSTAT, UBA (2014)		
		PNEC	FR	0.6	EFSA 2005		
23135-22-0	Oxamyl	PNEC		0.536	JRC derivation from EFSA report	0.536	
2385-85-5	Mirex	QC AQL-FRESH	USA	0.001	ETOX, UBA	0.001	
23950-58-5	Propyzamide	PNEC	INERIS	8.2	DG-SANCO 2003	8.2	
		PNEC		8.2	Von der Ohe, 2011		
24017-47-8	Triazophos	EQS	NL	0.001	NL Specific Pollutants	0.001	
		EQS	BE	0.03	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	0.03	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	0.001	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	0.03	RBSP-ECOSTAT, UBA (2014)		
		PNEC	FR	0.032	International Commission for the Protection of the Rhine		
		PNEC		0.032	Von der Ohe, 2011		
24579-73-5	Propamocarb	EQS	CH	1030	ETOX, UBA	1030	
25057-89-0	Bentazone	PNEC		270	Substance factsheet (2015)	270	Substance ranking high during the last prioritisation exercise. WFD compliant, updated in the Bentazone working group under the SG-R (2015)
26225-79-6	Ethofumesate	EQS	CH	22	Swiss ECOTOX Centre		
		EQS	SK	6.4	RBSP-ECOSTAT, UBA (2014)	6.4	
		PNEC	FR	25	Pesticide Ecotoxicity Database, US-EPA		
		PNEC		25	Von der Ohe, 2011		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
2642-71-9	Azinphos-ethyl	EQS	NL	0.0011	NL Specific Pollutants	0.0011	
		EQS	BE	0.01	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	0.01	RBSP-ECOSTAT, UBA (2014)		
		EQS	IT	0.01	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	0.1	RBSP-ECOSTAT, UBA (2014)		
29122-68-7	Atenolol	EQS	CH	150	Swiss ECOTOX Centre	150	
29232-93-7	Pirimiphos-methyl	EQS	NL	0.0005	NL Specific Pollutants	0.005	**Syngenta:** Proposed PNEC = 0.005 µg/L; Extra data on chronic fish and algae study provided. AF 10 applied.
298-04-4	Disulfoton	EQS	BE	0.01	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	0.004	RBSP-ECOSTAT, UBA (2014)	0.004	
		EQS	NL	0.082	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	0.004	RBSP-ECOSTAT, UBA (2014)		
		PNEC	FR	0.0037	RED, US-EPA 2000		
		PNEC		0.0037	Von der Ohe, 2011		
298-46-4	Carbamazepine	PNEC		0.5	Substance factsheet (2015)	0.5	Substance ranking high during the last prioritisation exercise. WFD compliant, updated in the Carbamazepine working group under the SG-R (2015)
301-12-2	Oxydemeton-methyl	EQS	FR_NEW	0.56	INERIS, 2012	0.035	
		EQS	BE	0.4	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	0.1	RBSP-ECOSTAT, UBA (2014)		
		EQS	IT	0.5	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	0.035	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	0.1	RBSP-ECOSTAT, UBA (2014)		
		PNEC		0.56	Von der Ohe, 2011		
30125-63-4	Desethylterbuthylazine	EQS	JDS3	0.0024	RIVM, 2014	0.25	**Syngenta:** document sent, proposed PNEC 0.25 µg/L. **NL:** indicative value under revision; agree with proposed value Syngenta

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
302-17-0	Chloral hydrate	EQS	BE	500	RBSP-ECOSTAT, UBA (2014)	10	
		EQS	DE	10	RBSP-ECOSTAT, UBA (2014)		**DE:** 10 µg/L need to be reviewed (no datasheet available). No longer proposed as RBSP in DE.
		EQS	NL	500	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	10	RBSP-ECOSTAT, UBA (2014)		
3060-89-7	Metobromuron	PNEC_ st	INERIS	0.26	Agritox	0.26	
		PNEC_ st		0.26	Von der Ohe, 2011		
307-24-4	Perfluorohexanoic acid (PFHxA)	EQS	IT	140	Italian EQS Working Group, 2015	140	
314-40-9	Bromacil	EQS	JDS3	0.01	INERIS, 2013	0.01	
		EQS	DE	0.6	RBSP-ECOSTAT, UBA (2014)		
32809-16-8	Procymidone	EQS	FR	1.2	INERIS, 2014	1.2	
330-55-2	Linuron	EQS	NL	0.17	NL Specific Pollutants		
		EQS	CH	0.26	Swiss ECOTOX Centre		
		EQS	FR	1	INERIS, 2013		
		EQS	BE	0.3	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	0.1	RBSP-ECOSTAT, UBA (2014)	0.1	
		EQS	FR	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	IE	0.7	RBSP-ECOSTAT, UBA (2014)		
		EQS	IT	0.5	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	0.1	RBSP-ECOSTAT, UBA (2014)		
		EQS	UK	0.5	RBSP-ECOSTAT, UBA (2014)		
333-41-5	Diazinon	EQS	DE	0.01	ECOSTAT	0.01	
		EQS	IE	0.01	ECOSTAT		
		EQS	UK	0.01	ECOSTAT		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
		EQS	NL	0.037	EQS DUTCH SPECIFIC POLLUTANTS		
		EQS	CH	0.015	Swiss ecotox centre		
		PNEC	INERIS	0.017	EFSA 2006		
335-67-1	Perfluorooctanoic acid (PFOA)	EQS	IT	0.1	Italian EQS Working Group, 2015	0.1	
3380-34-5	Triclosan	PNEC		0.053	Substance factsheet (2015)	0.02	
		EQS	DE	0.02			https://webetox.uba.de/webETOX/public/search/ziel.do
		EQS	CH	0.02			
3397-62-4	Desisopropyldesethyl atrazine	EQS	DK	0.01	RBSP-ECOSTAT, UBA (2014)	0.01	
3424-82-6	DDE, o,p'	EQS	CZ	0.01	RBSP-ECOSTAT, UBA (2014)	0.01	
		EQS	LV	0.025	RBSP-ECOSTAT, UBA (2014)		
		PNEC	FR	0.03	COMMPS database		
		PNEC_ st		0.03	Von der Ohe, 2011		
34256-82-1	Acetochlor	EQS	FR	0.013	INERIS, 2014	0.013	**Monsanto:** proposed a PNEC 1.4 µg/l based on SSD approach
		EQS	CZ	0.4	RBSP-ECOSTAT, UBA (2014)		
35367-38-5	Diflubenzuron	PNEC		0.004	EU_REPO_2012 0.004		
35554-44-0	Imazalil	PNEC		0.8	JRC derivation from EFSA report	0.8	
		PNEC_ st	INERIS	0.87	FOOTPRINT Database		
36734-19-7	Iprodione	PNEC	INERIS	0.35	RED, US-EPA 1998	0.35	**BASF:** proposed PNEC 5.4 µg/l based on a geomean of 3 NOEC, then using AF 3

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
37350-58-6	Metoprolol	EQS	CH	64	Swiss ECOTOX Centre		**DE:** https://webetox.uba.de/webETOX/public/basics/literatur.do?id=24268.
		EQS	NL	62	RIVM, 2016	62	
375-73-5	Perfluorobutane sulfonic acid (PFBS)	EQS	IT	372	Italian EQS Working Group, 2015	372	
40487-42-1	Pendimethalin	EQS	DK	0.01	RBSP-ECOSTAT, UBA (2014)		**DE:** The PNEC of 0,01 µg/L (DK) may overestimate the risk. Lowest NOEC's algae and fish are 3 µg/L and 6,3 µg/L **BASF:** proposed PNEC 0.7 µg/L based on mesocosm data
		EQS	SK	0.3	RBSP-ECOSTAT, UBA (2014)		
		EQS	SI	0.3	RBSP-ECOSTAT, UBA (2014)		
		EQS	UK	0.3	RBSP-ECOSTAT, UBA (2014)		
		PNEC	INERIS	0.07	Pesticide Ecotoxicity Database, US-EPA		
		EQS	NL	0.018	RIVM (2015)	0.018	http://www.rivm.nl/bibliotheek/rapporten/2015-0124.pdf
41394-05-2	Metamitron	EQS	CH	4	Swiss ECOTOX Centre	4	
		EQS	FR	4	INERIS, 2014		
		EQS	FI	32	RBSP-ECOSTAT, UBA (2014)		
		EQS	SE	10	RBSP-ECOSTAT, UBA (2014)		
		PNEC		3.8	Von der Ohe, 2011		
41859-67-0	Bezafibrate	EQS	CH	0.46	Swiss ECOTOX Centre	0.46	
		EQS	DE	2.3	UBA (DE)		**DE:** https://webetox.uba.de/webETOX/public/basics/literatur.do?id=24265

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
43121-43-3	Triadimefon	PNEC	INERIS	4.1	RED, US-EPA 2006	4.1	
439-14-5	Diazepam	PNEC		0.291	JRC derivation from ECOTOX US EPA	0.291	
50-00-0	Formaldehyde	EQS	FR	10.2	INERIS, 2015	10.2	
		EQS	DK	9.2	RBSP-ECOSTAT, UBA (2014)		
		EQS	PL	50	RBSP-ECOSTAT, UBA (2014)		
		EQS	SK	5	RBSP-ECOSTAT, UBA (2014)		**Cefic:** 5 µg/L value is ± 90 times lower than the PNEC value included in the REACH registration dossier of formaldehyde (440 µg/l)
		EQS	SI	130	RBSP-ECOSTAT, UBA (2014)		
50-28-2	17-beta-Estradiol	PNEC		4.00E-04	Substance factsheet (2015)	4.00E-04	Substance ranking high during the last prioritisation exercise
50471-44-8	Vinclozolin	PNEC	INERIS	1.2	Pesticide Ecotoxicity Database, US-EPA	1.2	
51218-45-2	Metolachlor	EQS	NL	0.4	NL Specific Pollutants	0.91	**Syngenta:** The STE exercise used a PNEC of 0.1 µg/L but it is not clear how this PNEC was derived. Syngenta evaluated the available data and derived: using the default AF of 5 an AA-EQS of 0.91 µg/L, and using an AF of 3, based on the fact that the most sensitive group is covered gives an AA-EQS of 1.51 µg/L. Both values are well above the 0.1 µg/l used in the original STE assessment.
	S-Metolachlor 87392-12-9	EQS	DE	0.2	RBSP-ECOSTAT, UBA (2014)		
		EQS	ES	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	LU	0.1	RBSP-ECOSTAT, UBA (2014)		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
		EQS	SI	0.27	RBSP database WRc, 2012		
		PNEC	CZ	0.2	RBSP-ECOSTAT, UBA (2014)		
		PNEC	INERIS	0.07	Pesticide Ecotoxicity Database, US-EPA		
51235-04-2	Hexazinone	EQS	CZ	0.048	RBSP-ECOSTAT, UBA (2014)	0.048	
		EQS	DE	0.07	RBSP-ECOSTAT, UBA (2014)		
		PNEC	INERIS	0.4	Pesticide Ecotoxicity Database, US-EPA		
525-66-6	Propranolol	PNEC	JRC	0.411	JRC derivation from ECOTOX US EPA	0.411	
52645-53-1	Permethrin	EQS	UK	0.0015	WFD UK Specific Pollutant	0.0015	
52-68-6	Trichlorfon	PNEC		0.00057	Substance factsheet (2015)	0.00057	
52888-80-9	Prosulfocarb	EQS	FR	0.5	INERIS, 2014	0.5	
		EQS	DK	0.01	RBSP-ECOSTAT, UBA (2014)		**DE:** Derivation should be check by DK. **Syngenta:** the DK RBSP value of 0.01 µg/L does not seem to be eco-base and we proposed the INERIS value of 0.5 µg/L.
52918-63-5	Deltamethrin	EQS	NL	0.0000031	NL Specific Pollutants	0.0000031	**Bayer Cropscience:** proposed PNEC of 0.7 ng/L based on SSDs and chronic exposure. JRC: **NL:** had a stringent quality assessment in EQS derivation (http://www.rivm.nl/bibliotheek/rapporten/601716015.pdf) and the test with *Gammarus fusciatus* passed these criteria. The assessment factor is according to the TGD and EQS guidance.

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
		PNEC	INERIS	0.0001	Pesticide Ecotoxicity Database, US-EPA		
		PNEC		0.0007	EU_REPO_2011		
53112-28-0	Pyrimethanil	EQS	CH	6	Swiss ECOTOX Centre	2	
		EQS	FR	2	INERIS, 2014		
53-16-7	Estrone	PNEC		0.0036	Swiss ECOTOX centre proposal	0.0036	
53-19-0	DDD, o,p'	PNEC	INERIS	0.00064	COMMPS database	0.00064	
534-52-1	Dinitro-o-cresol (DNOC)	EQS	DK	0.01	RBSP-ECOSTAT, UBA (2014)		
		PNEC	INERIS	1	ECOTOX database, US-EPA		
		PNEC		1	Von der Ohe, 2011		
		EQS	NL	9	RIVM (2016)	9	
53-70-3	Dibenz(a,h)anthracene	EQS	BE	0.5	RBSP-ECOSTAT, UBA (2014)		
		EQS	CZ	0.016	RBSP-ECOSTAT, UBA (2014)		
		EQS	DK	0.0014	RBSP-ECOSTAT, UBA (2014)	0.0014	
		PNEC	INERIS	0.0014	EU RAR 2007 (draft)		
		PNEC		0.0014	Verbruggen et al. 2008		
540-59-0	1,2-Dichloroethene	EQS	AT	10	RBSP-ECOSTAT, UBA (2014)		
	cis-1,2-Dichloroethylene	EQS	BE	10	RBSP-ECOSTAT, UBA (2014)		
	156-59-2	EQS	DE	10	RBSP-ECOSTAT, UBA (2014)		
	trans-1,2-Dichloroethylene	EQS	DK	6.8	RBSP-ECOSTAT, UBA (2014)		
	156-60-5	EQS	NL	6.8	RBSP-ECOSTAT, UBA (2014)	6.8	

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
		EQS	RO	10	RBSP-ECOSTAT, UBA (2014)		
541-73-1	1,3-Dichlorobenzene	EQS	FR	6	INERIS, 2012		
		EQS	BE	20	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	IT	2	RBSP-ECOSTAT, UBA (2014)	2	
		EQS	NL	250	RBSP-ECOSTAT, UBA (2014)		
		PNEC	CZ	0.1	RBSP-ECOSTAT, UBA (2014)		
		PNEC		6	Von der Ohe, 2011		
542-75-6	cis-1,3-Dichloropropene	EQS	FR	1.6	INERIS, 2012	1.5	**Dow AgroSciences:** the PNEC value for 1,3 dichloropropene should be 1.5 µg/L. This is based on an AF of 10 applied to the lowest NOEC where chronic data from three trophic levels is available (cf. TGD 2003)
	10061-01-5	EQS	BE	2	RBSP-ECOSTAT, UBA (2014)		
	trans-1,3-Dichloropropene	EQS	DE	10	RBSP-ECOSTAT, UBA (2014)		
	10061-02-6	EQS	NL	0.18	RBSP database WRc, 2012		
		EQS	RO	10	RBSP-ECOSTAT, UBA (2014)		
55179-31-2	Bitertanol	PNEC		0.152	JRC derivation from EFSA report	0.152	
55219-65-3	Triadimenol	PNEC	FR	2	EFSA 2008	2	
55335-06-3	Triclopyr	EQS	FR	700	INERIS, 2014	700	
		PNEC		3.3	DAR, EFSA 2005		
55-38-9	Fenthion	EQS	NL	0.003	NL Specific Pollutants		
		EQS	BE	0.0002	RBSP-ECOSTAT, UBA (2014)	0.0002	**DE:** Check, derivation and value: BE 0.0002 µg/l RBSP-ECOSTAT, UBA (2014) 0.0002 µg/l
		EQS	CZ	0.01	RBSP-ECOSTAT, UBA (2014)		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
		EQS	DE	0.004	RBSP-ECOSTAT, UBA (2014)		
		EQS	IT	0.01	RBSP-ECOSTAT, UBA (2014)		
		EQS	LU	0.004	RBSP-ECOSTAT, UBA (2014)		
		PNEC		0.0013	Von der Ohe, 2011		
5598-13-0	Chlorpyriphos methyl	PNEC	INERIS	0.001	DG-SANCO 2005	0.001	
		PNEC		0.001	Von der Ohe, 2011		
563-12-2	Ethion	PNEC_ st	INERIS	0.0005 6	Pesticide Ecotoxicity Database, US-EPA	0.00056	
		PNEC_ st		0.0005 6	Von der Ohe, 2011		
56-38-2	Parathion	EQS	NL	0.005	NL Specific Pollutants	0.0002	**DE**: PNEC 0.0002 µg/l need to be reviewed
	Parathion-methyl 298-00-0	EQS	BE	0.0002	RBSP-ECOSTAT, UBA (2014)		
		EQS	CZ	0.002	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	0.005	RBSP-ECOSTAT, UBA (2014)		
		EQS	IT	0.01	RBSP-ECOSTAT, UBA (2014)		
		EQS	LU	0.0002	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	0.0002	RBSP-ECOSTAT, UBA (2014)		
		PNEC	INERIS	0.0002	Pesticide Ecotoxicity Database, US-EPA		
		PNEC		0.0002	Von der Ohe, 2011		
56-55-3	Benzo(a)anthracene	EQS	NL	0.0002 3	NL Specific Pollutants	0.00023	**DE:** New value, RBSP (NL) http://wetten.overheid.nl/BWBR0027502/2015-11-19 PNEC and derivation need to be checked **NL:** the original value of 0.00023 ug/L (dissolved) can be found in: http://www.rivm.nl/bibliotheek/rapporten/601357009.pdf.
		EQS	BE	0.3	RBSP-ECOSTAT, UBA (2014)		
		EQS	CZ	0.03	RBSP-ECOSTAT, UBA (2014)		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
		EQS	DK	0.012	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	0.01	RBSP-ECOSTAT, UBA (2014)		
		PNEC	INERIS	0.012	EU RAR 2007 (draft)		
		PNEC		0.012	Verbruggen et al. 2008		
56-72-4	Coumaphos	EQS	BE	0.001	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	0.07	RBSP-ECOSTAT, UBA (2014)		
		EQS	DK	0.0007	RBSP-ECOSTAT, UBA (2014)	0.0007	
		EQS	NL	0.0034	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	0.07	RBSP-ECOSTAT, UBA (2014)		
		PNEC	INERIS	0.0034	RED, US-EPA 1996		
		PNEC		0.0034	Von der Ohe, 2011		
57018-04-9	Tolclofos-methyl	EQS	NL	1.2	NL Specific Pollutants	1.2	
57-12-5	Cyanide (as total CN)	PNEC		50	Substance factsheet (2015)	50	Substance ranking high during the last prioritisation exercise. WFD compliant, updated in the Cyanide working group under the SG-R (2015).
57-63-6	17-alpha-Ethinylestradiol	PNEC		3.50E-05	Substance factsheet (2015)	3.50E-05	Substance ranking high during the last prioritisation exercise
57-68-1	Sulfamethazine	EQS	CH	30	Swiss ECOTOX Centre	30	
57-74-9	Chlordane	EQS	FR	0.00005	INERIS, 2012	0.00005	
	trans-chlordane 5103-74-2	EQS	AT	0.002	RBSP-ECOSTAT, UBA (2014)		
	alpha-chlordane 5103-71-9	EQS	BE	0.002	RBSP-ECOSTAT, UBA (2014)		
	gamma-Chlordane 5566-34-7	EQS	DE	0.003	RBSP-ECOSTAT, UBA (2014)		
		EQS	LU	0.002	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	0.002	RBSP-ECOSTAT, UBA (2014)		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
		EQS	RO	0.003	RBSP-ECOSTAT, UBA (2014)		
57837-19-1	Metalaxyl	PNEC	INERIS	120	Pesticide Ecotoxicity Database, US-EPA	120	
	Metalaxyl-M 70630-17-0	PNEC		120	Von der Ohe, 2011		
58-08-2	Caffeine	PNEC		87	ECHA DOSSIER	87	
58-73-1	Diphenhydramine	PNEC		0.991	JRC derivation from ECOTOX US EPA	0.991	
58955-93-4	10,11-Dihydro-10,11-dihydroxycarbamazepine	PNEC	LfU Bayern	200	ETOX database, UBA	200	
5915-41-3	Terbuthylazine	EQS	NL	0.2	NL Specific Pollutants	0.32	**NL:** NL value will be revised to 0.32 µg/L for next round RBMP **Syngenta:** provided a document with PNEC 0.49 µg/L (SSD) and 0.22 µg/L (AF).
		EQS	CH	0.22	Swiss ECOTOX Centre		
		EQS	FR	0.06	INERIS, 2014		
		EQS	CZ	0.5	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	0.5	RBSP-ECOSTAT, UBA (2014)		
		EQS	DK	0.01	RBSP-ECOSTAT, UBA (2014)		
		EQS	ES	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	IT	0.5	RBSP-ECOSTAT, UBA (2014)		
		EQS	SI	0.5	RBSP-ECOSTAT, UBA (2014)		
		PNEC		0.22	PNEC 0.49 µg/L (SSD) and 0.22 µg/L (AF) proposed based on Huber (1994), Syngenta		
59-50-7	Chlorocresol (3-Methyl-4-chlorophenol)	EQS	FR	9.2	INERIS, 2011		
		EQS	BE	9	RBSP-ECOSTAT, UBA (2014)		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
		EQS	DE	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	6.4	RBSP-ECOSTAT, UBA (2014)	6.4	
		EQS	RO	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	UK	40	RBSP-ECOSTAT, UBA (2014)		
		PNEC	ECHA	15	ECHA DOSSIER		
60-00-4	Edetic acid (EDTA)	PNEC		2200	Substance factsheet (2015)	2200	Substance ranking high during the last prioritisation exercise. WFD compliant, updated in the Edetic acid (EDTA) working group under the SG-R (2015)
60168-88-9	Fenarimol	PNEC		0.00002	JRC derivation from ECOTOX US EPA	0.00002	
60207-90-1	Propiconazole	PNEC		6.1	Substance factsheet (2015)	6.1	Substance ranking high during the last prioritisation exercise. WFD compliant, updated in the Propiconazole working group under the SG-R (2015)
60-51-5	Dimethoate	EQS	NL	0.07	NL Specific Pollutants		**Cheminova A/S:** Proposed PNEC value is 2.4 µg/L. A proposal takes taking into account FMC/Cheminova studies is attached. (details under comment no. 92 in the List of comments) **BASF:** proposed a PNEC 0.48 µg/L based on NOEC of Daphnia magna with AF 50. **NL:** not agreed; acute values for insects are lower than chronic
		EQS	CH	0.07	Swiss ECOTOX Centre		
		EQS	FR	0. 1	INERIS, 2012		
		EQS	BE	0.02	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	0.1	RBSP-ECOSTAT, UBA (2014)		
		EQS	FI	0.7	RBSP-ECOSTAT, UBA (2014)		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
		EQS	IE	0.01	RBSP-ECOSTAT, UBA (2014)	0.01	**DE:** PNEC 0.01 µg/l RSBP (IE). Review of PNEC is needed
		EQS	IT	0.5	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	0.1	RBSP-ECOSTAT, UBA (2014)		
		EQS	SE	0.7	RBSP-ECOSTAT, UBA (2014)		
		EQS	UK	0.48	RBSP-ECOSTAT, UBA (2014)		
608-27-5	2,3-Dichloroaniline	EQS	DE	1	RBSP-ECOSTAT, UBA (2014)	1	
		EQS	LU	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	3	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	1	RBSP-ECOSTAT, UBA (2014)		
6190-65-4	Desethylatrazine	EQS	CZ	0.3	RBSP-ECOSTAT, UBA (2014)	0.2	
		EQS	LU	0.2	RBSP-ECOSTAT, UBA (2014)		
		PNEC		0.6	CIRCA data sheet, Dir. 2008/105/EC		
62-53-3	Aniline	EQS	CZ	5	RBSP-ECOSTAT, UBA (2014)	1.5	
		EQS	DE	0.8	RBSP-ECOSTAT, UBA (2014)		
		EQS	SK	1.5	RBSP-ECOSTAT, UBA (2014)		
		PNEC	ECHA	1200	ECHA DOSSIER		
		EQS	NL	1.5	RIVM 2016		
630-20-6	1,1,1,2-Tetrachloroethane	EQS	UK	140	RBSP-ECOSTAT, UBA (2014)	140	
63-25-2	Carbaryl	PNEC_ st	INERIS	0.015	Pesticide Ecotoxicity Database, US-EPA	0.015	
		PNEC_ st		0.015	Von der Ohe, 2011		
66230-04-4	Esfenvalerate	EQS	NL	0.0001	NL Specific Pollutants	0.0001	**Sumimoto Chemical Agro Europe S.A.:** request to change the PNEC value to 0.0005 µg/L. The statement is supported by EFSA *Conclusion on the peer review of the pesticide risk assessment of the active substance esfenvalerate.*

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
66246-88-6	Penconazole	EQS	FR	6	INERIS, 2013		**DE:** update may be required , The lowest NOEC 21-d for Daphnia magna reported in UBA ICS-database is 32 µg/L
		EQS	NL	1.7	RIVM	1.7	
668-34-8	Triphenyltin	MPC	RIVM (NL)	0.00023	RIVM report 601714018/2012	0.00023	
67129-08-2	Metazachlor	EQS	NL	0.08	NL Specific Pollutants	0.08	**BASF:** proposed PNEC 1.9 µg/L based on SSD from 19 primary producers NOEC/EC10, AF 1. **NL:** NL value 0.08 ug/L is also based on an SSD (10 chronic NOEC/EC10)
		EQS	CH	0.02	Swiss ECOTOX Centre		
		EQS	FR	0.019	INERIS, 2014		
		EQS	CZ	0.4	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	0.4	RBSP-ECOSTAT, UBA (2014)		
		EQS	LU	0.1	RBSP-ECOSTAT, UBA (2014)		
67306-00-7	Fenpropidin	PNEC		0.0032	JRC derivation based on EFSA conclusion	0.0032	
67564-91-4	Fenpropimorph	PNEC	ETOX	0.016	ETOX, UBA	0.016	**BASF:** proposed PNEC 0.03 µg/L based on the geomean NOECs of 2 ELS studies on Oncorhynchus mykiss
		PNEC		0.016	EFSA conclusions		
67-72-1	Hexachloroethane	EQS	FR	0.98	INERIS, 2012		
		EQS	BE	3	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	10	RBSP-ECOSTAT, UBA (2014)		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
		EQS	NL	0.44	RBSP-ECOSTAT, UBA (2014)	0.44	**NL:** 0.44 was derived for dissolved concentration
		EQS	RO	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	SI	24	RBSP-ECOSTAT, UBA (2014)		
67747-09-5	Prochloraz	EQS	FI	1	RBSP-ECOSTAT, UBA (2014)	1	
		PNEC	INERIS	0.32	DAR, EFSA 2007		
68359-37-5	Cyfluthrin	PNEC		0.001	ETOX database, UBA (UK standard)	0.001	
69377-81-7	Fluroxypyr	PNEC	FR	17.9	Pesticide Ecotoxicity Database, US-EPA	17.9	**DE:** Datasheet need to be updated. Lowest 14-d EyC50 Myriophyllum spicatum = 160 µg/L
709-98-8	Propanil	EQS	FR	0.2	INERIS, 2012	0.07	
		EQS	BE	0.2	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	0.1	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	0.07	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	0.1	RBSP-ECOSTAT, UBA (2014)		
		PNEC		0.2	Von der Ohe, 2011		
71-55-6	1,1,1-Trichloroethane	EQS	FR	26	INERIS, 2015	10	
		EQS	BE	100	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	DK	21	RBSP-ECOSTAT, UBA (2014)		
		EQS	ES	100	RBSP-ECOSTAT, UBA (2014)		
		EQS	IT	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	LU	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	21	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	UK	100	RBSP-ECOSTAT, UBA (2014)		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
		PNEC	ECHA	130	ECHA DOSSIER		
		PNEC		130	Von der Ohe, 2011		
723-46-6	Sulfamethoxazole	PNEC		0.4	Substance factsheet (2015)	0.4	Substance ranking high during the last prioritisation exercise. WFD compliant, updated in the Sulfamethoxazole working group under the SG-R (2015)
72-43-5	Methoxychlor	PNEC	INERIS	0.0005	ECOTOX database, US-EPA	0.0005	
		PNEC		0.0005	Von der Ohe, 2011		
7286-69-3	Sebuthylazine	EQS	AT	0.01	RBSP-ECOSTAT, UBA (2014)	0.01	
7287-19-6	Prometryn	EQS	DE	0.5	RBSP-ECOSTAT, UBA (2014)	0.5	
		PNEC	CZ	0.04	RBSP-ECOSTAT, UBA (2014)		
		PNEC		0.03	Pesticide Ecotoxicity Database, US-EPA		
731-27-1	Tolylfluanid	PNEC		0.26	Substance factsheet (2015)	0.26	Substance ranking high during the last prioritisation exercise. WFD compliant, updated in the Tolylfluanid working group under the SG-R (2015)
738-70-5	Trimethoprim	EQS	CH	60	Swiss ECOTOX Centre	60	
		EQS	DK	100	RBSP-ECOSTAT, UBA (2014)		
74223-64-6	Metsulfuron-methyl	EQS	NL	0.01	NL Specific Pollutants	0.01	**NL**: EQS=0.01 ug/L derivation: http://www.rivm.nl/bibliotheek/rapporten/601716020.pdf
		EQS	SE	0.02	RBSP-ECOSTAT, UBA (2014)		SDuPont: proposed EQS=PNEC =0.02 µg/L
		PNEC	FR	0.016	Pesticide Ecotoxicity Database, US-EPA		
74-95-3	Dibromomethane	PNEC	ECHA	45	ECHA DOSSIER	45	
75-01-4	Vinylchloride	EQS	BE	100	RBSP-ECOSTAT, UBA (2014)		
		EQS	CZ	1	RBSP-ECOSTAT, UBA (2014)		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
		EQS	DE	2	RBSP-ECOSTAT, UBA (2014)		**DE:** DE EQS=2 ug/L. OGewV. http://www.gesetze-im-internet.de/ogewv/BJNR142900011.html but the value could not be confirmed, when a new draft datasheet was prepared.
		EQS	DK	0.05	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	0.09	RBSP-ECOSTAT, UBA (2014)	0.09	The NL AA-EQS: http://www.rivm.nl/bibliotheek/rapporten/601782013.pdf
		EQS	RO	2	RBSP-ECOSTAT, UBA (2014)		
		PNEC	ECHA	77	ECHA DOSSIER		
75-25-2	Bromoform	PNEC	NL	11.3	RIVM, NL	11.3	
75-27-4	Dichlorobromomethane	PNEC		78	JRC derivation	78	
		PNEC		8	Japan risk assessment for water		
75-34-3	1,1-Dichloroethane	EQS	FR	92	INERIS, 2014		
		EQS	BE	100	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	10	RBSP-ECOSTAT, UBA (2014)	10	
		EQS	DK	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	LU	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	700	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	10	RBSP-ECOSTAT, UBA (2014)		
75-35-4	1,1-Dichloroethylene	EQS	FR	11.6	INERIS, 2013		
		EQS	BE	50	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	LU	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	9	RBSP-ECOSTAT, UBA (2014)		
		EQS	PL	5	RBSP-ECOSTAT, UBA (2014)	5	
		EQS	RO	10	RBSP-ECOSTAT, UBA (2014)		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
		PNEC	ECHA	9.12	ECHA DOSSIER		
76-03-9	Trichloroacetic acid	EQS	DK	0.01	RBSP-ECOSTAT, UBA (2014)	0.01	
		PNEC	ECHA	0.17	ECHA DOSSIER		
7664-41-7	Ammonia	PNEC	INERIS	67.5	US EPA		
		PNEC	ECHA	1.1	ECHA dossier	1.1	
76674-21-0	Flutriafol	EQS	DK	31	RBSP-ECOSTAT, UBA (2014)	31	
7786-34-7	Mevinphos	EQS	NL	0.00017	NL Specific Pollutants	0.00017	
		EQS	AT	0.01	RBSP-ECOSTAT, UBA (2014)		
		EQS	BE	0.002	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	0.0002	RBSP-ECOSTAT, UBA (2014)		
		EQS	IT	0.01	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	0.0002	RBSP-ECOSTAT, UBA (2014)		
78-51-3	Tris(2-butoxyethyl) phosphate (TBEP)	PNEC	ECHA	24	ECHA DOSSIER	24	
78587-05-0	Hexythiazox	PNEC		0.122	EFSA	0.122	
78-87-5	1,2-Dichloropropane	EQS	NL	280	NL Specific Pollutants	10	
		EQS	BE	400	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	10	RBSP-ECOSTAT, UBA (2014)		
		PNEC	ECHA	82	ECHA DOSSIER		
		PNEC	INERIS	409	ECOTOX database, US-EPA		
		PNEC		409	Von der Ohe, 2011		
79-00-5	1,1,2-Trichloroethane	EQS	FR	300	INERIS, 2013		
		EQS	BE	300	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	10	RBSP-ECOSTAT, UBA (2014)	10	
		EQS	LU	10	RBSP-ECOSTAT, UBA (2014)		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
		EQS	NL	22	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	SK	300	RBSP-ECOSTAT, UBA (2014)		
		EQS	UK	400	RBSP-ECOSTAT, UBA (2014)		
		PNEC		300	Von der Ohe, 2011		
79-11-8	Chloroacetic acid	EQS	FR	0.58	INERIS, 2014	0.6	
		EQS	AT	0.6	RBSP-ECOSTAT, UBA (2014)		
		EQS	BE	0.6	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	DK	0.58	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	0.58	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	10	RBSP-ECOSTAT, UBA (2014)		
		PNEC	ECHA	0.058	ECHA DOSSIER		
79241-46-6	Fluazifop-P-butyl	PNEC		0.477	JRC derivation based on EFSA conclusions	0.477	
79277-27-3	Thifensulfuron methyl	EQS	SE	0.05	RBSP-ECOSTAT, UBA (2014)	0.05	
		PNEC	INERIS	0.05	DEFRA 1995		
79-34-5	1,1,2,2-Tetrachloroethane	EQS	FR	140	INERIS, 2013		
		EQS	BE	100	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	DK	640	RBSP-ECOSTAT, UBA (2014)		
		EQS	LU	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	8	RBSP-ECOSTAT, UBA (2014)	8	
		EQS	UK	140	RBSP-ECOSTAT, UBA (2014)		
79622-59-6	Fluazinam	PNEC		0.058	JRC derivation based on EFSA dossier	0.058	

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
80-05-7	Bisphenol A	PNEC		0.24	Substance factsheet (2015)	0.24	Substance ranking high during the last prioritisation exercise. WFD compliant, updated in the Bisphenol A working group under the SG-R (2015)
80-09-1	Bisphenol S	PNEC	ECHA	270	ECHA DOSSIER	270	
8065-48-3	Demeton	EQS	DE	0.1	RBSP-ECOSTAT, UBA (2014)	0.1	
	Demeton-S-methyl 919-86-8						
	Demeton-S-methylsulfon 17040-19-6						
81103-11-9	Clarithromycin	PNEC		0.13	Substance factsheet (2015)	0.13	
81-15-2	Musk xylene	PNEC		1	Substance factsheet (2015)	1	Substance ranking high during the last prioritisation exercise
82097-50-5	Triasulfuron	PNEC_ st		0.0007	DG-SANCO 2000	0.0032	**Syngenta:** Applying an AF of 10 to the NOEC from the guideline 7 d Lemna study gives a PNEC of 0.008 µg/L. Applying an AF of 10 to NOEC from the older 14 d study gives a PNEC of 0.0032 µg/L. Both are above the INERIS PNEC used in the initial assessment of 0.0007 µg/L.
82558-50-7	Isoxaben	EQS	FR	0.6	INERIS, 2014	0.6	
82-68-8	Quintozene	EQS	AT	0.4	RBSP-ECOSTAT, UBA (2014)	0.4	
83121-18-0	Teflubenzuron	EQS	NL	0.0012	NL Specific Pollutants	0.0012	**BASF:** proposed PNEC 0.025 µg/L proposed based on mesocosm study AF 2. **NL:** NL also evaluated mesocosm study (cannot check if this is the same). NOEC was 0.005 µg/L and exposure was not chronic, derivation of NL EQS: http://www.rivm.nl/bibliotheek/rapporten/601716023.pdf

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
83164-33-4	Diflufenican	EQS	DE	0.009	RBSP-ECOSTAT, UBA (2014)	0.009	**DE:** DE EQS=0.009 ug/L. OGewV. Datasheet, Nendza 2003. https://webetox.uba.de/webETOX/public/basics/literatur.do?id=2202. The new Swedish EQS for diflufenican is 0,01 (revised in 2015; source: Karl Lilja)
		EQS	SE	0.01	RBSP-ECOSTAT, UBA (2014)		
83-32-9	Acenaphthene	EQS	BE	0.06	RBSP-ECOSTAT, UBA (2014)	0.06	**DE:** Derivation of this PNEC (BE EQS) need to be checked
		EQS	CZ	2.8	RBSP-ECOSTAT, UBA (2014)		
		EQS	DK	1.3	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	2.8	RBSP-ECOSTAT, UBA (2014)		
		PNEC	INERIS	3.8	EU RAR 2007 (draft)		
		PNEC		3.8	Von der Ohe, 2011		
		PNEC		3.8	Verbruggen et al. 2008		
834-12-8	Ametryn	EQS	BG	0.1	RBSP-ECOSTAT, UBA (2014)	0.1	
		EQS	CZ	3	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	0.5	RBSP-ECOSTAT, UBA (2014)		
		PNEC	ECHA	0.11	ECHA DOSSIER		
		PNEC	INERIS	0.114	RED, US-EPA 2005		
		PNEC		0.11	Von der Ohe, 2011		
84-66-2	Diethyl phthalate	PNEC		12	ECHA DOSSIER	12	
84-74-2	Di-n-butylphthalate	EQS	DK	2.3	RBSP-ECOSTAT, UBA (2014)		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
		EQS	FI	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	SK	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	SI	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	10	RBSP-ECOSTAT, UBA (2014)	10	https://webetox.uba.de/webETOX/public/basics/literatur.do?id=2207
		PNEC	ECHA	10	ECHA DOSSIER		
		PNEC	INERIS	10	EU RAR 2004 (final with addendum)		
		PNEC		10	Von der Ohe, 2011		
85-01-8	Phenanthrene	EQS	NL	1.1	NL Specific Pollutants	1.1	**DE:** NL AA-EQS = 1,2 µg/l. RBSP (NL), see: http://wetten.overheid.nl/BWBR0027502/2015-11-19 **NL:** The Dutch EQS takes all routes into account and is very up to date. The derivation can be found in: http://www.rivm.nl/bibliotheek/rapporten/601357007.pdf A factor of 40 could really make a difference in the prioritisation. The difference with other PAHs is caused by the fact that this one is not genotoxic carcinogenic and fish consumption is not critical.
		EQS	BE	0.1	RBSP-ECOSTAT, UBA (2014)		
		EQS	CZ	0.03	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	0.5	RBSP-ECOSTAT, UBA (2014)		
		EQS	DK	1.3	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	0.03	RBSP-ECOSTAT, UBA (2014)		
		EQS	SK	0.38	RBSP-ECOSTAT, UBA (2014)		
		PNEC	INERIS	1.3	EU RAR 2007 (draft)		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
		PNEC		1.3	Von der Ohe, 2011		
		PNEC		1.3	Verbruggen et al. 2008		
85509-19-9	Flusilazole	EQS	FR	0.3	INERIS	0.3	
85-68-7	Butylbenzyl phthalate	EQS	FI	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	UK	7.5	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	5.2	RBSP-ECOSTAT, UBA (2014)	5.2	**DE:** DE pEQS=5.2 µg/L. https://webetox.uba.de/webETOX/public/basics/literatur.do?id=2207
		PNEC	ECHA	7.5	ECHA DOSSIER		
		PNEC	INERIS	7.5	EU RAR 2007 (final)		
		PNEC		7.5	Von der Ohe, 2011		
86-50-0	Azinphos-methyl	EQS	DE	0.01	ECOSTAT		
		EQS	BE	0.002	ECOSTAT		
		EQS	RO	0.1	ECOSTAT		
		EQS	IT	0.01	ECOSTAT		
		EQS	LU	0.001	ECOSTAT		
		EQS	NL	0.0065	NL SPECIFIC POLLUTANTS	0.0065	**NL:** The value derived is a rather robust one, based on 25 species from fully evaluated chronic studies. Besides that, the importance of the routes fish consumption and secondary poisoning was considered. We propose to take this value (http://www.rivm.nl/bibliotheek/rapporten/601714004.pdf).
86-73-7	Fluorene	EQS	BE	2	RBSP-ECOSTAT, UBA (2014)	1.5	**NL:** The PNEC for direct ecotoxicity has been derived in: http://www.rivm.nl/bibliotheek/rapporten/607711007.pdf This value of 1.5 µg/l is a reliable value (AF 10). Fish consumption is not dealt with in this report, but with a TDI of 40 µg/kg bw/d and RIVM report cites four reliable BCF values of 1158, 1658, 818, 755

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
							(5% lipids), it appears that the PNEC for direct ecotoxicity is sufficient
		EQS	CZ	0.1	RBSP-ECOSTAT, UBA (2014)		
		EQS	DK	2.3	RBSP-ECOSTAT, UBA (2014)		
		PNEC	INERIS	2.5	EU RAR 2007 (draft)		
		PNEC		2.5	Von der Ohe, 2011		
87-65-0	2,6-Dichlorophenol	EQS	DK	3.4	RBSP-ECOSTAT, UBA (2014)	3.4	
87674-68-8	Dimethenamid	EQS	FR	0.2	INERIS, 2014	0.2	
		PNEC		0.2	Von der Ohe, 2011		
		Provisional PNEC		2.8	JRC Watch list report		
88-06-2	2,4,6-Trichlorophenol	EQS	CZ	0.1	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	IT	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	LU	0.1	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	0.26	RBSP-ECOSTAT, UBA (2014)	0.26	
882-09-7	Clofibric acid (Clofibrate)	QN-V	DE	5	ETOX, UBA	5	
88-72-2	o-Nitrotoluene	PNEC	INERIS	10	EU RAR 2008 (Final report)	10	
		PNEC		10	Von der Ohe, 2011		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
88-73-3	1-Cloro-2-nitrobenzene	EQS	FR	5.28	INERIS, 2012		
		EQS	BE	3	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	IT	1	RBSP-ECOSTAT, UBA (2014)	1	
		EQS	NL	29	RBSP-ECOSTAT, UBA (2014)		
		PNEC		26	Von der Ohe, 2011		
88-85-7	Dinoseb	PNEC	ECHA	0.29	ECHA DOSSIER	0.29	
89-59-8	4-Chloro-2-nitrotoluene	EQS	DE	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	IT	1	RBSP-ECOSTAT, UBA (2014)	1	
		EQS	NL	4	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	UK	10	RBSP-ECOSTAT, UBA (2014)		
		PNEC	INERIS	6	ECOTOX database, US-EPA		
		PNEC		6	Von der Ohe, 2011		
89-63-4	4-Chloro-2-nitroaniline	EQS	FR	6.3	INERIS, 2013		
		EQS	BE	2	RBSP-ECOSTAT, UBA (2014)		
		EQS	CZ	1	RBSP-ECOSTAT, UBA (2014)	1	
		EQS	DE	3	RBSP-ECOSTAT, UBA (2014)		
		EQS	DK	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	LU	3	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	3	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	3	RBSP-ECOSTAT, UBA (2014)		
90-12-0	1-Methylnaphthalene	EQS	DK	0.12	RBSP-ECOSTAT, UBA (2014)	0.12	
90-13-1	1-Chloronaphthalene	EQS	FR	0.325	INERIS, 2011		
		EQS	BE	1	RBSP-ECOSTAT, UBA (2014)		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
		EQS	CZ	0.1	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	0.01	RBSP-ECOSTAT, UBA (2014)	0.01	
		EQS	DK	2.7	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	0.77	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	0.01	RBSP-ECOSTAT, UBA (2014)		
90717-03-6	Quinmerac	PNEC	JRC	31.6	JRC derivation based on EFSA dossier	31.6	
91465-08-6	lambda-Cyhalothrin	EQS	NL	0.00002	NL Specific Pollutants	0.0002	**NL:** NL value is WFD compliant. Chronic NOEC with AF 100 because chronic studies with insects were not available. JRC: AF 10 used: Data set on acute and chronic toxicity with insects available
		EQS	FR	0.00019	INERIS, 2014		**Syngenta:** The PNEC used previously in the STE was 0.00002 µg/L. This value is based on the mysid chronic NOEC of 0.00022 µg/l. This is an estuarine/marine organism, whereas the FW PNEC should be based on a FW organism. Of the 3 trophic levels available, the lowest FW NOEC is for aquatic invertebrates and the screening level PNEC should be 0.0002 µg/L, as in biocides DAR. Admittedly, it is likely to have little impact on the assessment of lambda-cyhalothrin as the value is still well below LOD/LOQ.
919-86-8	Demeton-S-methyl	EQS	DE	0.1	ECOSTAT	0.1	
		EQS	RO	0.1	ECOSTAT		
92-52-4	Biphenyl	EQS	FR	3.4	INERIS, 2013		
		EQS	BE	2	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	1	RBSP-ECOSTAT, UBA (2014)	1	
		EQS	LU	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	1.5	RBSP-ECOSTAT, UBA (2014)		
		EQS	SK	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	UK	25	RBSP-ECOSTAT, UBA (2014)		
		PNEC	ECHA	17	ECHA DOSSIER		
		PNEC		1.7	Von der Ohe, 2011		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
933-75-5	2,3,6-Trichlorphenol	EQS	DE	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	LU	0.1	RBSP-ECOSTAT, UBA (2014)	0.1	
933-78-8	2,3,5-Trichlorphenol	EQS	DE	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	LU	0.1	RBSP-ECOSTAT, UBA (2014)	0.1	
93-65-2	Mecoprop	PNEC		3.6	Substance factsheet (2015)	3.6	Substance ranking high during the last prioritisation exercise. WFD compliant, updated in the Mecoprop working group under the SG-R (2015)
93-72-1	Fenoprop	PNEC_ st	FR	0.6	ECOTOX database, US-EPA	0.6	
93-76-5	2,4,5-Trichlorophenoxyacetic acid	EQS	FR	5	INERIS, 2013		
		EQS	BE	2	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	0.1	RBSP-ECOSTAT, UBA (2014)	0.1	
		EQS	IT	0.5	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	9	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	0.1	RBSP-ECOSTAT, UBA (2014)		
94361-06-5	Cyproconazole	EQS	CH	1.25	Swiss ECOTOX Centre		
		EQS	FR	0.6	INERIS, 2013	0.6	
94-74-6	2-Methyl-4-chlorophenoxyacetic acid (MCPA)	EQS	NL	1.4	NL Specific Pollutants		
		EQS	FR	0.5	INERIS, 2013		
		EQS	BE	0.7	RBSP-ECOSTAT, UBA (2014)		
		EQS	CZ	0.1	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	0.1	RBSP-ECOSTAT, UBA (2014)	0.1	
		EQS	DK	0.01	RBSP-ECOSTAT, UBA (2014)		**DE:** Derivation should be checked by DK
		EQS	IT	0.5	RBSP-ECOSTAT, UBA (2014)		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
		EQS	RO	0.1	RBSP-ECOSTAT, UBA (2014)		
		EQS	SE	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	CH	1.34	Swiss ECOTOX Centre		
		EQS	SK	1.6	RBSP-ECOSTAT, UBA (2014)		
94-75-7	2,4-Dichlorophenoxyacetic acid (2,4-D)	EQS	CH	0.2	Swiss ECOTOX Centre	0.1	
		EQS	FR	2.7	INERIS, 2013		
		EQS	BE	20	RBSP-ECOSTAT, UBA (2014)		
		EQS	CZ	0.1	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	0.1	RBSP-ECOSTAT, UBA (2014)		
		EQS	IT	0.5	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	26	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	0.1	RBSP-ECOSTAT, UBA (2014)		
		EQS	UK	0.3	RBSP-ECOSTAT, UBA (2014)		
94-81-5	4-(4-Chloro-o-tolyloxy) butyric acid	EQS	CZ	0.1	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	0.43	RBSP-ECOSTAT, UBA (2014)	0.43	**DE:** DE pEQS=0.43 ug/L. AF = 1000. https://webetox.uba.de/webETOX/public/basics/literatur.do?id=2645
		PNEC	INERIS	0.5	Pesticide Ecotoxicity Database, US-EPA		
		PNEC		0.5	Von der Ohe, 2011		
94-82-6	4-(2,4-Dichlorophenoxy)butyric acid (2,4-DB)	PNEC	INERIS	0.932	RED, US-EPA 2005	0.932	
		PNEC_st		0.93	Von der Ohe, 2011		
950-37-8	Methidathion	PNEC	INERIS	0.0022	RED, US-EPA 2006	0.0022	
		PNEC		0.0022	Von der Ohe, 2011		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
95-14-7	1H-Benzotriazole	EQS	CH	30	Swiss ECOTOX Centre	30	
		PNEC	ECHA	19.4	ECHA DOSSIER		
95-49-8	2-Chlorotoluene	EQS	FR	8	INERIS, 2012		
		EQS	BE	3	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	1	RBSP-ECOSTAT, UBA (2014)	1	
		EQS	IT	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	310	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	1	RBSP-ECOSTAT, UBA (2014)		
		PNEC	ECHA	2.8	ECHA DOSSIER		
		PNEC		14	Von der Ohe, 2011		
95-50-1	1,2-Dichlorobenzene	EQS	BE	20	RBSP-ECOSTAT, UBA (2014)		
		EQS	BG	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	CZ	1	RBSP-ECOSTAT, UBA (2014)	1	
		EQS	DE	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	FI	7.4	RBSP-ECOSTAT, UBA (2014)		
		EQS	IT	2	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	250	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	10	RBSP-ECOSTAT, UBA (2014)		
		PNEC	ECHA	3.7	ECHA DOSSIER		
		PNEC	INERIS	6.3	SIDS, OECD 2001		
		PNEC		6.3	Von der Ohe, 2011		
95-51-2	2-Chloroaniline	EQS	FR	0.64	INERIS, 2013		
		EQS	BE	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	CZ	0.3	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	3	RBSP-ECOSTAT, UBA (2014)		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
		EQS	IT	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	0.2	RBSP-ECOSTAT, UBA (2014)	0.2	
		EQS	RO	3	RBSP-ECOSTAT, UBA (2014)		
		PNEC		0.64	Von der Ohe, 2011		
95-57-8	2-Chlorophenol	EQS	FR	6	INERIS, 2012		
		EQS	BE	20	RBSP-ECOSTAT, UBA (2014)		
		EQS	CZ	3	RBSP-ECOSTAT, UBA (2014)	3	
		EQS	DE	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	IT	4	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	35	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	UK	50	RBSP-ECOSTAT, UBA (2014)		
95-63-6	1,2,4-Trimethylbenzene	EQS	SI	2	RBSP-ECOSTAT, UBA (2014)	2	
		PNEC	ECHA	120	ECHA DOSSIER		
95-76-1	3,4-Dichloroaniline	EQS	FR_NEW	0.02	INERIS, 2012	0.02	
		EQS	CZ	0.2	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	0.5	RBSP-ECOSTAT, UBA (2014)		
		EQS	IT	0.5	RBSP-ECOSTAT, UBA (2014)		
		EQS	LU	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	3	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	UK	0.2	RBSP-ECOSTAT, UBA (2014)		
95-85-2	2-Amino-4-chlorophenol	EQS	BE	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	10	RBSP-ECOSTAT, UBA (2014)		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
		EQS	RO	3	RBSP-ECOSTAT, UBA (2014)	3	
95-94-3	1,2,4,5-Tetrachlorobenzene	EQS	BE	9	RBSP-ECOSTAT, UBA (2014)		
		EQS	CZ	0.32	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	0.0016	RIVM (2010)	0.0016	**NL:** A newer derivation on EQS has been made in 2010. The resulting EQS, which takes into account all routes is much lower than this old EQS, but also than the EQSs of the other MS. The value is 0.0016 µg/L. The derivation can be found in: http://www.rivm.nl/bibliotheek/rapporten/601782020.pdf
		EQS	RO	10	RBSP-ECOSTAT, UBA (2014)		
95-95-4	2,4,5-Trichlorophenol	EQS	FR	10.8	INERIS, 2012		
		EQS	CZ	0.89	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	IT	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	LU	0.1	RBSP-ECOSTAT, UBA (2014)	0.1	
		EQS	NL	0.13	RBSP-ECOSTAT, UBA (2014)		
96-18-4	1,2,3-Trichloropropane	PNEC	ECHA	88	ECHA DOSSIER		
		PNEC		4.1	Von der Ohe, 2011		
		PNEC_st	INERIS	4.1	ECOTOX database, US-EPA	4.1	
96525-23-4	Flurtamone	EQS		0.23	UBA, DE	0.23	
97-00-7	1-Chloro-2,4-dinitrobenzene	EQS	FR	1.6	INERIS, 2013		
		EQS	BE	5	RBSP-ECOSTAT, UBA (2014)		
		EQS	CZ	5	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	5	RBSP-ECOSTAT, UBA (2014)		
		EQS	DK	5	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	0.54	RBSP-ECOSTAT, UBA (2014)	0.54	

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/l)	Comments
		EQS	RO	5	RBSP-ECOSTAT, UBA (2014)		
98-82-8	Isopropylbenzene	EQS	FR	22	INERIS, 2014		
		EQS	AT	22	RBSP-ECOSTAT, UBA (2014)		
		EQS	BE	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	CZ	0.7	RBSP-ECOSTAT, UBA (2014)	0.7	
		EQS	DE	10	RBSP-ECOSTAT, UBA (2014)		
		EQS	DK	22	RBSP-ECOSTAT, UBA (2014)		
		EQS	NL	4.2	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	10	RBSP-ECOSTAT, UBA (2014)		
		PNEC	ECHA	35	ECHA DOSSIER		
98-87-3	alpha,alpha-Dichlorotoluene	EQS	NL	0.034	NL Specific Pollutants	0.034	
		EQS	BE	5	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	10	RBSP-ECOSTAT, UBA (2014)		**DE:** DE EQS=10 µg/L. OGewV value, no datasheet available. https://webetox.uba.de/webETOX/public/basics/literatur.do?id=24172
98-95-3	Nitrobenzene	EQS	CZ	3	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	0.1	RBSP-ECOSTAT, UBA (2014)	0.1	
		PNEC	ECHA	38	ECHA DOSSIER		
99-87-6	p-Cymene	PNEC	JRC	4.4	JRC derivation based on ECOTOX US EPA	4.4	

Table III-2. List of PNEC/EQS$_{fw, eco}$ metals

The values stated under the column "Selected PNEC/EQS$_{fw,eco}$" were used in the STE.

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/L)	Comments
7429-90-5	Aluminium	EQS	CZ	1000	UBA, 2014	40	**Eurometaux:** The PNEC assessment for Al should take into account the pH, which strongly affects its solubility. The values quoted are valid for a specific set of circumstances. There is solid evidence for a value higher than 40 µg/l in the REACH files **European Aluminium;** provided additional comments specific to aluminium (details under comment no. 66 in the List of comments), and considers that that a PNEC of 40 µg/l is not realistic and suggests to revise it accordingly for the risk prioritisation stage. **DE:** PNEC 40 µg/L RBSP (PL). Ecotox is influenced by pH; value should be compared with dissolved concentration only.
		EQS	LU	200	UBA, 2014		
		EQS	PL	40	UBA, 2014		
		PNEC	INERIS	50	Environment Canada 1999		
7439-89-6	Iron	EQS	CZ	1000	UBA, 2014		
		EQS	LU	200	UBA, 2014	200	
		EQS	UK	1000	UBA, 2014		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/L)	Comments
		PNEC	INERIS	300	Environment Canada, US-EPA		
7439-95-4	Magnesium	EQS	CZ	120000	UBA, 2014		
		EQS	LU	75000	UBA, 2014	75000	
		EQS	PL	100000	UBA, 2014		
		PNEC	ECHA	410	ECHA DOSSIER		**DE:** PNEC 410 µg/L: Value not plausible! Background concentration, mean 19300 µg/L 90P = 27 300 µg/L (FOREGS, 2005)
7439-96-5	Manganese	EQS	BG	100	UBA, 2014		
		EQS	CZ	300	UBA, 2014		
		EQS	LU	50	UBA, 2014	50	
		EQS	UK	123	UBA, 2014		
		PNEC	ECHA	34	ECHA DOSSIER		
7439-98-7	Molybdenum	AA-EQS	NL	136	NL Specific Pollutants		
		EQS	BE	340	UBA, 2014		
		EQS	CZ	18	UBA, 2014		
		EQS	NL	136	UBA, 2014	136	
		EQS	PL	40	UBA, 2014		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/L)	Comments
		EQS	RO	3.6	UBA, 2014		
		EQS	SI	24	UBA, 2014		
		PNEC	ECHA	12700	ECHA DOSSIER		**DE:** The value is fare above the background listed in (FOREGS, 2005) and not acceptable **Eurometaux**: Value in ECHA dossier (12.7 mg/l) considered more reasonable due to the most comprehensive and robust ecotoxicity data set used in the analysis, and to the reliability of the derivation process
		PNEC	INERIS	340	Van Vlaardingen and Verbruggen, 2009		
7440-22-4	Silver	AA-EQS	NL	0.01	NL Specific Pollutants		
		EQS	AT	0.1	UBA, 2014		
		EQS	BE	0.08	UBA, 2014		
		EQS	CZ	3.5	UBA, 2014		
		EQS	DE	0.02	UBA, 2014		**DE:** the EQS in Germany for Silver = 0.02 [µg/l] dissolved annual average
		EQS	DK	0.017	UBA, 2014	0.017	**EPMF:** We consider the REACH freshwater PNEC ECHA / UK EQS more robust (details under comment no. 67(3), in the List of comments) **Eurometaux:** Value in ECHA dossier considered more reasonable due to the most comprehensive and robust data set used in the analysis,

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/L)	Comments
							and the reliability and relevance of studies used for its derivation, using measured dissolved silver concentrations
		EQS	PL	5	UBA, 2014		
		EQS	UK	0.04			
		PNEC	ECHA	0.04	ECHA DOSSIER		
		PNEC	INERIS	0.05	SSD all available valid data mainly from ECOTOX US-EPA		
7440-23-5	Sodium	EQS	LU	200000	UBA, 2014	200000	
7440-24-6	Strontium	EQS	DK	210	UBA, 2014	210	
7440-28-0	Thallium	AA-EQS	NL	0.05	NL Specific Pollutants	0.05	
		EQS	BE	0.2	UBA, 2014		
		EQS	DE	0.2	UBA, 2014		
		EQS	DK	0.48	UBA, 2014		
		EQS	PL	2	UBA, 2014		
		EQS	RO	2	UBA, 2014		
7440-31-5	Tin	AA-EQS	NL	0.6	NL Specific Pollutants	0.6	

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/L)	Comments
		EQS	CZ	25	UBA, 2014		
		EQS	DK	2	UBA, 2014		
		EQS	EE	3	UBA, 2014		
		EQS	RO	2.2	UBA, 2014		
		PNEC	INERIS	1.5	ECOTOX database, US-EPA		
7440-32-6	Titanium	AA-EQS	NL	20	NL Specific Pollutants	20	
		EQS	BE	20	UBA, 2014		
		EQS	PL	50	UBA, 2014		
		PNEC	ECHA	76	ECHA DOSSIER	ECHA DOSSIER	
7440-36-0	Antimony	AA-EQS	NL	5.6	NL Specific Pollutants	5.6	**NL:** NL AA-EQS=5.6 µg/L value derived according to guidance, includes hh
		PNEC	ECHA	113	ECHA DOSSIER		**Eurometaux:** Value in ECHA dossier (0.113 mg/L) considered more reasonable due to the range of natural background concentrations
		AA-EQS	FR	113	INERIS, 2014		
		EQS	BE	100	UBA, 2014		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/L)	Comments
		EQS	CZ	250	UBA, 2014		
		EQS	DK	113	UBA, 2014		
		EQS	PL	2	UBA, 2014		
		EQS	SI	3.2	UBA, 2014		
		PNEC	ECHA	113	ECHA DOSSIER		
7440-38-2	Arsenic	AA-EQS	NL	0.5	NL Specific Pollutants		
		EQS	AT	24	UBA, 2014		
		EQS	BE	3	UBA, 2014		
		EQS	BG	10-20	UBA, 2014		
		EQS	CZ	11	UBA, 2014		
		EQS	DE	40 mg/kg	UBA, 2014		**DE:** Value refers to suspended matter concentration
		EQS	DK	4.3	UBA, 2014		
		EQS	EE	10	UBA, 2014		
		EQS	ES	50	UBA, 2014		
		EQS	FR	4.2	UBA, 2014		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/L)	Comments
		EQS	IE	25	UBA, 2014		
		EQS	IT	10	UBA, 2014		
		EQS	LU	10	UBA, 2014		
		EQS	LV	150	UBA, 2014		
		EQS	PL	50	UBA, 2014		
		EQS	RO	7.2	UBA, 2014		
		EQS	SK	7.5	UBA, 2014		
		EQS	SI	7	UBA, 2014		
		EQS	UK	50	UBA, 2014		
		PNEC	ECHA	13	ECHA DOSSIER	13	**Eurometaux:** Value in ECHA dossier (13 µg/L) considered more reasonable due to the range of natural background concentrations. A PNEC of 0.5 µg/l is lower than mid-range of European inland ambient background concentrations for arsenic, reported for European stream waters in FOREGS (http://weppi.gtk.fi/publ/foregsatlas/) and will therefore lead to many false positive results when performing compliance checks **DE:** a value of 13 µg/L for arsenic is not acceptable, compare datasheet: https://webetox.uba.de/webETOX/public/basics/literatur.do?id=24345 and Dutch regulations

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/L)	Comments
							http://wetten.overheid.nl/BWBR0027502/geldigheidsdatum_08-02-2016/afdrukken
7440-39-3	Barium	AA-EQS	NL	73	NL Specific Pollutants		
		EQS	BE	60	UBA, 2014		
		EQS	CZ	180	UBA, 2014		
		EQS	DK	9.3	UBA, 2014	9.3	
		EQS	EE	50	UBA, 2014		
		EQS	PL	500	UBA, 2014		
		EQS	RO	200	UBA, 2014		
		PNEC	INERIS	58	ECOTOX database, US-EPA		
7440-41-7	Beryllium	AA-EQS	NL	0.08	NL Specific Pollutants	0.08	
		EQS	BE	0.08	UBA, 2014		
		EQS	CZ	0.5	UBA, 2014		
		EQS	PL	0.8	UBA, 2014		
		EQS	RO	0.05	UBA, 2014		**DE:** PNEC 0.05 µg/L. Background NL 0,02 µg/l (Osté, 2013) 90P =0,056 (FOREGS, 2005) RBSP, NL 0,08 µg/l. Review of PNEC may be indicated

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/L)	Comments
							Eurometaux: An EQS value of 33 µg/L at a water hardness of 200 mg/L CaCO3 is considered more reasonable due to the dependendency of Be toxicity upon the hardness of the water body, and the range of natural background concentrations
		PNEC	INERIS	0.038	ECOTOX database, US-EPA		
7440-42-8	Boron	AA-EQS	NL	180	NL Specific Pollutants	180	**DE:** PNEC for Biocides is 180 µg/L **Eurometaux:** Value in ECHA dossier (2.9 mg/l) considered more reasonable due to the range of natural background concentrations
		EQS	BE	700	UBA, 2014		
		EQS	CY	1000	UBA, 2014		
		EQS	CZ	300	UBA, 2014		
		EQS	DK	94	UBA, 2014		
		EQS	PL	2000	UBA, 2014		
		EQS	SI	180	UBA, 2014		
		PNEC	ECHA	2900	ECHA DOSSIER		
7440-47-3	Chromium	AA-EQS	NL	3.4	NL Specific Pollutants		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/L)	Comments
		EQS	AT	9	UBA, 2014		
		EQS	BE	5	UBA, 2014		
		EQS	BG	100	UBA, 2014		
		EQS	CZ	18	UBA, 2014		
		EQS	DE	640 mg/kg	UBA, 2014		**DE:** Suspended matter concentration
		EQS	DK	3.4	UBA, 2014		
		EQS	EE	5	UBA, 2014		
		EQS	ES	50	UBA, 2014		
		EQS	FR	3.4	UBA, 2014		
		EQS	IT	7	UBA, 2014		
		EQS	LT	10	UBA, 2014		
		EQS	LU	18	UBA, 2014		
		EQS	LV	11	UBA, 2014		
		EQS	PL	50	UBA, 2014		
		EQS	RO	2.5	UBA, 2014	2.5	**DE:** CAS No. 18540-29-9, Chromium 6+; PNEC 2.5 µg/L: Review derivation. Check if only dissolved concentrations are used to calculate STE score

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/L)	Comments
		EQS	SE	3	UBA, 2014		
		EQS	SK	9	UBA, 2014		
		EQS	SI	12	UBA, 2014		
		PNEC	ECHA	6.5	ECHA DOSSIER		
18540-29-9	Chromium (VI)	EQS		0.47	EU-RAR, 2005	0.47	*Ceriodaphnia dubia* / 7d, NOEC: 0.0047mg/L , AF of 10
				3.4	EU-RAR, 2005, Watch list report		Application of SSD and AF of 3
7440-48-4	Cobalt	AA-EQS	NL	0.2	NL Specific Pollutants		
		EQS	BE	0.5	UBA, 2014		
		EQS	CZ	3	UBA, 2014		
		EQS	DK	0.28	UBA, 2014		
		EQS	LU	3.1	UBA, 2014		
		EQS	PL	50	UBA, 2014		
		EQS	RO	0.7	UBA, 2014		
		EQS	SI	0.3	UBA, 2014		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/L)	Comments
		PNEC	ECHA	0.6	ECHA DOSSIER	0.6	**Eurometaux:** Value in ECHA dossier (0.6 µg/l) considered more reasonable due to the range of natural background concentrations.
		PNEC	INERIS	0.5	ECOTOX database, US-EPA		
7440-50-8	Copper	AA-EQS	NL	2.4	NL Specific Pollutants		
		EQS	AT	1.6-9.3	UBA, 2014		
		EQS	BE	7	UBA, 2014		
		EQS	BG	5-112	UBA, 2014		
		EQS	CYP	60	UBA, 2014		
		EQS	CZ	14	UBA, 2014		
		EQS	DE	160 mg/kg	UBA, 2014		**DE:** Value refers to suspended matter concentration
		EQS	DK	1	UBA, 2014		
		EQS	EE	15	UBA, 2014		
		EQS	ES	5-120	UBA, 2014		
		EQS	FR	1.4	UBA, 2014		
		EQS	IE	3.4	UBA, 2014		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/L)	Comments
		EQS	LT	10	UBA, 2014		
		EQS	LU	10	UBA, 2014		
		EQS	LV	9	UBA, 2014		
		EQS	PL	50	UBA, 2014		
		EQS	RO	1.3	UBA, 2014		
		EQS	SE	4	UBA, 2014		
		EQS	SK	1.1	UBA, 2014		
		EQS	SI	8.2	UBA, 2014		
		EQS	UK	1-28	UBA, 2014		
		PNEC	ECHA	7.8	ECHA DOSSIER	7.8	**DE:** The PNEC of 7.8 µg/l is not acceptable. It is above the 90 percentile of 2.45 µg/L cited for Europe by (FOREGS, 2005). The recently derived AA-EQS 2.4 by NL is the better option http://wetten.overheid.nl/BWBR0027502/2015-11-19 **Eurometaux:** Value in ECHA dossier was derived for waters across whole Europe and is considered more reasonable due to the most comprehensive and robust data set used in the analysis, the range of natural background concentrations, and to Cu homeostase range. The indicated EQS ranges may be related to different bio-availabilities and/or ambient background levels. If bio-availability data are available, an EQS bio-available should be derived and used

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/L)	Comments
7440-61-1	Uranium	AA-EQS	NL	0.5	NL Specific Pollutants	0.5	**JRC:** The value from NL (which includes correction to the backgroud concentration for NL) is used now: The QSfw, eco is determined as QSfw, eco = QSadded, eco + Cb = 0.17 + 0.33 = 0.5 µg/L. http://www.rivm.nl/bibliotheek/rapporten/270006003.pdf
		EQS	BE	1	UBA, 2014		
		EQS	CZ	24	UBA, 2014		
		EQS	DK	0.015	UBA, 2014		
		PNEC	INERIS	0.3	Pickett et al. (1993)		
		AA-EQS	DE	0.44	Wenzel et al. 2015		**DE:** PNEC DK is not plausible regarding the Background value. DE 0,44 µg/L; https://webetox.uba.de/webETOX/public/basics/literatur.do?id=24363
7440-62-2	Vanadium	AA-EQS	NL	3.5	NL Specific Pollutants	3.5	
		EQS	BE	4	UBA, 2014		
		EQS	CZ	18	UBA, 2014		
		EQS	DK	4.1	UBA, 2014		
		EQS	PL	50	UBA, 2014		
		EQS	RO	1.2	UBA, 2014		**DE:** 1.2 µg/L may be too low. Final review needed

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/L)	Comments
		PNEC	ECHA	7.6	ECHA DOSSIER		**Eurometaux:** Value in ECHA dossier (7.6 µg/L) considered more reasonable due to the range of natural background concentrations
		PNEC	INERIS	2.5	ECOTOX database, US-EPA		
7440-66-6	Zinc	PNEC		10.9	Substance factsheet (2015)	10.9	Substance ranking high during the last prioritisation exercise. WFD compliant, updated in the Zinc working group under the SG-R (2015)
7440-70-2	Calcium	EQS	CZ	190000	RBSP-ECOSTAT, UBA (2014)	190000	
		EQS	LU	200000	RBSP-ECOSTAT, UBA (2014)		
		EQS	PL	200000	RBSP-ECOSTAT, UBA (2014)		
7782-49-2	Selenium	EQS	NL	0.05	NL Specific Pollutants	0.05	**Eurometaux:** Value in ECHA dossier considered more reasonable due to the most comprehensive and robust data set used in the analysis, to the reliability of the derivation process, and the typical natural background concentration of Se in fresh surface water (0.32 µg Se/L) **DE:** The PNEC: 0.05 µg/L to low compared with Background water 90P = 1.10 µg/L (FOREGS, 2005) STE score should be calculated with 1.1 µg/L. Netherlands 10P = 0.2 µg/L. (Osté, 2013)
		EQS	AT	5.3	RBSP-ECOSTAT, UBA (2014)		

CAS number	Substance name	Type	MS/ Institution	Value (µg/L)	Reference	Selected PNEC/EQS fw, eco (µg/L)	Comments
		EQS	BE	2	RBSP-ECOSTAT, UBA (2014)		
		EQS	CZ	2	RBSP-ECOSTAT, UBA (2014)		
		EQS	DE	2.5	RBSP-ECOSTAT, UBA (2014)		
		EQS	ES	1	RBSP-ECOSTAT, UBA (2014)		
		EQS	LU	2.9	RBSP-ECOSTAT, UBA (2014)		
		EQS	PL	20	RBSP-ECOSTAT, UBA (2014)		
		EQS	RO	0.07	RBSP-ECOSTAT, UBA (2014)		
		EQS	SI	6	RBSP-ECOSTAT, UBA (2014)		
		PNEC	ECHA	2.67	ECHA DOSSIER		
		PNEC	INERIS	0.88	SSD with all available valid data, mainly from the ECOTOX US EPA		

Table III-3. List of PNEC/EQS$_{dw, hh}$ and drinking water guideline values.

PNEC$_{dw, hh}$ were selected following the TGD-EQS (2011): (1) WHO guideline value, (2) parametric value (RIVM or US-EPA) and (3) parametric precautionary value of 0.1 µg/L according to Dir. 98/83/EC for substances used as PPP.

CAS	Substance	PNEC/EQS dw, hh (µg/L)	Reference
106-93-4	1,2-Dibromoethane	0.4	WHO, 2011
52918-63-5	Deltamethrin	0.1	Dir. 98/83/EC
60168-88-9	Fenarimol	0.1	Dir. 98/83/EC
57-74-9	Chlordane	0.2	WHO, 2011
66230-04-4	Esfenvalerate	0.1	Dir. 98/83/EC
52-68-6	Trichlorfon	0.1	Dir. 98/83/EC
68359-37-5	Cyfluthrin	0.1	Dir. 98/83/EC
56-72-4	Coumaphos	0.1	Dir. 98/83/EC
83121-18-0	Teflubenzuron	0.1	Dir. 98/83/EC
24017-47-8	Triazophos	0.1	Dir. 98/83/EC
82097-50-5	Triasulfuron	0.1	Dir. 98/83/EC
950-37-8	Methidathion	3.5	US-EPA
102851-06-9	Tau-fluvalinate	0.1	Dir. 98/83/EC
150-68-5	Monuron	0.1	Dir. 98/83/EC
298-04-4	Disulfoton	0.14	US-EPA
35367-38-5	Diflubenzuron	0.1	Dir. 98/83/EC
2385-85-5	Mirex	0.7	US-EPA
67306-00-7	Fenpropidin	0.1	Dir. 98/83/EC
3397-62-4	Desisopropyldesethylatrazine	0.1	Dir. 98/83/EC
14816-18-3	Phoxim	0.1	Dir. 98/83/EC
301-12-2	Oxydemeton-methyl	0.1	Dir. 98/83/EC
79-11-8	Chloroacetic acid	20	WHO, 2011
173159-57-4	Foramsulfuron	0.1	Dir. 98/83/EC
145701-23-1	Florasulam	0.1	Dir. 98/83/EC
2303-17-5	Triallate	0.1	Dir. 98/83/EC
52645-53-1	Permethrin	175	RIVM
55-38-9	Fenthion	0.1	Dir. 98/83/EC
56-55-3	Benzo(a)anthracene	0.175	RIVM
1113-02-6	Omethoate	1.4	US-EPA

7440-61-1	Uranium	30	WHO, 2011
7782-49-2	Selenium	40	WHO, 2011
2642-71-9	Azinphos-ethyl	0.1	Dir. 98/83/EC
7786-34-7	Mevinphos	0.1	Dir. 98/83/EC
2163-68-0	2-Hydroxyatrazine	200	WHO, 2011
563-12-2	Ethion	1.75	US-EPA
121-75-5	Malathion	70	US-EPA
7440-28-0	Thallium	0.245	US-EPA
114-26-1	Propoxur	0.1	Dir. 98/83/EC
129-00-0	Pyrene	105	US-EPA
7440-22-4	Silver	17.5	US-EPA
14797-65-0	Nitrite (NO2)	3000	WHO, 2011
91465-08-6	lambda-Cyhalothrin	2	Dir. 98/83/EC
56-38-2	Parathion	21	US-EPA
7440-39-3	Barium	700	WHO, 2011
72-43-5	Methoxychlor	20	RIVM
5598-13-0	Chlorpyriphos-methyl	35	RIVM
111991-09-4	Nicosulfuron	0.1	Dir. 98/83/EC
7429-90-5	Aluminium	200	Dir. 98/83/EC
29232-93-7	Pirimiphos-methyl	0.1	Dir. 98/83/EC
668-34-8	Triphenyltin	0.1	Dir. 98/83/EC
83164-33-4	Diflufenican	700	RIVM
138261-41-3	Imidacloprid	0.1	Dir. 98/83/EC
76-03-9	Trichloroacetic acid	200	WHO, 2011
314-40-9	Bromacil	0.1	Dir. 98/83/EC
1007-28-9	6-Deisopropylatrazine	70	RIVM
2032-65-7	Methiocarb	0.1	Dir. 98/83/EC
74223-64-6	Metsulfuron-methyl	0.1	Dir. 98/83/EC
7440-41-7	Beryllium	7	US-EPA
1031-07-8	Endosulfan sulfate	21	RIVM
7439-96-5	Manganese	50	Dir. 98/83/EC
15307-86-5	Diclofenac	5600	US-EPA
50-28-2	17-beta-Estradiol	0.175	US-EPA
333-41-5	Diazinon	0.7	RIVM
111988-49-9	Thiacloprid	0.1	Dir. 98/83/EC
7439-89-6	Iron	200	Dir. 98/83/EC

60-51-5	Dimethoate	6	WHO, 2011
7664-41-7	Ammonia	500	Dir. 98/83/EC
53-70-3	Dibenz(a,h)anthracene	1.75	RIVM
106-47-8	4-Chloroaniline	0.0315	RIVM
141776-32-1	Sulfosulfuron	0.1	Dir. 98/83/EC
98-95-3	Nitrobenzene	1.75	US-EPA
79277-27-3	Thifensulfuron methyl	0.1	Dir. 98/83/EC
7286-69-3	Sebuthylazine	0.1	Dir. 98/83/EC
7440-66-6	Zinc	1050	US-EPA
7440-23-5	Sodium	200000	Dir. 98/83/EC
95-50-1	1,2-Dichlorobenzene	1000	WHO, 2011
7440-24-6	Strontium	2100	US-EPA
7440-48-4	Cobalt	4.9	RIVM
86-73-7	Fluorene	140	RIVM
75-01-4	Chloroethene	0.3	WHO, 2011
21725-46-2	Cyanazine	0.6	WHO, 2011
108-95-2	Phenol	140	RIVM
7439-95-4	Magnesium	672000	US-EPA
63-25-2	Carbaril	0.1	Dir. 98/83/EC
121-14-2	2,4-Dinitrotoluene	7	RIVM
335-67-1	Perfluorooctanoic acid (PFOA)	0.35	RIVM
1014-69-3	Desmetryn	0.1	Dir. 98/83/EC
106-46-7	1,4-Dichlorobenzene	300	WHO, 2011
16887-00-6	Chloride	250000	Dir. 98/83/EC
3380-34-5	Triclosan	17.5	US-EPA
78-87-5	1,2-Dichloropropane	40	WHO, 2011
85-01-8	Phenanthrene	140	RIVM
95-94-3	1,2,4,5-Tetrachlorobenzene	0.735	RIVM
7440-31-5	Tin	700	RIVM
3424-82-6	2,2-(2-Chlorophenyl-4'-chlorophenyl)-1,1-dichloroethene (DDE, o,p')	2	Dir. 98/83/EC
208-96-8	Acenaphthylene	175	RIVM
53-19-0	DDD, o,p'	2	Dir. 98/83/EC
7440-47-3	Chromium	50	WHO, 2011

7440-62-2	Vanadium	3.5	US-EPA
1330-78-5	Tricresyl Phosphate	245	RIVM
108-90-7	Chlorobenzene	70	US-EPA
16984-48-8	Fluoride	1500	WHO, 2011
7440-42-8	Boron	2400	WHO, 2011
80-05-7	Bisphenol A	14	RIVM
90-12-0	1-Methylnaphthalene	140	RIVM
298-46-4	Carbamazepine	56	RIVM
139-13-9	Nitrilotriacetic acid	200	WHO, 2011
118134-30-8	Spiroxamine	87.5	RIVM
723-46-6	Sulfamethoxazole	455	RIVM
10605-21-7	Carbendazim	0.1	Dir. 98/83/EC
75-34-3	1,1-Dichloroethane	700	US-EPA
126-73-8	Tributyl phosphate	280	RIVM
83-32-9	Acenaphthene	210	US-EPA
34256-82-1	Acetochlor	70	Dir. 98/83/EC
142459-58-3	Flufenacet	14	RIVM
7440-50-8	Copper	2000	WHO, 2011
7440-38-2	Arsenic	10	WHO, 2011
100-41-4	Ethylbenzene	300	WHO, 2011
19937-59-8	Metoxuron	0.1	Dir. 98/83/EC
94-74-6	2-Methyl-4-chlorophenoxyacetic acid (aka MCPA)	2	WHO, 2011
1563-66-2	Carbofuran	7	WHO, 2011
19666-30-9	Oxadiazon	12.6	RIVM
16752-77-5	Methomyl	0.1	Dir. 98/83/EC
7440-36-0	Antimony	20	WHO, 2011
15545-48-9	Chlorotoluron	30	WHO, 2011
541-73-1	1,3-Dichlorobenzene	10.5	US-EPA
139-40-2	Propazine	0.1	Dir. 98/83/EC
50-00-0	Formaldehyde	700	Dir. 98/83/EC
330-55-2	Linuron	0.1	Dir. 98/83/EC
94-75-7	2,4-Dichlorophenoxyacetic acid (aka 2,4-D)	0.1	Dir. 98/83/EC
108-42-9	3-Chloroaniline	0.0315	RIVM

67129-08-2	Metazachlor	0.1	Dir. 98/83/EC
15687-27-1	Ibuprofen	385	RIVM
92-52-4	Biphenyl	175	US-EPA
100-42-5	Styrene	20	WHO, 2011
122931-48-0	Rimsulfuron	0.1	Dir. 98/83/EC
122-39-4	Diphenylamine	87.5	Dir. 98/83/EC
67-72-1	Hexachloroethane	2.45	RIVM
86-50-0	Azinphos-methyl	0.1	Dir. 98/83/EC
10265-92-6	Methamidophos	0.1	Dir. 98/83/EC
122-14-5	Fenitrothion	0.1	Dir. 98/83/EC
933-78-8	2,3,5-Trichlorphenol	10.5	RIVM
144550-36-7	Iodosulfuron	0.1	Dir. 98/83/EC
13684-56-5	Desmedipham	0.1	Dir. 98/83/EC
933-75-5	2,3,6-Trichlorphenol	10.5	RIVM
106-89-8	Epichlorhydrin (1-chloro-2,3-epoxypropane)	0.4	WHO, 2011
40487-42-1	Pendimethalin	20	WHO, 2011
142-28-9	1,3-Dichloropropane	70	US-EPA
95-51-2	2-Chloroaniline	0.0315	RIVM
542-75-6	1,3-Dichloropropene	20	WHO, 2011
709-98-8	Propanil	0.1	Dir. 98/83/EC
95-95-4	2,4,5-Trichlorophenol	350	RIVM
1746-81-2	Monolinuron	0.1	Dir. 98/83/EC
67564-91-4	Fenpropimorph	10.5	RIVM
18691-97-9	Methabenzthiazuron	0.1	Dir. 98/83/EC
98-82-8	Isopropylbenzene	350	RIVM
540-59-0	1,2-Dichloroethene	50	WHO, 2011
133-07-3	Folpet	0.1	Dir. 98/83/EC
51235-04-2	Hexazinone	0.1	Dir. 98/83/EC
88-06-2	2,4,6-Trichlorophenol	200	WHO, 2011
133855-98-8	Epoxiconazole	28	RIVM
59-50-7	Chlorocresol	0.1	Dir. 98/83/EC
120-83-2	2,4-Dichlorophenol	10.5	Dir. 98/83/EC
85509-19-9	Flusilazole	7	RIVM
101200-48-0	Tribenuron-methyl	0.1	Dir. 98/83/EC
101205-02-1	Cycloxydim	0.1	Dir. 98/83/EC

101-21-3	Chlorpropham	0.1	Dir. 98/83/EC
103-90-2	Acetaminophen (Paracetamol)	1190	RIVM
106-48-9	4-Chlorophenol	10.5	RIVM
1066-51-9	Aminomethylphosphonic acid (AMPA)	1050	Dir. 98/83/EC
1071-83-6	Glyphosate	350	Dir. 98/83/EC
107534-96-3	Tebuconazole	105	RIVM
108-43-0	3-Chlorophenol	10.5	RIVM
1085-98-9	Dichlofluanide	1225	RIVM
108-88-3	Toluene	700	WHO, 2011
110488-70-5	Dimethomorph	0.1	Dir. 98/83/EC
115-96-8	Tris(2-chloroethyl)phosphate (TCEP)	1540	RIVM
116-06-3	Aldicarb	10	WHO, 2011
116-29-0	Tetradifon	52.5	RIVM
117428-22-5	Picoxystrobin	0.1	Dir. 98/83/EC
119446-68-3	Difenoconazole	35	RIVM
1194-65-6	Dichlobenil	0.1	Dir. 98/83/EC
120-32-1	Chlorophene	0.1	Dir. 98/83/EC
120-36-5	Diclorprop	100	WHO, 2011
120923-37-7	Amidosulfuron	0.1	Dir. 98/83/EC
121552-61-2	Cyprodinil	0.1	Dir. 98/83/EC
123-91-1	1,4-Dioxane	50	WHO, 2011
124-48-1	Dibromochloromethane	100	WHO, 2011
126535-15-7	Triflusulfuron-methyl	0.1	Dir. 98/83/EC
126-71-6	Triisobutyl phosphate	7455	RIVM
126833-17-8	Fenhexamid	0.1	Dir. 98/83/EC
128639-02-1	Carfentrazone-ethyl	0.1	Dir. 98/83/EC
131-11-3	Dimethyl phthalate	32900	RIVM
131341-86-1	Fludioxonil	1295	RIVM
131860-33-8	Azoxystrobin	0.1	Dir. 98/83/EC
131983-72-7	Triticonazole	0.1	Dir. 98/83/EC
1330-20-7	Xylene (mixed isomers)	500	WHO, 2011
133-06-2	Captan	0.1	Dir. 98/83/EC
134-62-3	Diethyltoluamide (DEET)	2625	RIVM

13684-63-4	Phenmedipham	0.1	Dir. 98/83/EC
141517-21-7	Trifloxystrobin	350	RIVM
143390-89-0	Kresoxim-methyl	0.1	Dir. 98/83/EC
152019-73-3	Metolachlor OA	0.1	Dir. 98/83/EC
15299-99-7	Napropamide	0.1	Dir. 98/83/EC
153719-23-4	Thiamethoxam	0.1	Dir. 98/83/EC
15950-66-0	2,3,4-Trichlorphenol	10.5	RIVM
1610-18-0	Prometon	52.5	Dir. 98/83/EC
1634-04-4	Methyl-tert-butyl ether (MTBE)	1050	RIVM
1646-88-4	Aldicarb sulfone	3.5	Dir. 98/83/EC
1689-84-5	Bromoxynil	0.1	Dir. 98/83/EC
1698-60-8	Chloridazon	0.1	Dir. 98/83/EC
1702-17-6	Clopyralid	0.1	Dir. 98/83/EC
17040-19-6	Demeton-S-methylsulfon	0.1	Dir. 98/83/EC
171118-09-5	Metolachlor ESA	0.1	Dir. 98/83/EC
17254-80-7	Chloridazon methyl-desphenyl	0.1	Dir. 98/83/EC
175013-18-0	Pyraclostrobine	105	RIVM
188425-85-6	Boscalid	0.1	Dir. 98/83/EC
1897-45-6	Chlorothalonil	0.1	Dir. 98/83/EC
1918-00-9	Dicamba	105	Dir. 98/83/EC
1982-47-4	Chloroxuron	0.1	Dir. 98/83/EC
2008-58-4	2,6-Dichlorobenzamide	0.1	Dir. 98/83/EC
21087-64-9	Metribuzin	0.1	Dir. 98/83/EC
210880-92-5	Clothianidin	0.1	Dir. 98/83/EC
2164-08-1	Lenacil	0.1	Dir. 98/83/EC
2212-67-1	Molinate	6	WHO, 2011
23103-98-2	Pirimicarb	0.1	Dir. 98/83/EC
23135-22-0	Oxamyl	87.5	Dir. 98/83/EC
23950-58-5	Propyzamide	0.1	Dir. 98/83/EC
24579-73-5	Propamocarb	0.1	Dir. 98/83/EC
25057-89-0	Bentazone	0.1	Dir. 98/83/EC
26225-79-6	Ethofumesate	0.1	Dir. 98/83/EC
26259-45-0	Secbumeton	0.1	Dir. 98/83/EC
30125-63-4	Desethylterbuthylazine	14	RIVM

30125-63-4	Terbutylazine-desethyl	14	RIVM
302-17-0	Chloral hydrate	350	Dir. 98/83/EC
3060-89-7	Metobromuron	0.1	Dir. 98/83/EC
307-24-4	Perfluorohexanoic acid (PFHxA)	0.1	RIVM
32809-16-8	Procymidone	0.1	Dir. 98/83/EC
35554-44-0	Imazalil	87.5	RIVM
36734-19-7	Iprodione	210	RIVM
37350-58-6	Metoprolol	9.8	RIVM
375-73-5	Perfluorobutanesulfonate (PFBS)	3	RIVM
41394-05-2	Metamitron	0.1	Dir. 98/83/EC
41859-67-0	Bezafibrate	35	RIVM
43121-43-3	Triadimefon	0.1	Dir. 98/83/EC
50471-44-8	Vinclozolin	87.5	Dir. 98/83/EC
51218-45-2	Metolachlor	10	WHO, 2011
52888-80-9	Prosulfocarb	0.1	Dir. 98/83/EC
53112-28-0	Pyrimethanil	0.1	Dir. 98/83/EC
534-52-1	Dinitro-o-cresol (DNOC)	0.1	Dir. 98/83/EC
55179-31-2	Bitertanol	10.5	RIVM
55219-65-3	Triadimenol	0.1	Dir. 98/83/EC
55335-06-3	Triclopyr	0.1	Dir. 98/83/EC
57018-04-9	Tolclofos-methyl	224	RIVM
57-12-5	Cyanides (as total CN)	50	Dir. 98/83/EC
57837-19-1	Metalaxyl	0.1	Dir. 98/83/EC
5915-41-3	Terbuthylazine	7	RIVM
60-00-4	Edetic acid (EDTA)	600	WHO, 2011
60207-90-1	Propiconazole	140	RIVM
6190-65-4	Desethylatrazine	70	RIVM
62-53-3	Aniline	5.04	RIVM
630-20-6	1,1,1,2-Tetrachloroethane	105	US-EPA
66246-88-6	Penconazole	105	RIVM
67747-09-5	Prochloraz	35	RIVM
69377-81-7	Fluroxypyr	0.1	Dir. 98/83/EC
71-55-6	1,1,1-Trichloroethane	980	US-EPA
7287-19-6	Prometryn	14	Dir. 98/83/EC

731-27-1	Tolylfluanid	350	RIVM
738-70-5	Trimethoprim	14.7	RIVM
7439-98-7	Molybdenum	17.5	US-EPA
75-25-2	Bromoform	100	WHO, 2011
75-27-4	Dichlorobromomethane	60	WHO, 2011
76674-21-0	Flutriafol	0.1	Dir. 98/83/EC
78587-05-0	Hexythiazox	0.1	Dir. 98/83/EC
79-00-5	1,1,2-Trichloroethane	14	US-EPA
79241-46-6	Fluazifop-P-butyl	0.1	Dir. 98/83/EC
79622-59-6	Fluazinam	0.1	Dir. 98/83/EC
80-09-1	Bisphenol S	1750	RIVM
8065-48-3	Demeton	0.1	Dir. 98/83/EC
82558-50-7	Isoxaben	0.1	Dir. 98/83/EC
82-68-8	Quintozene	0.1	Dir. 98/83/EC
834-12-8	Ametryn	0.1	Dir. 98/83/EC
84-66-2	Diethyl phthalate	2625	RIVM
84-74-2	Di-n-butylphthalate	182	RIVM
87-65-0	2,6-Dichlorophenol	0.1	Dir. 98/83/EC
87674-68-8	Dimethenamid	0.1	Dir. 98/83/EC
88-72-2	o-Nitrotoluene	35	US-EPA
88-85-7	Dinoseb	3.5	Dir. 98/83/EC
90717-03-6	Quinmerac	0.1	Dir. 98/83/EC
919-86-8	Demeton-S-methyl	0.1	Dir. 98/83/EC
93-65-2	Mecoprop	10	WHO, 2011
93-72-1	Fenoprop	9	RIVM
93-76-5	2,4,5-Trichlorophenoxyacetic acid	9	WHO, 2011
94361-06-5	Cyproconazole	0.1	Dir. 98/83/EC
94-81-5	2-Methyl-4-chlorophenoxybutyric acid (aka MCPB)	0.1	Dir. 98/83/EC
94-82-6	4-(2,4-Dichlorophenoxy)butyric acid (aka 2,4-DB)	90	RIVM
95-57-8	2-Chlorophenol	17.5	RIVM
96-12-8	1,2-Dibromo-3-chloropropane	1	WHO, 2011

96-18-4	1,2,3-Trichloropropane	28	US-EPA
96525-23-4	Flurtamone	0.1	Dir. 98/83/EC
99-87-6	p-Cymene	140	RIVM

Table III-4. List of PNEC/EQS$_{water, hh food}$

CAS	Substance	PNEC/EQS (µg/L)	Source/ Reference
1031-07-8	Endosulfan sulfate	2.04	RIVM (NL) as a tentative EQS hh food
107534-96-3	Tebuconazole	23.41	RIVM (NL) as a tentative EQS hh food
1085-98-9	Dichlofluanid	295.89	RIVM (NL) as a tentative EQS hh food
116-29-0	Tetradifon	0.59	RIVM (NL) as a tentative EQS hh food
118134-30-8	Spiroxamine	17.49	RIVM (NL) as a tentative EQS hh food
119446-68-3	Difenoconazole	1.84	RIVM (NL) as a tentative EQS hh food
129-00-0	Pyrene	20.20	RIVM (NL) as a tentative EQS hh food
131341-86-1	Fludioxonil	61.53	RIVM (NL) as a tentative EQS hh food
1330-78-5	Tricresyl Phosphate	5.37	RIVM (NL) as a tentative EQS hh food
133855-98-8	Epoxiconazole	486.96	RIVM (NL) as a tentative EQS hh food
141517-21-7	Trifloxystrobin	14.12	RIVM (NL) as a tentative EQS hh food
142459-58-3	Flufenacet	2.56	RIVM (NL) as a tentative EQS hh food
15687-27-1	Ibuprofen	230.88	RIVM (NL) as a tentative EQS hh food
175013-18-0	Pyraclostrobine	2.59	RIVM (NL) as a tentative EQS hh food
19666-30-9	Oxadiazon	0.18	RIVM (NL) as a tentative EQS hh food
208-96-8	Acenaphthylene	11.23	RIVM (NL) as a tentative EQS hh food
333-41-5	Diazinon	0.17	RIVM (NL) as a tentative EQS hh food
35554-44-0	Imazalil	27.03	RIVM (NL) as a tentative EQS hh food
36734-19-7	Iprodione	10.87	RIVM (NL) as a tentative EQS hh food
41859-67-0	Bezafibrate	2.36	RIVM (NL) as a tentative EQS hh food
52645-53-1	Permethrin	6.79	RIVM (NL) as a tentative EQS hh food
53-70-3	Dibenz(a,h)anthracene	0.02	RIVM (NL) as a tentative EQS hh food
55179-31-2	Bitertanol	1.07	RIVM (NL) as a tentative EQS hh food
5598-13-0	Chlorpyriphos methyl	0.34	RIVM (NL) as a tentative EQS hh food
56-55-3	Benzo(a)anthracene	0.01	RIVM (NL) as a tentative EQS hh food
57018-04-9	Tolclofos-methyl	5.41	RIVM (NL) as a tentative EQS hh food
60207-90-1	Propiconazole	13.53	RIVM (NL) as a tentative EQS hh food
66246-88-6	Penconazole	5.71	RIVM (NL) as a tentative EQS hh food
67564-91-4	Fenpropimorph	0.18	RIVM (NL) as a tentative EQS hh food
67-72-1	Hexachloroethane	0.08	RIVM (NL) as a tentative EQS hh food
67747-09-5	Prochloraz	2.25	RIVM (NL) as a tentative EQS hh food
72-43-5	Methoxychlor	0.97	RIVM (NL) as a tentative EQS hh food

CAS	Substance	PNEC/EQS (µg/L)	Source/ Reference
731-27-1	Tolylfluanid	82.26	RIVM (NL) as a tentative EQS hh food
80-05-7	Bisphenol A	5.56	RIVM (NL) as a tentative EQS hh food
83164-33-4	Diflufenican	8.53	RIVM (NL) as a tentative EQS hh food
84-74-2	Di-n-butylphthalate	18.95	RIVM (NL) as a tentative EQS hh food
85509-19-9	Flusilazole	0.49	RIVM (NL) as a tentative EQS hh food
86-73-7	Fluorene	4.64	RIVM (NL) as a tentative EQS hh food
90-12-0	1-Methylnaphthalene	10.42	RIVM (NL) as a tentative EQS hh food
92-52-4	Biphenyl	69.72	RIVM (NL) as a tentative EQS hh food
93-72-1	Fenoprop	0.99	RIVM (NL) as a tentative EQS hh food
94-82-6	4-(2,4-Dichlorophenoxy)butyric acid (2,4-DB)	7.44	RIVM (NL) as a tentative EQS hh food
95-94-3	1,2,4,5-Tetrachlorobenzene	0.00	RIVM (NL) as a tentative EQS hh food
95-95-4	2,4,5-Trichlorophenol	11.42	RIVM (NL) as a tentative EQS hh food
98-82-8	Isopropylbenzene	171.55	RIVM (NL) as a tentative EQS hh food
99-87-6	p-Cymene	9.98	RIVM (NL) as a tentative EQS hh food

Table III-5. List of PNEC/EQS$_{sw, eco}$

CAS number	Substance name	Available PNEC/EQS				Selected PNEC/EQS
		PNEC/EQS (µg/L)	Country / Institution	Water type	Reference	µg/L
7440-50-8	Copper	5.2	ECHA	Marine water	Copper ECHA dossier	
		7.0	BE	Transitional water	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	
		3.8	BE	Coastal water	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	
		5.0	IE	Transitional / coastal water	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	
		5.0	UK	Transitional / coastal water	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	
		3.76	UK	Coastal water	Environment Agency UK, 2016	3.76
7440-66-6	Zinc	6.1	ECHA	Marine water	Zinc ECHA dossier	
		3.0	NL	Transitional / coastal water	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	3.0
		20.0	BE	Transitional water	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	
		3.0	BE	Coastal water	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	3.0
		40.0	IE	Transitional / coastal water	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	
		8.0	SE	Transitional / coastal water	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	
		40.0	UK	Transitional / coastal water	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	
		6.8	UK	Coastal water	Environment Agency UK, 2016	
7440-47-3	Chromium	0.6	NL	Transitional / coastal water	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	0.6
		5.0	BE	Transitional waters	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	
		4.0	IT	Transitional / coastal water	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	

CAS number	Substance name	Available PNEC/EQS				Selected PNEC/EQS
		PNEC/EQS (µg/L)	Country / Institution	Water type	Reference	µg/L
		3.0	SE	Transitional / coastal water	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	
18540-29-9	Chromium (VI)	0.6	UK	Transitional / coastal water	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	
		0.6	UK	Coastal water	Environment Agency UK, 2016	0.6
7440-38-2	Arsenic	3.0	BE	Transitional water	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	3.0
		20.0	IE	Transitional / coastal water	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	
		5.0	IT	Transitional / coastal water	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	
		25.0	UK	Transitional / coastal water	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	
		25.0	UK	Coastal water	Environment Agency UK, 2016	
129-00-0	Pyrene	0.04	BE	Transitional water	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	0.04
		0.04	BE	Marine water	Ghekiere A et al., 2013	
56-55-3	Benzo(a)anthracene	0.3	BE	Transitional water	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	0.3
		0.3	BE	Marine water	Ghekiere A et al., 2013	
85-01-8	Phenanthrene	0.1	BE	Transitional water	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	0.1
		0.03	RO	Transitional / coastal water	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	
		1.3	BU	Transitional water	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	
		0.1	BE	Marine water	Ghekiere A et al., 2013	
218-01-9	Chrysene	1.0	BE	Transitional water	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	1.0
		1.0	BE	Marine water	Ghekiere A et al., 2013	
108-88-3	Toluene	680		Marine water	Toluene ECHA dossier	
		74	UK	Coastal water	Environment Agency UK, 2016	74

CAS number	Substance name	Available PNEC/EQS				Selected PNEC/EQS
		PNEC/EQS (µg/L)	Country / Institution	Water type	Reference	µg/L
330-55-2	Linuron	0.5	UK	Coastal water	Environment Agency UK, 2016	
		0.5	UK	Salt water	Crane M et al., 2007	
		0.3	BE	Marine water	Ghekiere A et al., 2013	0.3

Table III-6. List of PNEC/EQS$_{sed, eco}$

CAS number	Substance name	Available PNEC/EQS				Selected PNEC/EQS	
		PNEC/EQS_sed (µg/kg) dw	Country / Institution	Sediment type	Reference	µg/kg ww	Comments
7440-47-3	Chromium	90000	US, ECHA	fresh water	US-EPA, 2000; EU risk assessment report, 2005	90000	
		640000	DE		DG Environment report, 2012, Johnson, I., et al., WRcRef: UC8981/1		
		205700	ECHA		Chromium ECHA dossier		
53-19-0	DDD, o,p'	0.99			James et al., 2009	0.99	EqP INERIS
56-55-3	Benzo(a)anthracene	27.7			James et al., 2009	27.7	EqP INERIS
		10000	DK		DG Environment report, 2012, Johnson, I., et al., WRcRef: UC8981/1		
7440-38-2	Arsenic	7240	UK; CAN	marine water	Cole et al., 1999		
		12000	IT	coastal water	Maggi et al., 2012		
		17000	US, ECHA	fresh water	US-EPA, 2000	17000	
		25000	FR		Mamindy-Pajany, Y., et al., 2013		
7440-50-8	Copper	87000	ECHA		Copper ECHA dossier	87000	
		160000	DE		DG Environment report, 2012, Johnson, I., et al., WRcRef: UC8981/1		
		197000	US	fresh water	US-EPA, 2000		
7440-66-6	Zinc	117800	ECHA		Zinc ECHA dossier	117800	
		315000	US	fresh water	US-EPA, 2000		
85-01-8	Phenanthrene	2708			James et al., 2009	2708	EqP INERIS
		3000	DK		DG Environment report, 2012, Johnson, I., et al., WRcRef: UC8981/1		
1002-53-5	Dibutyltin (dichloride)	7.0	ECHA	fresh water	Dibutyltin dichloride ECHA dossier	6.526	

CAS number	Substance name	Available PNEC/EQS				Selected PNEC/EQS	
		PNEC/EQS_sed (µg/kg) dw	Country / Institution	Sediment type	Reference	µg/kg ww	Comments
	Dibutyltin	100	DE		DG Environment report, 2012, Johnson, I., et al., WRcRef: UC8981/1		
1163-19-5	Decabromodiphenyl ether (BDE-209)	384000	ECHA	fresh water	BDE-209 ECHA dossier	384000	
1461-25-2	Tetrabutyltin	0.202			James et al., 2009	0.202	EqP INERIS
207122-16-5	2,2',3,4,4',5',6-Heptabromodiphenyl ether (BDE-183)	266			EqP (calculated by JRC)	266	
		49000			BDE EQS datasheet, 2005		
668-34-8	Triphenyltin	25.6			EqP (calculated by JRC)		
		20	DE		DG Environment report, 2012, Johnson, I., et al., WRcRef: UC8981/1	20	
78763-54-9	Monobutyltin	1.17			James et al., 2009	1.17	EqP INERIS
1336-36-3	Polychlorinated biphenyls (PCB) sum	0.403			James et al., 2009		EqP INERIS; STE score is not reported since PCBs were measured only in 3MS

Note: EqP= Equillibrium Partitioning

Table III-7. List of PNEC/EQS$_{biota(fish),\ secpois}$

CAS number	Substance name	Available PNEC/EQS				Selected PNEC/EQS	
		PNEC/EQS µg/kg) ww	Country / Institution	Taxom	Reference	µg/kg ww	Comments
7440-66-6	Zinc	500	DK	Bivalves; marine	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	n.a.	Not relevant, because essential element
35065-27-1	2,2',4,4',5,5'-Hexachlorobiphenyl (PCB-153)	0.5	DK	Bivalves; marine	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	0.5	Insufficient data available on effects of exposure to single NDL-PCBs
35065-28-2	2,2',3,4,4',5'-Hexachlorobiphenyl (PCB-138)	0.5	DK	Bivalves; marine	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	0.5	Insufficient data available on effects of exposure to single NDL-PCBs
35065-29-3	2,2',3,4,4',5,5'-Heptachlorobiphenyl (PCB-180)	0.5	DK	Bivalves; marine	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	0.5	Insufficient data available on effects of exposure to single NDL-PCBs
35693-99-3	2,2',5,5'-Tetrachlorobiphenyl (PCB-52)	0.2	DK	Bivalves; marine	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	0.2	Insufficient data available on effects of exposure to single NDL-PCBs
37680-73-2	2,2',4,5,5'-Pentachlorobiphenyl (PCB-101)	0.5	DK	Bivalves; marine	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	0.5	Insufficient data available on effects of exposure to single NDL-PCBs
7012-37-5	2,4,4'-Trichlorobiphenyl (PCB-28)	0.2	DK	Bivalves; marine	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	0.2	Insufficient data available on effects of exposure to single NDL-PCBs
7440-50-8	Copper	200	DK	Fish, marine	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	n.a.	Not relevant, because essential element
7440-38-2	Arsenic	missing				missing	
7440-47-3	Chromium	50	DK	Bivalves; marine	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	n.a.	Not relevant
		17000	ECB		European Chemicals Bureau, Chromium EU risk assessment report, 2005	17000	secondary poisoning Cr(VI)
182346-21-0	BDE-85 (2,2',3,4,4'-pentabromodiphenyl ether)	0.0085			Directive 2013/39/EU	0.0085	

Table III-8. List of PNEC/EQS biota(mollusc), secpois

CAS number	Substance name	Available PNEC/EQS				Selected PNEC/EQS	
		PNEC/EQS µg/kg ww	Country / Institution	Taxom	Reference	µg/kg ww	Comments
7440-50-8	Copper	200	DK	Bivalves; marine	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	n.a.	not pose a risk for secondary poisoning (REACH dossier)
		1.49	RO	not clear	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1		unrealisticly low value; not pose a risk for secondary poisoning (REACH dossier)
		2727	UK	Bivalves; marine	Warn T et al., 2010		prefered in Sc2_PNEC QC
7440-66-6	Zinc	500	DK	Bivalves; marine	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	n.a.	not pose a risk for secondary poisoning (REACH dossier)
		45455	UK	Bivalves; marine	Warn T et al., 2010		prefered in Sc2_PNEC QC
35065-27-1	2,2',4,4',5,5'-Hexachlorobiphenyl (PCB-153)	0.05	DK	Bivalves; marine	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	0.05	Insufficient data available on effects of exposure to single NDL-PCBs
35065-28-2	2,2',3,4,4',5'-Hexachlorobiphenyl (PCB-138)	0.05	DK	Bivalves; marine	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	0.05	Insufficient data available on effects of exposure to single NDL-PCBs
7440-47-3	Chromium	50	DK	Bivalves; marine	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1		very low PNEC from DK
		17000	ECB	Mouse secpois	European Chemicals Bureau, Chromium EU risk assessment report, 2005		Mouse secondary poisoning by Cr(VI)
		1091	UK	Bivalves; marine	Warn T et al., 2010	1091	prefered in Sc2_PNEC QC
35065-29-3	2,2',3,4,4',5,5'-Heptachlorobiphenyl (PCB-180)	0.05	DK	Bivalves; marine	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	0.05	Insufficient data available on effects of exposure to single NDL-PCBs
35693-99-3	2,2',5,5'-Tetrachlorobiphenyl (PCB-52)	0.05	DK	Bivalves; marine	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	0.05	Insufficient data available on effects of exposure to single NDL-PCBs
37680-73-2	2,2',4,5,5'-Pentachlorobiphenyl (PCB-101)	0.05	DK	Bivalves; marine	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	0.05	Insufficient data available on effects of exposure to single NDL-PCBs
7012-37-5	2,4,4'-Trichlorobiphenyl (PCB-28)	0.02	DK	Bivalves; marine	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	0.02	Insufficient data available on effects of exposure to single NDL-PCBs
7440-38-2	Arsenic	5455	UK	Bivalves; marine	Warn T et al., 2010	5455	

CAS number	Substance name	Available PNEC/EQS				Selected PNEC/EQS	
		PNEC/EQS µg/kg ww	Country / Institution	Taxom	Reference	µg/kg ww	Comments
129-00-0	Pyrene	1.00	DK	Bivalves; marine	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	1.00	very low PNEC from DK
56-55-3	Benzo(a)anthracene	0.50	DK	Bivalves; marine	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	0.50	very low PNEC from DK
85-01-8	Phenanthrene	1.00	DK	Bivalves; marine	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	1.00	very low PNEC from DK
218-01-9	Chrysene	0.50	DK	Bivalves; marine	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	0.50	very low PNEC from DK
53-70-3	Dibenzo(a,h)anthracene	0.50	DK	Bivalves; marine	DG Environment report, 2012, Johnson I et al., WRcRef: UC8981/1	0.50	very low PNEC from DK

Annex IV: STE results

Table IV-1. STEfw, eco results - inland whole water monitoring data, $PNEC_{fw, eco}$.

For each substance, two scenarios are presented. Top/shaded: Sc2 (all monitoring records; non-quantified records set as half LOD/Q); Bottom/white: Sc2-PNEC QC (quantified records plus non-quantified samples excluding those for which ½LOD/Q > PNEC).

Note: n/a for some substances in Sc2-PNECQC indicates that they are not considered in STE since did not fulfilled the representativeness criteria for data

[1] RQ_P90 is the risk quotient between the 90th percentile of all monitoring records and the selected PNEC.
[2] RQ_P95 is the risk quotient between the 95th percentile of all monitoring records and the selected PNEC.
[3] Fspat, Ftemp and Fext stand for the spatial, temporal and extend of PNEC exceedance factors in the STE approach, calculated as described in Section 2.1, while the Final STE score is the sum of the individual factors.
[4] Only STE scores using Sc2-PNEC QC were used for the risk-based ranking of substances.

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
100-00-5	1-Chloro-4-nitrobenzene	1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
1002-53-5	Dibutyltin	0.01	1.95E+00	2.50E+00	4.93E-02	7.26E-01	7.00E-02	0.845
			7.50E-01	1.00E+00	4.18E-03	2.41E-01	4.00E-02	0.285
100-41-4	Ethylbenzene	1	7.03E-01	2.50E+00	1.82E-02	7.56E-01	7.00E-02	0.844
			5.00E-01	5.00E-01	2.00E-04	1.04E-01	4.00E-02	0.145
100-42-5	Styrene	0.63	7.94E-01	7.94E-01	5.20E-02	2.96E-01	4.00E-02	0.388
			3.97E-01	7.94E-01	7.28E-04	1.05E-01	0.00E+00	0.106
1007-28-9	6-Desisopropylatrazine	0.01	5.00E+00	5.00E+00	3.57E-01	8.92E-01	1.10E-01	1.359
			1.00E+00	1.00E+00	6.43E-03	2.93E-01	1.10E-01	0.409
101200-48-0	Tribenuron-methyl	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
101205-02-1	Cycloxydim	2150	1.16E-05	1.16E-05	0.00E+00	0.00E+00	0.00E+00	0.000
			1.16E-05	1.16E-05	0.00E+00	0.00E+00	0.00E+00	0.000
101-21-3	Chlorpropham	4	1.25E-02	1.25E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			1.25E-02	1.25E-02	0.00E+00	0.00E+00	0.00E+00	0.000
1014-69-3	Desmetryn	0.025	5.00E-01	1.00E+00	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-01	1.00E+00	0.00E+00	0.00E+00	0.00E+00	0.000
10265-92-6	Methamidophos	0.016	3.13E+00	3.13E+00	5.27E-01	8.03E-01	7.00E-02	1.400
			7.81E-01	7.81E-01	0.00E+00	0.00E+00	0.00E+00	0.000
102851-06-9	Tau-fluvalinate	0.0021	1.19E+01	1.19E+01	1.00E+00	9.99E-01	1.80E-01	2.179
			n/a	n/a	n/a	n/a	n/a	n/a
1031-07-8	Endosulfan sulfate	0.005	2.00E+00	5.00E+00	2.42E-01	7.70E-01	1.10E-01	1.123
			1.00E+00	1.00E+00	0.00E+00	0.00E+00	0.00E+00	0.000
103-65-1	n-Propylbenzene	35	1.43E-01	1.43E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			1.43E-01	1.43E-01	0.00E+00	0.00E+00	0.00E+00	0.000
103-90-2	Acetaminophen (Paracetamol)	136	2.21E-04	4.41E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			2.21E-04	4.41E-04	0.00E+00	0.00E+00	0.00E+00	0.000
104-35-8	4-Nonylphenol mono-ethoxylate (NP1EO)	0.05	3.00E+00	3.00E+00	3.80E-02	4.37E-01	7.00E-02	0.545
			1.00E+00	1.00E+00	1.13E-02	1.48E-01	4.00E-02	0.199
104-51-8	n-Butylbenzene	3.3	3.03E-01	3.03E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			3.03E-01	3.03E-01	0.00E+00	0.00E+00	0.00E+00	0.000
10605-21-7	Carbendazim	0.15	3.33E-01	1.00E+00	2.09E-02	3.67E-01	4.00E-02	0.428
			3.33E-01	1.00E+00	1.98E-02	3.50E-01	4.00E-02	0.409
106-43-4	4-Chlorotoluene	1	5.00E-01	5.00E+00	2.25E-02	7.26E-01	7.00E-02	0.819
			2.50E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
106-46-7	1,4-Dichlorobenzene	1	5.00E-01	2.50E+00	4.30E-02	4.50E-01	7.00E-02	0.563
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
106-47-8	4-Chloroaniline	0.05	1.00E+00	3.00E+00	4.51E-02	8.50E-01	7.00E-02	0.965
			1.00E+00	1.00E+00	0.00E+00	0.00E+00	0.00E+00	0.000
106-48-9	4-Chlorophenol	2	2.50E-02	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-02	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.000
1066-51-9	Aminomethylphosphonic acid (AMPA)	540	1.85E-03	3.80E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			1.85E-03	3.80E-03	0.00E+00	0.00E+00	0.00E+00	0.000
106-89-8	Epichlorhydrin (1-Chloro-2,3-epoxypropane)	0.65	3.85E+00	7.69E+00	1.33E-01	7.35E-01	1.10E-01	0.978
			7.69E-01	7.69E-01	0.00E+00	0.00E+00	0.00E+00	0.000
106-93-4	1,2-Dibromoethane	0.002	6.25E+02	1.25E+03	1.00E+00	1.00E+00	1.00E+00	3.000
			n/a	n/a	n/a	n/a	n/a	n/a
1071-83-6	Glyphosate	56	4.64E-03	9.46E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			4.64E-03	9.46E-03	0.00E+00	0.00E+00	0.00E+00	0.000
107534-96-3	Tebuconazole	0.578	8.65E-02	8.65E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			8.65E-02	8.65E-02	0.00E+00	0.00E+00	0.00E+00	0.000
108-41-8	3-Chlorotoluene	1	5.00E+00	5.00E+00	5.10E-02	7.40E-01	7.00E-02	0.861
			2.50E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
108-42-9	3-Chloroaniline	0.41	1.22E-01	1.22E-01	8.58E-04	4.03E-01	0.00E+00	0.404
			1.22E-01	1.22E-01	3.82E-04	1.66E-01	0.00E+00	0.167
108-43-0	3-Chlorophenol	2	5.00E-02	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-02	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.000
1085-98-9	Dichlofluanid	0.26	7.69E-02	7.69E-02	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
			7.69E-02	7.69E-02	0.00E+00	0.00E+00	0.00E+00	0.000
108-60-1	Dichloroisopropyl ether (Propane)	10	5.00E-01	5.00E-01	6.12E-04	0.00E+00	0.00E+00	0.001
			5.00E-01	5.00E-01	6.12E-04	0.00E+00	0.00E+00	0.001
108-67-8	1,3,5-Trimethylbenzene	2	5.00E-01	1.25E+00	1.21E-02	9.65E-01	0.00E+00	0.978
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
108-88-3	Toluene	74	6.76E-03	6.76E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			6.76E-03	6.76E-03	0.00E+00	0.00E+00	0.00E+00	0.000
108-90-7	Chlorobenzene	1	5.00E-01	5.00E-01	4.77E-03	7.87E-01	0.00E+00	0.791
			5.00E-01	5.00E-01	4.80E-04	2.17E-01	0.00E+00	0.217
108-95-2	Phenol	1	1.00E+00	3.00E+00	6.05E-02	6.41E-01	1.10E-01	0.812
			6.03E-01	1.00E+00	2.49E-02	4.59E-01	1.10E-01	0.594
110488-70-5	Dimethomorph	5.6	8.93E-03	8.93E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			8.93E-03	8.93E-03	0.00E+00	0.00E+00	0.00E+00	0.000
1113-02-6	Omethoate	0.00084	5.95E+01	5.95E+01	9.99E-01	9.99E-01	4.10E-01	2.409
			1.19E+02	1.36E+02	9.47E-01	9.44E-01	5.60E-01	2.452
111988-49-9	Thiacloprid	0.01	1.00E+00	1.00E+00	7.92E-02	3.70E-01	7.00E-02	0.519
			1.00E+00	1.00E+00	1.90E-02	1.77E-01	4.00E-02	0.236
111991-09-4	Nicosulfuron	0.0087	2.87E+00	2.87E+00	9.82E-01	9.88E-01	1.10E-01	2.080
			1.03E+01	2.26E+01	8.32E-01	7.20E-01	2.80E-01	1.833
114-26-1	Propoxur	0.01	2.50E+00	2.50E+00	8.60E-01	9.57E-01	7.00E-02	1.887
			1.00E+00	1.00E+00	1.72E-01	1.70E-01	1.10E-01	0.452
115-86-6	Triphenyl phosphate (TPT)	3.7	6.76E-02	6.76E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			6.76E-02	6.76E-02	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
115-96-8	Tris(2-chloroethyl)phosphate (TCEP)	4	4.00E-02	6.25E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			4.00E-02	6.25E-02	0.00E+00	0.00E+00	0.00E+00	0.000
116-06-3	Aldicarb	0.08	6.25E-01	6.25E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			6.25E-01	6.25E-01	0.00E+00	0.00E+00	0.00E+00	0.000
116-29-0	Tetradifon	0.11	4.55E-01	4.55E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			4.55E-01	4.55E-01	0.00E+00	0.00E+00	0.00E+00	0.000
1163-19-5	Decabromodiphenyl ether (BDE-209)	0.046	5.43E+00	2.17E+01	1.95E-01	5.50E-01	2.80E-01	1.025
			n/a	n/a	n/a	n/a	n/a	n/a
117428-22-5	Picoxystrobin	0.8	6.25E-02	6.25E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			6.25E-02	6.25E-02	0.00E+00	0.00E+00	0.00E+00	0.000
117-84-0	Di-n-octyl phthalate	19.793	4.29E-01	4.29E-01	5.50E-03	1.78E-01	0.00E+00	0.183
			4.29E-01	4.29E-01	5.50E-03	1.78E-01	0.00E+00	0.183
118134-30-8	Spiroxamine	0.02	2.50E+00	2.50E+00	4.66E-01	9.39E-01	7.00E-02	1.474
			5.00E-01	1.32E+00	5.46E-02	2.86E-01	1.10E-01	0.451
119446-68-3	Difenoconazole	0.6	1.67E-01	1.67E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			1.67E-01	1.67E-01	0.00E+00	0.00E+00	0.00E+00	0.000
1194-65-6	Dichlobenil	0.63	3.97E-02	3.97E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			3.97E-02	3.97E-02	0.00E+00	0.00E+00	0.00E+00	0.000
120-32-1	Chlorophene	0.59	4.24E-01	4.24E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			4.24E-01	4.24E-01	0.00E+00	0.00E+00	0.00E+00	0.000
120-36-5	Dichlorprop	0.1	2.00E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.00E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
120-83-2	2,4-Dichlorophenol	0.54	9.26E-02	1.85E-01	5.88E-04	2.53E-01	0.00E+00	0.254
			9.26E-02	1.85E-01	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
120923-37-7	Amidosulfuron	0.18	2.78E-01	2.78E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.78E-01	2.78E-01	0.00E+00	0.00E+00	0.00E+00	0.000
121-14-2	2,4-Dinitrotoluene	2	6.25E-02	1.50E-01	4.88E-02	6.72E-01	4.00E-02	0.761
			6.25E-02	6.50E-02	3.60E-03	1.88E-01	0.00E+00	0.192
121552-61-2	Cyprodinil	0.16	1.56E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			1.56E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
121-73-3	1-Cloro-4-nitrobenzene	0.55	9.09E-01	9.09E-01	3.48E-04	2.42E-01	0.00E+00	0.242
			9.09E-01	9.09E-01	3.48E-04	2.42E-01	0.00E+00	0.242
121-75-5	Malathion	0.0002	1.00E+02	1.25E+02	9.98E-01	9.96E-01	5.60E-01	2.554
			2.00E+02	2.31E+02	6.70E-01	9.86E-01	5.60E-01	2.216
122-14-5	Fenitrothion	0.009	2.22E+00	2.50E+00	3.64E-01	8.02E-01	7.00E-02	1.236
			5.56E-01	5.56E-01	0.00E+00	0.00E+00	0.00E+00	0.000
122-39-4	Diphenylamine	1.6	3.13E-02	3.13E-02	3.28E-04	0.00E+00	0.00E+00	0.000
			3.13E-02	3.13E-02	3.28E-04	0.00E+00	0.00E+00	0.000
122931-48-0	Rimsulfuron	0.012	2.08E+00	2.08E+00	3.66E-01	9.91E-01	7.00E-02	1.428
			8.33E-01	8.33E-01	5.70E-03	3.38E-02	0.00E+00	0.039
123-91-1	1,4-Dioxane	10000	1.25E-04	1.55E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			1.25E-04	1.55E-04	0.00E+00	0.00E+00	0.00E+00	0.000
124-48-1	Dibromochloromethane	0.63	7.94E-01	7.94E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			7.94E-01	7.94E-01	0.00E+00	0.00E+00	0.00E+00	0.000
126535-15-7	Triflusulfuron-methyl	0.13	3.85E-01	3.85E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			3.85E-01	3.85E-01	0.00E+00	0.00E+00	0.00E+00	0.000
126-71-6	Triisobutyl phosphate	11	2.27E-02	5.73E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			2.27E-02	5.73E-02	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
126-73-8	Tributyl phosphate	0.1	5.00E+00	5.00E+00	1.04E-01	5.41E-01	2.80E-01	0.926
			5.00E-01	1.00E+00	2.57E-02	2.06E-01	4.00E-02	0.272
126833-17-8	Fenhexamid	1	2.50E-02	2.50E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-02	2.50E-02	0.00E+00	0.00E+00	0.00E+00	0.000
128639-02-1	Carfentrazone-ethyl	0.092	5.43E-01	5.43E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.43E-01	5.43E-01	0.00E+00	0.00E+00	0.00E+00	0.000
129-00-0	Pyrene	0.0023	1.00E+01	2.04E+01	9.86E-01	9.17E-01	4.10E-01	2.312
			1.87E+01	3.91E+01	7.93E-01	8.53E-01	5.60E-01	2.207
131-11-3	Dimethyl phthalate	192	2.60E-03	2.60E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			2.60E-03	2.60E-03	0.00E+00	0.00E+00	0.00E+00	0.000
131341-86-1	Fludioxonil	0.5	5.00E-02	1.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-02	1.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
131860-33-8	Azoxystrobin	0.2	1.25E-01	2.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			1.25E-01	2.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
131983-72-7	Triticonazole	1	5.00E-02	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-02	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.000
1330-20-7	Xylene	17.2	5.81E-02	5.81E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			5.81E-02	5.81E-02	0.00E+00	0.00E+00	0.00E+00	0.000
133-06-2	Captan	0.34	7.35E-02	3.68E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			7.35E-02	3.68E-01	0.00E+00	0.00E+00	0.00E+00	0.000
133-07-3	Folpet	0.0881	2.84E-01	5.68E-01	4.45E-03	6.38E-01	0.00E+00	0.643
			2.84E-01	5.68E-01	0.00E+00	0.00E+00	0.00E+00	0.000
1330-78-5	Tricresyl Phosphate	0.033	2.76E-01	4.18E-01	5.39E-03	5.00E-01	0.00E+00	0.505
			2.76E-01	4.18E-01	5.39E-03	5.00E-01	0.00E+00	0.505

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
1336-36-3	PCB-sum (Polychlorinated biphenyls)	0.007	2.36E+00	2.36E+00	5.02E-02	8.05E-01	7.00E-02	0.925
			5.71E-01	5.71E-01	1.48E-02	5.11E-01	0.00E+00	0.525
133855-98-8	Epoxiconazole	0.18	2.78E-01	2.78E-01	1.80E-03	4.62E-01	0.00E+00	0.464
			2.78E-01	2.78E-01	0.00E+00	0.00E+00	0.00E+00	0.000
134-62-3	Diethyltoluamide (DEET)	41	2.15E-03	3.41E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			2.15E-03	3.41E-03	0.00E+00	0.00E+00	0.00E+00	0.000
13674-84-5	Tris(1-chloro-2-propyl) phosphate (TCPP)	640	9.53E-04	1.41E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			9.53E-04	1.41E-03	0.00E+00	0.00E+00	0.00E+00	0.000
13674-87-8	Tris(1,3-dichloropropyl) phosphate (TDCPP)	10	1.00E-02	1.30E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			1.00E-02	1.30E-02	0.00E+00	0.00E+00	0.00E+00	0.000
13684-56-5	Desmedipham	0.13	1.15E+00	1.15E+00	4.95E-02	9.41E-01	4.00E-02	1.031
			3.85E-01	3.85E-01	0.00E+00	0.00E+00	0.00E+00	0.000
13684-63-4	Phenmedipham	113	4.42E-04	4.42E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			4.42E-04	4.42E-04	0.00E+00	0.00E+00	0.00E+00	0.000
136-85-6	5-Methyl-1H-benzotriazole	150	1.40E-03	1.73E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			1.40E-03	1.73E-03	0.00E+00	0.00E+00	0.00E+00	0.000
138261-41-3	Imidacloprid	0.0083	3.61E+00	8.43E+00	9.00E-01	8.43E-01	2.80E-01	2.023
			1.08E+01	3.01E+01	6.08E-01	5.29E-01	4.10E-01	1.547
139-13-9	Nitrilotriacetic acid	5	8.08E-01	1.52E+00	7.29E-02	2.61E-01	1.10E-01	0.444
			8.08E-01	1.52E+00	7.29E-02	2.61E-01	1.10E-01	0.444

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
139-40-2	Propazine	0.25	1.00E-01	1.00E-01	2.24E-04	4.08E-01	0.00E+00	0.408
			1.00E-01	1.00E-01	8.62E-05	2.55E-01	0.00E+00	0.255
141517-21-7	Trifloxystrobin	0.27	1.85E-01	1.85E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			1.85E-01	1.85E-01	0.00E+00	0.00E+00	0.00E+00	0.000
141776-32-1	Sulfosulfuron	0.05	1.00E+00	1.00E+00	0.00E+00	0.00E+00	0.00E+00	0.000
			1.00E+00	1.00E+00	0.00E+00	0.00E+00	0.00E+00	0.000
142-28-9	1,3-Dichloropropane	2	5.00E+00	5.00E+00	9.46E-02	7.79E-01	7.00E-02	0.944
			1.25E-01	1.25E-01	0.00E+00	0.00E+00	0.00E+00	0.000
142459-58-3	Flufenacet	0.04	1.25E+00	1.25E+00	6.93E-02	4.48E-01	7.00E-02	0.587
			6.25E-01	6.25E-01	1.52E-02	2.85E-01	7.00E-02	0.370
143390-89-0	Kresoxim-methyl	0.63	3.97E-02	7.94E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			3.97E-02	7.94E-02	0.00E+00	0.00E+00	0.00E+00	0.000
144550-36-7	Iodosulfuron	0.04	8.75E-01	8.75E-01	1.79E-02	9.85E-01	4.00E-02	1.043
			8.75E-01	8.75E-01	0.00E+00	0.00E+00	0.00E+00	0.000
145701-23-1	Florasulam	0.0126	3.97E+00	3.97E+00	1.16E-01	9.65E-01	7.00E-02	1.150
			n/a	n/a	n/a	n/a	n/a	n/a
1461-25-2	Tetrabutyltin	0.14	1.79E-01	1.79E-01	4.28E-05	8.00E-01	0.00E+00	0.800
			1.79E-01	1.79E-01	0.00E+00	0.00E+00	0.00E+00	0.000
14797-65-0	Nitrite (NO2)	6	1.47E+01	2.42E+01	8.85E-01	7.95E-01	4.10E-01	2.091
			1.48E+01	2.43E+01	8.83E-01	7.93E-01	4.10E-01	2.087
14816-18-3	Phoxim	0.008	6.25E+00	6.25E+00	7.24E-01	8.64E-01	1.10E-01	1.698
			n/a	n/a	n/a	n/a	n/a	n/a
150-68-5	Monuron	0.0065	3.85E+00	7.69E+00	1.00E+00	9.97E-01	1.10E-01	2.107
			n/a	n/a	n/a	n/a	n/a	n/a
152019-73-3	Metolachlor OA	0.2	2.25E-01	3.15E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.25E-01	3.15E-01	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
15299-99-7	Napropamide	5.1	4.90E-03	4.90E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			4.90E-03	4.90E-03	0.00E+00	0.00E+00	0.00E+00	0.000
15307-86-5	Diclofenac	0.05	7.00E+00	1.14E+01	2.81E-01	6.94E-01	2.80E-01	1.254
			7.00E+00	1.14E+01	2.75E-01	6.82E-01	1.80E-01	1.137
153719-23-4	Thiamethoxam	0.14	1.07E-01	1.79E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			1.07E-01	1.79E-01	0.00E+00	0.00E+00	0.00E+00	0.000
15545-48-9	Chlorotoluron	0.1	5.00E-01	6.30E-01	1.63E-02	1.69E-01	7.00E-02	0.255
			5.00E-01	5.70E-01	8.01E-03	1.65E-01	7.00E-02	0.243
1563-66-2	Carbofuran	0.016	1.56E+00	1.56E+00	2.02E-01	5.62E-01	7.00E-02	0.834
			7.81E-01	7.81E-01	1.55E-02	2.05E-01	7.00E-02	0.290
15687-27-1	Ibuprofen	0.3	3.65E-01	5.67E-01	5.85E-03	1.29E-01	0.00E+00	0.135
			3.65E-01	5.67E-01	5.85E-03	1.29E-01	0.00E+00	0.135
15950-66-0	2,3,4-Trichlorphenol	0.54	4.63E-01	4.63E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			4.63E-01	4.63E-01	0.00E+00	0.00E+00	0.00E+00	0.000
1610-18-0	Prometon	1	2.00E-02	2.00E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			2.00E-02	2.00E-02	0.00E+00	0.00E+00	0.00E+00	0.000
1634-04-4	Methyl-tert-butyl ether (MTBE)	2600	1.92E-03	1.92E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			1.92E-03	1.92E-03	0.00E+00	0.00E+00	0.00E+00	0.000
1646-88-4	Aldicarb sulfone	0.66	7.58E-02	7.58E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			7.58E-02	7.58E-02	0.00E+00	0.00E+00	0.00E+00	0.000
16752-77-5	Methomyl	0.04	1.25E+00	1.25E+00	1.14E-01	5.99E-01	4.00E-02	0.753
			6.25E-01	6.25E-01	4.16E-03	2.55E-01	0.00E+00	0.259
16887-00-6	Chloride	94000	1.34E-03	7.55E-02	4.37E-03	7.07E-01	0.00E+00	0.711
			1.34E-03	7.55E-02	4.37E-03	7.07E-01	0.00E+00	0.711
1689-84-5	Bromoxynil	0.5	5.00E-02	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-02	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
16984-48-8	Fluoride	500	6.80E-01	9.60E-01	2.63E-02	4.22E-01	4.00E-02	0.489
			6.80E-01	9.60E-01	2.63E-02	4.22E-01	4.00E-02	0.489
1698-60-8	Chloridazon	10	5.00E-03	2.50E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-03	2.50E-02	0.00E+00	0.00E+00	0.00E+00	0.000
1702-17-6	Clopyralid	70	7.14E-04	7.14E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			7.14E-04	7.14E-04	0.00E+00	0.00E+00	0.00E+00	0.000
17040-19-6	Demeton-S-methylsulfon	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
171118-09-5	Metolachlor ethanesulfonic acid (ESA)	0.2	5.25E-01	7.44E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.25E-01	7.44E-01	0.00E+00	0.00E+00	0.00E+00	0.000
17254-80-7	Chloridazon methyl-desphenyl	37	6.76E-03	8.35E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			6.76E-03	8.35E-03	0.00E+00	0.00E+00	0.00E+00	0.000
173159-57-4	Foramsulfuron	0.036	1.39E+00	1.39E+00	1.79E-01	9.91E-01	4.00E-02	1.210
			n/a	n/a	n/a	n/a	n/a	n/a
1746-81-2	Monolinuron	0.1	2.50E-01	2.50E-01	2.36E-03	8.12E-01	0.00E+00	0.815
			2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
175013-18-0	Pyraclostrobine	0.24	2.08E-01	2.08E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.08E-01	2.08E-01	0.00E+00	0.00E+00	0.00E+00	0.000
18691-97-9	Methabenzthiazuron	0.033	7.58E-01	7.58E-01	2.56E-02	6.63E-01	4.00E-02	0.728
			7.58E-01	7.58E-01	0.00E+00	0.00E+00	0.00E+00	0.000
188425-85-6	Boscalid	11.6	2.16E-03	6.20E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			2.16E-03	6.20E-03	0.00E+00	0.00E+00	0.00E+00	0.000
1897-45-6	Chlorothalonil	0.06	3.33E-01	4.17E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			3.33E-01	4.17E-01	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
1918-00-9	Dicamba	0.5	1.00E-01	1.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			1.00E-01	1.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
19666-30-9	Oxadiazon	0.088	2.84E-01	2.84E-01	7.32E-03	2.52E-01	0.00E+00	0.259
			2.84E-01	2.84E-01	6.69E-03	2.71E-01	0.00E+00	0.278
1982-47-4	Chloroxuron	0.27	9.26E-02	9.26E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			9.26E-02	9.26E-02	0.00E+00	0.00E+00	0.00E+00	0.000
19937-59-8	Metoxuron	0.064	3.91E-01	3.91E-01	2.45E-03	3.19E-01	0.00E+00	0.322
			3.91E-01	3.91E-01	2.07E-03	3.04E-01	0.00E+00	0.306
2008-58-4	2,6-Dichlorobenzamide	78	3.21E-04	3.99E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			3.21E-04	3.99E-04	0.00E+00	0.00E+00	0.00E+00	0.000
2032-65-7	Methiocarb	0.002	1.25E+01	1.25E+01	9.24E-01	9.71E-01	2.80E-01	2.176
			4.00E+00	7.00E+00	4.30E-01	6.65E-01	2.80E-01	1.374
208-96-8	Acenaphthylene	1.3	1.92E-02	3.85E-02	1.62E-03	9.43E-01	0.00E+00	0.945
			1.92E-02	3.85E-02	3.72E-04	5.45E-01	0.00E+00	0.546
21087-64-9	Metribuzin	0.12	2.08E-01	2.08E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.08E-01	2.08E-01	0.00E+00	0.00E+00	0.00E+00	0.000
210880-92-5	Clothianidin	0.13	1.92E-01	1.92E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			1.92E-01	1.92E-01	0.00E+00	0.00E+00	0.00E+00	0.000
2163-68-0	2-Hydroxyatrazine	0.002	2.50E+01	5.00E+01	9.99E-01	9.98E-01	5.60E-01	2.558
			5.00E+01	5.00E+01	9.94E-01	9.95E-01	4.10E-01	2.400
#2164-08-1	Lenacil	0.65	7.69E-02	7.69E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			7.69E-02	7.69E-02	0.00E+00	0.00E+00	0.00E+00	0.000
21725-46-2	Cyanazine	1	2.50E-02	2.50E-02	8.12E-04	7.66E-01	0.00E+00	0.767
			2.50E-02	2.50E-02	3.56E-04	8.61E-01	0.00E+00	0.862
218-01-9	Chrysene	0.0012	9.17E+00	2.08E+01	9.92E-01	9.75E-01	4.10E-01	2.377
			3.08E+01	8.33E+01	8.25E-01	9.53E-01	5.60E-01	2.338

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
2212-67-1	Molinate	3.8	1.32E-02	1.32E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			1.32E-02	1.32E-02	0.00E+00	0.00E+00	0.00E+00	0.000
22204-53-1	Naproxen	1.7	3.53E-02	5.88E-02	6.13E-04	0.00E+00	0.00E+00	0.001
			3.53E-02	5.88E-02	6.13E-04	0.00E+00	0.00E+00	0.001
2303-17-5	Triallate	0.41	6.10E-02	6.10E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			n/a	n/a	n/a	n/a	n/a	n/a
23103-98-2	Pirimicarb	0.09	2.78E-01	2.78E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.78E-01	2.78E-01	0.00E+00	0.00E+00	0.00E+00	0.000
23135-22-0	Oxamyl	0.536	9.33E-02	9.33E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			9.33E-02	9.33E-02	0.00E+00	0.00E+00	0.00E+00	0.000
2385-85-5	Mirex	0.001	5.00E+00	2.50E+01	7.46E-01	1.00E+00	2.80E-01	2.026
			n/a	n/a	n/a	n/a	n/a	n/a
23950-58-5	Propyzamide	8.2	3.05E-03	3.05E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			3.05E-03	3.05E-03	0.00E+00	0.00E+00	0.00E+00	0.000
24017-47-8	Triazophos	0.001	5.00E+01	5.00E+01	9.99E-01	1.00E+00	2.80E-01	2.279
			n/a	n/a	n/a	n/a	n/a	n/a
24579-73-5	Propamocarb	1030	4.85E-05	4.85E-05	0.00E+00	0.00E+00	0.00E+00	0.000
			4.85E-05	4.85E-05	0.00E+00	0.00E+00	0.00E+00	0.000
25057-89-0	Bentazone	270	1.11E-04	2.19E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			1.11E-04	2.19E-04	0.00E+00	0.00E+00	0.00E+00	0.000
25812-30-0	Gemfibrozil	3.846153846	3.25E-03	3.25E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			3.25E-03	3.25E-03	0.00E+00	0.00E+00	0.00E+00	0.000
26225-79-6	Ethofumesate	6.4	3.91E-03	9.38E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			3.91E-03	9.38E-03	0.00E+00	0.00E+00	0.00E+00	0.000
26259-45-0	Secbumeton	0.1	2.00E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.00E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
2642-71-9	Azinphos-ethyl	0.0011	2.27E+01	2.27E+01	1.00E+00	1.00E+00	2.80E-01	2.280
			2.73E+01	4.55E+01	1.00E+00	1.00E+00	4.10E-01	2.410

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
29122-68-7	Atenolol	150	3.07E-04	4.27E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			3.07E-04	4.27E-04	0.00E+00	0.00E+00	0.00E+00	0.000
29232-93-7	Pirimiphos-methyl	0.005	4.00E+00	5.00E+00	4.79E-01	8.50E-01	7.00E-02	1.399
			1.00E+00	1.00E+00	0.00E+00	0.00E+00	0.00E+00	0.000
298-04-4	Disulfoton	0.004	6.25E+00	1.25E+01	9.31E-01	9.91E-01	1.80E-01	2.101
			n/a	n/a	n/a	n/a	n/a	n/a
298-46-4	Carbamazepine	0.5	7.60E-01	1.36E+00	7.34E-03	4.02E-01	4.00E-02	0.449
			7.60E-01	1.36E+00	7.34E-03	4.02E-01	4.00E-02	0.449
301-12-2	Oxydemeton-methyl	0.035	1.43E+00	1.43E+00	5.10E-01	9.47E-01	4.00E-02	1.498
			n/a	n/a	n/a	n/a	n/a	n/a
30125-63-4	Desethylterbuthylazine	0.25	1.00E-01	1.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			1.00E-01	1.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
302-17-0	Chloral hydrate	10	5.00E-02	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-02	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.000
3060-89-7	Metobromuron	0.26	9.62E-02	9.62E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			9.62E-02	9.62E-02	0.00E+00	0.00E+00	0.00E+00	0.000
307-24-4	Perfluorohexanoic acid (PFHxA)	140	2.00E-04	4.64E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			2.00E-04	4.64E-04	0.00E+00	0.00E+00	0.00E+00	0.000
314-40-9	Bromacil	0.01	5.00E+00	5.00E+00	7.07E-01	9.14E-01	7.00E-02	1.692
			1.00E+00	1.00E+00	0.00E+00	0.00E+00	0.00E+00	0.000
32809-16-8	Procymidone	1.2	2.08E-02	2.08E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			2.08E-02	2.08E-02	0.00E+00	0.00E+00	0.00E+00	0.000
330-55-2	Linuron	0.1	2.50E-01	2.50E-01	9.22E-03	2.76E-01	0.00E+00	0.285
			2.50E-01	2.50E-01	2.84E-03	1.46E-01	0.00E+00	0.149
333-41-5	Diazinon	0.01	2.50E+00	4.00E+00	2.78E-01	7.04E-01	7.00E-02	1.052

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
			1.00E+00	1.00E+00	1.39E-02	3.18E-01	4.00E-02	0.372
335-67-1	Perfluorooctanoic acid (PFOA)	0.1	6.70E-01	1.40E+00	1.87E-02	3.92E-01	7.00E-02	0.481
			6.62E-01	1.40E+00	1.85E-02	3.92E-01	7.00E-02	0.480
3380-34-5	Triclosan	0.02	2.00E+00	2.33E+00	2.03E-01	7.07E-01	7.00E-02	0.980
			1.75E+00	2.60E+00	8.90E-02	4.51E-01	1.10E-01	0.650
3397-62-4	Desisopropyldesethylatrazine	0.01	5.00E+00	5.00E+00	7.97E-01	9.81E-01	7.00E-02	1.848
			n/a	n/a	n/a	n/a	n/a	n/a
3424-82-6	DDE, o,p'	0.01	5.00E-01	6.25E-01	3.52E-02	5.88E-01	4.00E-02	0.663
			5.00E-01	5.00E-01	2.86E-04	5.49E-01	0.00E+00	0.550
34256-82-1	Acetochlor	0.013	1.92E+00	1.92E+00	2.90E-01	4.13E-01	1.10E-01	0.813
			9.62E-01	9.62E-01	9.08E-02	1.66E-01	1.10E-01	0.367
35367-38-5	Diflubenzuron	0.004	6.25E+00	6.25E+00	9.90E-01	9.93E-01	1.10E-01	2.093
			n/a	n/a	n/a	n/a	n/a	n/a
35554-44-0	Imazalil	0.8	9.38E-02	9.38E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			9.38E-02	9.38E-02	0.00E+00	0.00E+00	0.00E+00	0.000
36734-19-7	Iprodione	0.35	7.14E-02	1.43E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			7.14E-02	1.43E-01	0.00E+00	0.00E+00	0.00E+00	0.000
37350-58-6	Metoprolol	62	7.26E-03	1.05E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			7.26E-03	1.05E-02	0.00E+00	0.00E+00	0.00E+00	0.000
375-73-5	Perfluorobutane sulfonic acid	372	8.03E-05	1.54E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			8.03E-05	1.54E-04	0.00E+00	0.00E+00	0.00E+00	0.000
40487-42-1	Pendimethalin	0.018	1.39E+00	1.39E+00	2.02E-01	7.11E-01	4.00E-02	0.953
			6.94E-01	6.94E-01	0.00E+00	0.00E+00	0.00E+00	0.000
41394-05-2	Metamitron	4	1.25E-02	1.25E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			1.25E-02	1.25E-02	0.00E+00	0.00E+00	0.00E+00	0.000
41859-67-0	Bezafibrate	0.46	2.11E-01	3.26E-01	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
			2.11E-01	3.26E-01	0.00E+00	0.00E+00	0.00E+00	0.000
43121-43-3	Triadimefon	4.1	1.22E-02	1.22E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			1.22E-02	1.22E-02	0.00E+00	0.00E+00	0.00E+00	0.000
439-14-5	Diazepam	0.291	4.30E-02	4.30E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			4.30E-02	4.30E-02	0.00E+00	0.00E+00	0.00E+00	0.000
50-00-0	Formaldehyde	10.2	2.45E-01	9.80E-01	1.95E-02	5.40E-01	7.00E-02	0.629
			2.45E-01	2.45E-01	1.03E-02	1.89E-01	0.00E+00	0.199
50-28-2	17-beta-Estradiol	0.0004	1.25E+00	1.25E+00	6.49E-01	9.89E-01	1.10E-01	1.747
			2.50E+00	4.85E+00	2.39E-01	8.36E-01	1.80E-01	1.255
50471-44-8	Vinclozolin	1.2	2.08E-02	2.08E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			2.08E-02	2.08E-02	0.00E+00	0.00E+00	0.00E+00	0.000
51218-45-2	Metolachlor	0.91	2.75E-02	5.49E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			2.75E-02	5.49E-02	0.00E+00	0.00E+00	0.00E+00	0.000
51235-04-2	Hexazinone	0.048	5.21E-01	1.04E+00	1.15E-02	5.28E-01	4.00E-02	0.580
			5.21E-01	5.21E-01	0.00E+00	0.00E+00	0.00E+00	0.000
525-66-6	Propranolol	0.411	3.65E-02	4.87E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			3.65E-02	4.87E-02	0.00E+00	0.00E+00	0.00E+00	0.000
52645-53-1	Permethrin	0.0015	1.67E+01	1.67E+01	9.82E-01	9.88E-01	1.80E-01	2.151
			6.67E+00	1.33E+01	4.44E-01	2.87E-01	4.10E-01	1.140
52-68-6	Trichlorfon	0.00057	8.77E+01	8.77E+01	1.00E+00	9.99E-01	4.10E-01	2.408
			n/a	n/a	n/a	n/a	n/a	n/a
52888-80-9	Prosulfocarb	0.5	1.00E-01	1.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			1.00E-01	1.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
52918-63-5	Deltamethrin	0.0000031	1.61E+04	1.61E+04	1.00E+00	1.00E+00	1.00E+00	3.000
			n/a	n/a	n/a	n/a	n/a	n/a
53112-28-0	Pyrimethanil	2	1.25E-02	2.50E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			1.25E-02	2.50E-02	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
53-16-7	Estrone	0.0036	6.94E-01	6.94E+00	5.48E-02	3.56E-01	1.10E-01	0.521
			6.94E-01	1.39E+00	5.35E-02	3.34E-01	1.10E-01	0.497
53-19-0	DDD, o,p'	0.00064	7.81E+00	1.56E+01	8.29E-01	9.25E-01	2.80E-01	2.034
			7.81E-01	7.81E-01	1.02E-01	3.27E-01	1.10E-01	0.540
534-52-1	Dinitro-o-cresol (DNOC)	9	2.78E-03	4.44E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			2.78E-03	4.44E-03	0.00E+00	0.00E+00	0.00E+00	0.000
53-70-3	Dibenz(a,h)anthracene	0.0014	3.57E+00	3.57E+00	9.58E-01	8.71E-01	1.10E-01	1.939
			1.07E+00	5.01E+00	3.73E-01	4.13E-01	4.10E-01	1.196
540-59-0	1,2-Dichloroethene	6.8	1.84E+00	2.94E+00	1.17E-02	5.62E-01	7.00E-02	0.644
			7.35E-01	7.35E-01	0.00E+00	0.00E+00	0.00E+00	0.000
541-73-1	1,3-Dichlorobenzene	2	2.50E-01	5.00E-01	2.10E-02	1.67E-01	4.00E-02	0.228
			2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
542-75-6	1,3-Dichloropropene	1.5	6.67E-01	1.00E+00	0.00E+00	0.00E+00	0.00E+00	0.000
			6.67E-01	6.67E-01	0.00E+00	0.00E+00	0.00E+00	0.000
55179-31-2	Bitertanol	0.152	1.64E-01	1.64E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			1.64E-01	1.64E-01	0.00E+00	0.00E+00	0.00E+00	0.000
55219-65-3	Triadimenol	2	2.50E-02	2.50E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-02	2.50E-02	0.00E+00	0.00E+00	0.00E+00	0.000
55335-06-3	Triclopyr	700	3.57E-05	3.57E-05	0.00E+00	0.00E+00	0.00E+00	0.000
			3.57E-05	3.57E-05	0.00E+00	0.00E+00	0.00E+00	0.000
55-38-9	Fenthion	0.0002	1.25E+02	1.25E+02	1.00E+00	1.00E+00	5.60E-01	2.560
			1.50E+02	2.50E+02	1.00E+00	9.95E-01	5.60E-01	2.555

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
5598-13-0	Chlorpyriphos methyl	0.001	2.00E+01	2.50E+01	8.72E-01	1.00E+00	2.80E-01	2.152
			1.00E+01	2.00E+01	4.11E-01	9.76E-01	2.80E-01	1.667
563-12-2	Ethion	0.00056	1.79E+01	4.46E+01	1.00E+00	1.00E+00	2.80E-01	2.280
			3.57E+01	3.57E+01	1.00E+00	1.00E+00	2.80E-01	2.280
56-38-2	Parathion	0.0002	1.25E+02	1.25E+02	9.99E-01	9.68E-01	5.60E-01	2.527
			2.50E+01	2.50E+01	3.08E-01	9.78E-01	5.60E-01	1.846
56-55-3	Benzo(a)anthracene	0.00023	6.52E+01	1.22E+02	9.99E-01	1.00E+00	1.00E+00	2.998
			1.30E+02	2.30E+02	9.97E-01	1.00E+00	5.60E-01	2.557
56-72-4	Coumaphos	0.0007	3.57E+01	3.57E+01	1.00E+00	1.00E+00	2.80E-01	2.280
			n/a	n/a	n/a	n/a	n/a	n/a
57018-04-9	Tolclofos-methyl	1.2	2.08E-02	4.17E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			2.08E-02	4.17E-02	0.00E+00	0.00E+00	0.00E+00	0.000
57-12-5	Cyanide (as total CN)	50	1.00E-01	1.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			1.00E-01	1.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
57-63-6	17-alpha-Ethinylestradiol	0.000035	1.43E+01	1.57E+01	1.88E-01	9.72E-01	2.80E-01	1.440
			n/a	n/a	n/a	n/a	n/a	n/a
57-68-1	Sulfamethazine	30	8.33E-04	8.33E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			8.33E-04	8.33E-04	0.00E+00	0.00E+00	0.00E+00	0.000
57-74-9	Chlordane	0.00005	2.00E+02	5.00E+02	1.00E+00	1.00E+00	5.60E-01	2.560
			n/a	n/a	n/a	n/a	n/a	n/a
57837-19-1	Metalaxyl	120	2.08E-04	2.08E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			2.08E-04	2.08E-04	0.00E+00	0.00E+00	0.00E+00	0.000
58-08-2	Caffeine	87	3.79E-03	5.75E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			3.79E-03	5.75E-03	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
58-73-1	Diphenhydramine	0.991	9.59E-04	9.59E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			9.59E-04	9.59E-04	0.00E+00	0.00E+00	0.00E+00	0.000
58955-93-4	10,11-Dihydro-10,11-dihydroxycarbamazepine	200	3.05E-03	4.09E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			3.05E-03	4.09E-03	0.00E+00	0.00E+00	0.00E+00	0.000
5915-41-3	Terbuthylazine	0.32	7.81E-02	2.06E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			7.81E-02	2.03E-01	0.00E+00	0.00E+00	0.00E+00	0.000
59-50-7	Chlorocresol (3-Methyl-4-chlorophenol)	6.4	1.95E-02	3.91E-02	5.18E-04	3.68E-01	0.00E+00	0.369
			1.95E-02	3.91E-02	0.00E+00	0.00E+00	0.00E+00	0.000
60-00-4	Edetic acid (EDTA)	2200	5.00E-03	7.73E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-03	7.73E-03	0.00E+00	0.00E+00	0.00E+00	0.000
60168-88-9	Fenarimol	0.00002	2.50E+03	2.50E+03	1.00E+00	1.00E+00	1.00E+00	3.000
			n/a	n/a	n/a	n/a	n/a	n/a
60207-90-1	Propiconazole	6.1	8.20E-03	8.20E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			8.20E-03	8.20E-03	0.00E+00	0.00E+00	0.00E+00	0.000
60-51-5	Dimethoate	0.01	2.50E+00	5.00E+00	4.07E-01	6.90E-01	7.00E-02	1.167
			1.00E+00	1.00E+00	3.28E-02	3.04E-01	7.00E-02	0.407
608-27-5	2,3-Dichloroaniline	1	5.00E-02	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-02	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.000
6190-65-4	Desethylatrazine	0.2	2.50E-01	4.05E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-01	4.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
62-53-3	Aniline	1.5	3.33E-01	3.33E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			3.33E-01	3.33E-01	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
630-20-6	1,1,1,2-Tetrachloroethane	140	1.79E-02	1.79E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			1.79E-02	1.79E-02	0.00E+00	0.00E+00	0.00E+00	0.000
63-25-2	Carbaryl	0.015	1.67E+00	1.67E+00	2.78E-01	8.16E-01	7.00E-02	1.164
			6.67E-01	6.67E-01	3.65E-02	3.36E-01	4.00E-02	0.412
66230-04-4	Esfenvalerate	0.0001	5.00E+02	5.00E+02	1.00E+00	9.99E-01	5.60E-01	2.559
			n/a	n/a	n/a	n/a	n/a	n/a
66246-88-6	Penconazole	1.7	1.47E-02	2.94E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			1.47E-02	2.94E-02	0.00E+00	0.00E+00	0.00E+00	0.000
668-34-8	Triphenyltin	0.00023	7.39E+01	7.39E+01	3.87E-01	1.00E+00	4.10E-01	1.797
			5.88E+01	8.02E+01	2.23E-01	1.00E+00	4.10E-01	1.633
67129-08-2	Metazachlor	0.08	3.13E-01	3.50E-01	9.30E-03	1.13E-01	4.00E-02	0.163
			3.13E-01	3.50E-01	9.10E-03	1.12E-01	4.00E-02	0.161
67306-00-7	Fenpropidin	0.0032	7.81E+00	7.81E+00	7.88E-01	9.80E-01	1.80E-01	1.948
			n/a	n/a	n/a	n/a	n/a	n/a
67564-91-4	Fenpropimorph	0.016	1.56E+00	1.56E+00	2.12E-01	4.91E-01	7.00E-02	0.773
			7.81E-01	7.81E-01	0.00E+00	0.00E+00	0.00E+00	0.000
67-72-1	Hexachloroethane	0.44	5.68E-01	5.68E-01	4.20E-03	1.00E+00	0.00E+00	1.004
			5.68E-01	5.68E-01	1.38E-04	0.00E+00	0.00E+00	0.000
67747-09-5	Prochloraz	1	3.50E-02	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			3.50E-02	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.000
68359-37-5	Cyfluthrin	0.001	2.50E+01	1.00E+02	9.58E-01	9.83E-01	4.10E-01	2.350
			n/a	n/a	n/a	n/a	n/a	n/a
69377-81-7	Fluroxypyr	17.9	1.40E-03	2.79E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			1.40E-03	2.79E-03	0.00E+00	0.00E+00	0.00E+00	0.000
709-98-8	Propanil	0.07	7.14E-01	7.14E-01	3.02E-03	9.18E-01	0.00E+00	0.921
			7.14E-01	7.14E-01	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
71-55-6	1,1,1-Trichloroethane	10	2.50E-02	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-02	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.000
723-46-6	Sulfamethoxazole	0.4	5.00E-01	2.93E+00	3.28E-03	4.14E-01	0.00E+00	0.418
			5.00E-01	3.04E+00	3.28E-03	4.20E-01	0.00E+00	0.423
72-43-5	Methoxychlor	0.0005	5.00E+01	5.00E+01	8.53E-01	9.97E-01	2.80E-01	2.130
			1.00E+00	1.00E+00	1.34E-01	2.53E-01	2.80E-01	0.667
7286-69-3	Sebuthylazine	0.01	2.00E+00	2.50E+00	1.41E-01	9.52E-01	7.00E-02	1.163
			1.00E+00	1.00E+00	4.32E-03	9.48E-01	4.00E-02	0.993
7287-19-6	Prometryn	0.5	5.00E-02	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-02	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.000
731-27-1	Tolylfluanid	0.26	1.92E-01	1.92E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			1.92E-01	1.92E-01	0.00E+00	0.00E+00	0.00E+00	0.000
738-70-5	Trimethoprim	60	6.67E-04	1.12E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			6.67E-04	1.12E-03	0.00E+00	0.00E+00	0.00E+00	0.000
74223-64-6	Metsulfuron-methyl	0.01	5.00E+00	5.00E+00	4.87E-01	8.66E-01	7.00E-02	1.423
			1.00E+00	1.00E+00	0.00E+00	0.00E+00	0.00E+00	0.000
74-95-3	Dibromomethane	45	5.56E-03	5.56E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			5.56E-03	5.56E-03	0.00E+00	0.00E+00	0.00E+00	0.000
75-01-4	Vinylchloride	0.09	1.39E+01	5.56E+01	7.45E-01	9.68E-01	4.10E-01	2.124
			5.56E-01	1.11E+00	3.68E-02	6.52E-01	1.80E-01	0.869
75-25-2	Bromoform	11.3	4.42E-02	4.42E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			4.42E-02	4.42E-02	0.00E+00	0.00E+00	0.00E+00	0.000
75-27-4	Dichlorobromomethane	78	3.21E-03	6.41E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			3.21E-03	6.41E-03	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
75-34-3	1,1-Dichloroethane	10	5.00E-01	1.00E+00	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-01	1.00E+00	0.00E+00	0.00E+00	0.00E+00	0.000
75-35-4	1,1-Dichloroethylene	5	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
76-03-9	Trichloroacetic acid	0.01	1.80E+01	2.40E+01	8.52E-01	6.98E-01	2.80E-01	1.830
			2.10E+01	2.80E+01	7.75E-01	5.00E-01	2.80E-01	1.555
7664-41-7	Ammonia	67.5	3.11E+00	5.58E+00	4.14E-01	5.72E-01	1.80E-01	1.166
			3.11E+00	5.58E+00	4.14E-01	5.72E-01	1.80E-01	1.166
76674-21-0	Flutriafol	31	1.61E-03	1.61E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			1.61E-03	1.61E-03	0.00E+00	0.00E+00	0.00E+00	0.000
7786-34-7	Mevinphos	0.00017	1.18E+02	1.47E+02	1.00E+00	1.00E+00	5.60E-01	2.559
			5.88E+01	1.18E+02	7.53E-01	1.00E+00	5.60E-01	2.313
78-51-3	Tris(2-butoxyethyl) phosphate (TBEP)	24	4.17E-03	8.15E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			4.17E-03	8.15E-03	0.00E+00	0.00E+00	0.00E+00	0.000
78587-05-0	Hexythiazox	0.122	4.10E-01	4.10E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			4.10E-01	4.10E-01	0.00E+00	0.00E+00	0.00E+00	0.000
78-87-5	1,2-Dichloropropane	10	1.00E+00	1.00E+00	0.00E+00	0.00E+00	0.00E+00	0.000
			1.00E+00	1.00E+00	0.00E+00	0.00E+00	0.00E+00	0.000
79-00-5	1,1,2-Trichloroethane	10	1.25E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			1.25E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
79-11-8	Chloroacetic acid	0.6	8.33E+00	1.67E+01	3.44E-01	9.32E-01	1.80E-01	1.456
			n/a	n/a	n/a	n/a	n/a	n/a
79241-46-6	Fluazifop-P-butyl	0.477	5.24E-02	5.24E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			5.24E-02	5.24E-02	0.00E+00	0.00E+00	0.00E+00	0.000
79277-27-3	Thifensulfuron methyl	0.05	1.00E+00	1.00E+00	3.81E-03	4.66E-01	4.00E-02	0.510
			1.00E+00	1.00E+00	3.81E-03	4.66E-01	4.00E-02	0.510
79-34-5	1,1,2,2-Tetrachloroethane	8	3.13E-01	3.13E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			3.13E-01	3.13E-01	0.00E+00	0.00E+00	0.00E+00	0.000
79622-59-6	Fluazinam	0.058	4.31E-01	4.31E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			4.31E-01	4.31E-01	0.00E+00	0.00E+00	0.00E+00	0.000
80-05-7	Bisphenol A	0.24	1.04E+00	1.31E+00	7.93E-02	3.63E-01	1.10E-01	0.553
			5.00E-01	9.37E-01	6.12E-02	2.85E-01	1.10E-01	0.457
80-09-1	Bisphenol S	270	1.85E-04	2.85E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			1.85E-04	2.85E-04	0.00E+00	0.00E+00	0.00E+00	0.000
8065-48-3	Demeton	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
81103-11-9	Clarithromycin	0.13	1.08E+00	1.31E+02	4.50E-02	3.86E-01	7.00E-02	0.501
			n/a	n/a	n/a	n/a	n/a	n/a
81-15-2	Musk xylene	1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
82097-50-5	Triasulfuron	0.0032	1.56E+01	1.56E+01	1.00E+00	1.00E+00	1.80E-01	2.180
			n/a	n/a	n/a	n/a	n/a	n/a
82558-50-7	Isoxaben	0.6	8.33E-02	8.33E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			8.33E-02	8.33E-02	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
82-68-8	Quintozene	0.4	3.13E-02	6.25E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			3.13E-02	6.25E-02	0.00E+00	0.00E+00	0.00E+00	0.000
83121-18-0	Teflubenzuron	0.0012	2.08E+01	2.08E+01	1.00E+00	1.00E+00	2.80E-01	2.280
			n/a	n/a	n/a	n/a	n/a	n/a
83164-33-4	Diflufenican	0.009	2.78E+00	2.89E+00	8.30E-01	9.48E-01	1.10E-01	1.888
			6.00E+00	1.11E+01	5.93E-01	8.19E-01	1.80E-01	1.592
83-32-9	Acenaphthene	0.06	2.08E-01	4.17E-01	4.70E-03	4.64E-01	0.00E+00	0.469
			2.08E-01	4.17E-01	1.95E-03	3.82E-01	0.00E+00	0.383
834-12-8	Ametryn	0.1	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
84-66-2	Diethyl phthalate	12	4.17E-02	4.17E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			4.17E-02	4.17E-02	0.00E+00	0.00E+00	0.00E+00	0.000
84-74-2	Di-n-butylphthalate	10	5.00E-02	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-02	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.000
85-01-8	Phenanthrene	1.1	1.91E-02	4.55E-02	1.12E-02	9.08E-01	7.00E-02	0.989
			1.73E-02	2.73E-02	2.28E-03	6.35E-01	0.00E+00	0.637
85509-19-9	Flusilazole	0.3	1.67E-01	1.67E-01	3.52E-04	1.16E-01	0.00E+00	0.116
			1.67E-01	1.67E-01	0.00E+00	0.00E+00	0.00E+00	0.000
85-68-7	Butylbenzyl phthalate	5.2	9.62E-02	9.62E-02	5.23E-03	5.38E-01	0.00E+00	0.544
			9.62E-02	9.62E-02	5.82E-04	1.48E-01	0.00E+00	0.148
86-50-0	Azinphos-methyl	0.0065	3.85E+00	3.85E+00	3.93E-01	9.34E-01	1.10E-01	1.437
			7.69E-01	7.69E-01	0.00E+00	0.00E+00	0.00E+00	0.000
86-73-7	Fluorene	1.5	6.67E-03	8.33E-03	7.50E-04	8.67E-01	0.00E+00	0.868
			6.67E-03	6.67E-03	7.50E-04	8.67E-01	0.00E+00	0.868
87-65-0	2,6-Dichlorophenol	3.4	1.47E-02	1.47E-02	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
			1.47E-02	1.47E-02	0.00E+00	0.00E+00	0.00E+00	0.000
87674-68-8	Dimethenamid	0.2	1.25E-01	1.25E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			1.25E-01	1.25E-01	0.00E+00	0.00E+00	0.00E+00	0.000
88-06-2	2,4,6-Trichlorophenol	0.26	4.81E-01	4.81E-01	1.18E-03	5.18E-01	0.00E+00	0.519
			4.81E-01	4.81E-01	0.00E+00	0.00E+00	0.00E+00	0.000
882-09-7	Clofibric acid (Clofibrate)	5	3.00E-03	5.00E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			3.00E-03	5.00E-03	0.00E+00	0.00E+00	0.00E+00	0.000
88-72-2	o-Nitrotoluene	10	2.50E-02	2.50E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-02	2.50E-02	0.00E+00	0.00E+00	0.00E+00	0.000
88-73-3	1-Cloro-2-nitrobenzene	1	5.00E-01	5.00E-01	3.72E-04	1.31E-01	0.00E+00	0.131
			5.00E-01	5.00E-01	3.72E-04	1.31E-01	0.00E+00	0.131
88-85-7	Dinoseb	0.29	8.62E-02	8.62E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			8.62E-02	8.62E-02	0.00E+00	0.00E+00	0.00E+00	0.000
89-59-8	4-Chloro-2-nitrotoluene	1	2.50E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
89-63-4	4-Chloro-2-nitroaniline	1	5.00E-02	1.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-02	1.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
90-12-0	1-Methylnaphthalene	0.12	8.33E-02	8.33E-02	6.15E-03	4.47E-01	0.00E+00	0.453
			8.33E-02	8.33E-02	6.15E-03	4.47E-01	0.00E+00	0.453
90-13-1	1-Chloronaphthalene	0.01	2.50E+01	2.50E+01	4.69E-01	9.16E-01	2.80E-01	1.665
			n/a	n/a	n/a	n/a	n/a	n/a
90717-03-6	Quinmerac	31.6	7.91E-04	1.08E-03	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
			7.91E-04	1.08E-03	0.00E+00	0.00E+00	0.00E+00	0.000
91465-08-6	lambda-Cyhalothrin	0.0002	2.50E+02	2.50E+02	9.97E-01	9.98E-01	5.60E-01	2.555
			5.00E+01	2.50E+02	5.42E-01	9.23E-01	5.60E-01	2.025
919-86-8	Demeton-S-methyl	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
92-52-4	Biphenyl	1	5.00E-02	5.00E-02	9.94E-03	9.43E-01	0.00E+00	0.953
			5.00E-02	5.00E-02	2.49E-03	1.19E-01	0.00E+00	0.122
933-75-5	2,3,6-Trichlorphenol	0.1	2.50E+00	2.50E+00	1.99E-01	7.52E-01	7.00E-02	1.021
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
933-78-8	2,3,5-Trichlorphenol	0.1	1.25E+00	1.25E+00	1.54E-01	9.83E-01	4.00E-02	1.177
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
93-65-2	Mecoprop	3.6	6.94E-03	1.11E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			6.94E-03	1.11E-02	0.00E+00	0.00E+00	0.00E+00	0.000
93-72-1	Fenoprop	0.6	4.17E-02	4.17E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			4.17E-02	4.17E-02	0.00E+00	0.00E+00	0.00E+00	0.000
93-76-5	2,4,5-Trichlorophenoxyacetic acid	0.1	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
94361-06-5	Cyproconazole	0.6	4.17E-02	4.17E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			4.17E-02	4.17E-02	0.00E+00	0.00E+00	0.00E+00	0.000
94-74-6	2-Methyl-4-chlorophenoxyacetic acid (MCPA)	0.1	2.50E-01	5.12E-01	4.24E-02	1.84E-01	7.00E-02	0.296
			2.50E-01	5.00E-01	4.07E-02	1.73E-01	7.00E-02	0.284

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
94-75-7	2,4-Dichlorophenoxyacetic acid (2,4-D)	0.1	2.50E-01	4.00E-01	5.50E-03	1.48E-01	4.00E-02	0.193
			2.50E-01	3.70E-01	0.00E+00	0.00E+00	0.00E+00	0.000
94-81-5	4-(4-Chloro-o-tolyloxy) butyric acid	0.43	5.81E-02	5.81E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			5.81E-02	5.81E-02	0.00E+00	0.00E+00	0.00E+00	0.000
94-82-6	4-(2,4-Dichlorophenoxy)butyric acid (2,4-DB)	0.932	2.15E-02	2.68E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			2.15E-02	2.68E-02	0.00E+00	0.00E+00	0.00E+00	0.000
950-37-8	Methidathion	0.0022	1.14E+01	1.14E+01	1.00E+00	1.00E+00	1.80E-01	2.180
			n/a	n/a	n/a	n/a	n/a	n/a
95-14-7	1H-Benzotriazole	30	5.67E-02	9.33E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			5.67E-02	9.33E-02	0.00E+00	0.00E+00	0.00E+00	0.000
95-49-8	2-Chlorotoluene	1	5.00E-01	5.00E+00	1.94E-02	7.38E-01	7.00E-02	0.827
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
95-50-1	1,2-Dichlorobenzene	1	5.00E-01	1.00E+00	4.60E-02	2.66E-01	7.00E-02	0.382
			2.50E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
95-51-2	2-Chloroaniline	0.2	5.00E-01	1.25E+00	1.47E-02	8.94E-01	4.00E-02	0.948
			2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
95-57-8	2-Chlorophenol	3	1.67E-02	3.33E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			1.67E-02	3.33E-02	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
95-63-6	1,2,4-Trimethylbenzene	2	5.00E-01	5.00E-01	9.95E-03	9.53E-01	0.00E+00	0.963
			2.50E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
95-76-1	3,4-Dichloroaniline	0.02	2.50E+00	7.50E+00	5.45E-01	9.62E-01	1.10E-01	1.617
			5.00E-01	1.00E+00	8.43E-03	6.68E-01	0.00E+00	0.677
95-85-2	2-Amino-4-chlorophenol	3	3.33E-01	3.33E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			3.33E-01	3.33E-01	0.00E+00	0.00E+00	0.00E+00	0.000
95-94-3	1,2,4,5-Tetrachlorobenzene	0.0016	3.13E+02	3.13E+02	9.37E-01	9.96E-01	5.60E-01	2.493
			6.25E-01	6.25E-01	1.88E-02	6.00E-01	0.00E+00	0.619
95-95-4	2,4,5-Trichlorophenol	0.1	6.50E-01	1.25E+00	3.98E-02	7.42E-01	7.00E-02	0.851
			6.50E-01	6.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
96-12-8	1,2-Dibromo-3-chloropropane	1	6.50E-01	6.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			6.50E-01	6.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
96-18-4	1,2,3-Trichloropropane	4.1	6.10E-01	6.10E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			6.10E-01	6.10E-01	0.00E+00	0.00E+00	0.00E+00	0.000
96525-23-4	Flurtamone	0.23	1.09E-01	1.09E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			1.09E-01	1.09E-01	0.00E+00	0.00E+00	0.00E+00	0.000
97-00-7	1-Chloro-2,4-dinitrobenzene	0.54	9.26E-01	9.26E-01	3.82E-03	7.56E-01	0.00E+00	0.759
			9.26E-01	9.26E-01	0.00E+00	0.00E+00	0.00E+00	0.000
98-82-8	Isopropylbenzene	0.7	7.14E-01	1.43E+00	4.00E-02	6.44E-01	4.00E-02	0.723
			3.57E-01	7.14E-01	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
98-87-3	alpha,alpha-Dichlorotoluene	0.034	1.47E+02	1.47E+02	4.29E-01	1.00E+00	5.60E-01	1.989
			n/a	n/a	n/a	n/a	n/a	n/a
98-95-3	Nitrobenzene	0.1	2.50E+00	2.50E+00	4.45E-01	6.53E-01	1.10E-01	1.208
			1.00E+00	1.00E+00	2.92E-02	3.64E-01	4.00E-02	0.433
99-87-6	p-Cymene	4.4	2.27E-01	2.27E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.27E-01	2.27E-01	0.00E+00	0.00E+00	0.00E+00	0.000

Table IV-2. STEfw, eco results - inland whole water monitoring data for metals, $PNEC_{fw, eco}$.

For each substance, two scenarios are presented. Top/shaded: Sc2 (all monitoring records; non-quantified records set as half LOD/Q); Bottom/white: Sc2-PNEC QC (quantified records plus non-quantified samples excluding those for which ½LOD/Q > PNEC).

[1] RQ_P90 is the risk quotient between the 90th percentile of all monitoring records and the selected PNEC.
[2] RQ_P95 is the risk quotient between the 95th percentile of all monitoring records and the selected PNEC.
[3] Fspat, Ftemp and Fext stand for the spatial, temporal and extend of PNEC exceedance factors in the STE approach, calculated as described in Section 2.1, while the Final STE score is the sum of the individual factors.
[4] Only STE scores using Sc2-PNEC QC were used for the risk-based ranking of substances.

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
18540-29-9	Chromium 6+	0.47	3.19E+01	3.19E+01	9.77E-01	9.92E-01	2.80E-01	2.249
			1.06E+01	1.28E+01	8.88E-01	9.62E-01	1.80E-01	2.030
7439-95-4	Magnesium	75000	7.65E-02	1.33E-01	1.47E-03	8.27E-01	0.00E+00	0.828
			7.65E-02	1.33E-01	1.47E-03	8.27E-01	0.00E+00	0.828
7440-22-4	Silver	0.017	7.35E+01	1.47E+02	9.91E-01	9.84E-01	5.60E-01	2.536
			2.94E+01	4.41E+01	7.51E-01	9.47E-01	4.10E-01	2.108
7440-23-5	Sodium	200000	1.90E-02	2.10E-01	3.68E-03	9.49E-01	0.00E+00	0.952
			1.90E-02	2.10E-01	3.68E-03	9.49E-01	0.00E+00	0.952
7440-24-6	Strontium	210	2.14E+00	2.48E+00	1.16E-01	7.14E-01	7.00E-02	0.899
			2.14E+00	2.48E+00	1.16E-01	7.14E-01	7.00E-02	0.899
7440-28-0	Thallium	0.05	2.50E+01	5.00E+01	6.63E-01	8.65E-01	2.80E-01	1.808
			1.00E+00	2.40E+00	1.85E-01	3.70E-01	5.60E-01	1.116
7440-31-5	Tin	0.6	8.33E+00	4.17E+01	6.00E-01	7.28E-01	2.80E-01	1.608
			8.33E-01	1.17E+00	1.38E-01	2.68E-01	1.80E-01	0.586
7440-32-6	Titanium	20	7.50E-01	1.25E+00	8.10E-02	3.46E-01	4.00E-02	0.467
			6.50E-01	1.12E+00	3.74E-02	2.98E-01	4.00E-02	0.375
7440-36-0	Antimony	5.6	2.68E-01	4.46E-01	7.29E-03	2.64E-01	0.00E+00	0.271
			2.68E-01	4.46E-01	3.56E-03	2.56E-01	0.00E+00	0.260

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
7440-41-7	Beryllium	0.08	1.56E+01	3.13E+01	7.19E-01	8.22E-01	2.80E-01	1.820
			1.50E+00	3.00E+00	4.23E-01	3.88E-01	5.60E-01	1.371
7440-61-1	Uranium	0.5	5.00E+00	2.00E+02	7.21E-01	8.71E-01	1.00E+00	2.592
			4.00E+00	8.60E+00	5.54E-01	7.66E-01	1.00E+00	2.321
7440-70-2	Calcium	190000	2.56E-02	2.42E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.56E-02	2.42E-01	0.00E+00	0.00E+00	0.00E+00	0.000

Table IV-3. STEfw, eco results - inland water (dissolved fraction) monitoring data, $PNEC_{fw,\ eco}$.

For each substance, two scenarios are presented. Top/shaded: Sc2 (all monitoring records; non-quantified records set as half LOD/Q); Bottom/white: Sc2-PNEC QC (quantified records plus non-quantified samples excluding those for which ½LOD/Q > PNEC).

[1] RQ_P90 is the risk quotient between the 90th percentile of all monitoring records and the selected PNEC.
[2] RQ_P95 is the risk quotient between the 95th percentile of all monitoring records and the selected PNEC.
[3] Fspat, Ftemp and Fext stand for the spatial, temporal and extend of PNEC exceedance factors in the STE approach, calculated as described in Section 2.1, while the Final STE score is the sum of the individual factors.
[4] Only STE scores using Sc2-PNEC QC were used for the risk-based ranking of substances.

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
7429-90-5	Aluminium	40	4.20	6.96	0.709	0.854	0.18	1.743
			6.50	9.89	0.561	0.716	0.18	1.457
7439-89-6	Iron	200	4.35	7.10	0.157	0.566	0.11	0.833
			4.35	7.10	0.157	0.566	0.11	0.833
7439-96-5	Manganese	50	2.20	3.36	0.327	0.494	0.11	0.931
			2.20	3.36	0.327	0.494	0.11	0.931
7439-98-7	Molybdenum	136	0.01	0.04	0.000	0.000	0	0.000
			0.01	0.04	0.000	0.000	0	0.000
7440-38-2	Arsenic	13	0.38	0.77	0.000	0.000	0	0.000
			0.38	0.77	0.000	0.000	0	0.000
7440-39-3	Barium	9.3	7.84	9.03	0.773	0.977	0.18	1.931
			7.84	9.03	0.773	0.977	0.18	1.931
7440-42-8	Boron	180	0.83	1.39	0.104	0.525	0.04	0.669
			0.83	1.23	0.069	0.489	0.04	0.598
7440-47-3	Chromium	2.5	2.00	4.00	0.088	0.429	0.11	0.627

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
			1.00	1.00	0.030	0.245	0.07	0.345
7440-48-4	Cobalt	0.6	41.67	41.67	0.510	0.883	0.28	1.674
			0.87	1.38	0.119	0.366	0.07	0.555
7440-50-8	Copper	7.8	1.12	3.85	0.070	0.420	0.11	0.600
			0.64	0.77	0.044	0.292	0.07	0.406
7440-62-2	Vanadium	3.5	1.43	1.43	0.140	0.567	0.04	0.747
			0.40	0.66	0.045	0.378	0.04	0.463
7440-66-6	Zinc	10.9	4.59	4.59	0.439	0.572	0.11	1.120
			2.57	4.45	0.390	0.499	0.18	1.069
7782-49-2	Selenium	0.05	108.00	250.00	0.913	0.995	1	2.908
			70.00	102.25	0.652	0.994	0.56	2.206

Table IV-4. STEdw, hh results - inland whole water monitoring data, $PNEC_{dw, hh}$.

For each substance, two scenarios are presented. Top/shaded: Sc2 (all monitoring records; non-quantified records set as half LOD/Q); Bottom/white: Sc2-PNEC QC (quantified records plus non-quantified samples excluding those for which ½LOD/Q > PNEC).

Note: n/a for some substances in Sc2-PNECQC indicates that they are not considered in STE since did not fulfilled the representativeness criteria

[1] RQ_P90 is the risk quotient between the 90th percentile of all monitoring records and the selected PNEC.
[2] RQ_P95 is the risk quotient between the 95th percentile of all monitoring records and the selected PNEC.
[3] Fspat, Ftemp and Fext stand for the spatial, temporal and extend of PNEC exceedance factors in the STE approach, calculated as described in Section 2.1, while the Final STE score is the sum of the individual factors.
[4] Only STE scores using Sc2-PNEC QC were used for the risk-based ranking of substances.

CAS	Substance	PNEC (µg/L	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
100-41-4	Ethylbenzene	300	2.34E-03	8.33E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			1.67E-03	1.67E-03	0.00E+00	0.00E+00	0.00E+00	0.000
100-42-5	Styrene	20	2.50E-02	2.50E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			1.25E-02	2.50E-02	0.00E+00	0.00E+00	0.00E+00	0.000
1007-28-9	6-Deisopropylatrazine	70	7.14E-04	7.14E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			1.43E-04	1.43E-04	0.00E+00	0.00E+00	0.00E+00	0.000
101200-48-0	Tribenuron-methyl	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
101205-02-1	Cycloxydim	0.1	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
101-21-3	Chlorpropham	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
1014-69-3	Desmetryn	0.1	1.25E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			1.25E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
10265-92-6	Methamidophos	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			1.25E-01	1.25E-01	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
102851-06-9	Tau-fluvalinate	0.1	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			n/a	n/a	n/a	n/a	n/a	n/a
1031-07-8	Endosulfan sulfate	21	4.76E-04	1.19E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			2.38E-04	2.38E-04	0.00E+00	0.00E+00	0.00E+00	0.000
103-90-2	Acetaminophen (Paracetamol)	1190	2.52E-05	5.04E-05	0.00E+00	0.00E+00	0.00E+00	0.000
			2.52E-05	5.04E-05	0.00E+00	0.00E+00	0.00E+00	0.000
10605-21-7	Carbendazim	0.1	5.00E-01	1.50E+00	2.52E-02	3.82E-01	7.00E-02	0.477
			5.00E-01	1.50E+00	2.41E-02	3.69E-01	4.00E-02	0.433
106-46-7	1,4-Dichlorobenzene	300	1.67E-03	8.33E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			1.67E-03	1.67E-03	0.00E+00	0.00E+00	0.00E+00	0.000
106-47-8	4-Chloroaniline	0.0315	1.59E+00	4.76E+00	4.81E-01	7.98E-01	1.10E-01	1.389
			1.59E+00	1.59E+00	3.28E-01	7.72E-01	4.00E-02	1.140
106-48-9	4-Chlorophenol	10.5	4.76E-03	9.52E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			4.76E-03	9.52E-03	0.00E+00	0.00E+00	0.00E+00	0.000
1066-51-9	Aminomethylphosphonic acid (AMPA)	1050	9.52E-04	1.95E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			9.52E-04	1.95E-03	0.00E+00	0.00E+00	0.00E+00	0.000
106-89-8	Epichlorhydrin (1-chloro-2,3-epoxypropane)	0.4	6.25E+00	1.25E+01	2.95E-01	9.33E-01	1.80E-01	1.408
			1.25E+00	1.25E+00	9.89E-02	9.17E-01	7.00E-02	1.086
106-93-4	1,2-Dibromoethane	0.4	3.13E+00	6.25E+00	1.95E-01	5.85E-01	1.80E-01	0.960
			n/a	n/a	n/a	n/a	n/a	n/a
1071-83-6	Glyphosate	350	7.43E-04	1.51E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			7.43E-04	1.51E-03	0.00E+00	0.00E+00	0.00E+00	0.000
107534-96-3	Tebuconazole	105	4.76E-04	4.76E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			4.76E-04	4.76E-04	0.00E+00	0.00E+00	0.00E+00	0.000
108-42-9	3-Chloroaniline	0.0315	1.59E+00	1.59E+00	4.42E-01	8.46E-01	7.00E-02	1.358
			1.59E+00	1.59E+00	4.42E-01	8.46E-01	7.00E-02	1.357

CAS	Substance	PNEC (µg/L	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
108-43-0	3-Chlorophenol	10.5	9.52E-03	9.52E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			9.52E-03	9.52E-03	0.00E+00	0.00E+00	0.00E+00	0.000
1085-98-9	Dichlofluanide	1225	1.63E-05	1.63E-05	0.00E+00	0.00E+00	0.00E+00	0.000
			1.63E-05	1.63E-05	0.00E+00	0.00E+00	0.00E+00	0.000
108-88-3	Toluene	700	7.14E-04	7.14E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			7.14E-04	7.14E-04	0.00E+00	0.00E+00	0.00E+00	0.000
108-90-7	Chlorobenzene	70	7.14E-03	7.14E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			7.14E-03	7.14E-03	0.00E+00	0.00E+00	0.00E+00	0.000
108-95-2	Phenol	140	7.14E-03	2.14E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			4.31E-03	7.14E-03	0.00E+00	0.00E+00	0.00E+00	0.000
110488-70-5	Dimethomorph	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
1113-02-6	Omethoate	1.4	3.57E-02	3.57E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			7.14E-02	8.14E-02	0.00E+00	0.00E+00	0.00E+00	0.000
111988-49-9	Thiacloprid	0.1	1.00E-01	1.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			1.00E-01	1.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
111991-09-4	Nicosulfuron	0.1	2.50E-01	2.50E-01	2.56E-03	1.05E-01	0.00E+00	0.107
			8.97E-01	1.97E+00	1.40E-01	3.10E-01	7.00E-02	0.520
114-26-1	Propoxur	0.1	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			1.00E-01	1.00E-01	2.30E-03	4.21E-02	0.00E+00	0.044
115-96-8	Tris(2-chloroethyl)phosphate (TCEP)	1540	1.04E-04	1.62E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			1.04E-04	1.62E-04	0.00E+00	0.00E+00	0.00E+00	0.000
116-06-3	Aldicarb	10	5.00E-03	5.00E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-03	5.00E-03	0.00E+00	0.00E+00	0.00E+00	0.000
116-29-0	Tetradifon	52.5	9.52E-04	9.52E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			9.52E-04	9.52E-04	0.00E+00	0.00E+00	0.00E+00	0.000
117428-22-5	Picoxystrobin	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
118134-30-8	Spiroxamine	87.5	5.71E-04	5.71E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			1.14E-04	3.01E-04	0.00E+00	0.00E+00	0.00E+00	0.000
119446-68-3	Difenoconazole	35	2.86E-03	2.86E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			2.86E-03	2.86E-03	0.00E+00	0.00E+00	0.00E+00	0.000
1194-65-6	Dichlobenil	0.1	2.50E-01	2.50E-01	1.23E-03	1.64E-01	0.00E+00	0.166
			2.50E-01	2.50E-01	1.23E-03	1.64E-01	0.00E+00	0.166
120-32-1	Chlorophene	0.1	2.50E+00	2.50E+00	1.00E+00	0.00E+00	7.00E-02	1.070
			2.50E+00	2.50E+00	1.00E+00	0.00E+00	7.00E-02	1.070
120-36-5	Diclorprop	100	2.00E-04	2.50E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			2.00E-04	2.50E-04	0.00E+00	0.00E+00	0.00E+00	0.000
120-83-2	2,4-Dichlorophenol	10.5	4.76E-03	9.52E-03	2.74E-04	4.40E-01	0.00E+00	0.440
			4.76E-03	9.52E-03	0.00E+00	0.00E+00	0.00E+00	0.000
120923-37-7	Amidosulfuron	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
121-14-2	2,4-Dinitrotoluene	7	1.79E-02	4.29E-02	1.68E-03	1.11E-01	0.00E+00	0.113
			1.79E-02	1.86E-02	1.80E-03	1.11E-01	0.00E+00	0.113
121552-61-2	Cyprodinil	0.1	2.50E-01	4.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-01	4.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
121-75-5	Malathion	70	2.86E-04	3.57E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			5.71E-04	6.59E-04	0.00E+00	0.00E+00	0.00E+00	0.000
122-14-5	Fenitrothion	0.1	2.00E-01	2.25E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-02	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.000
122-39-4	Diphenylamine	87.5	5.71E-04	5.71E-04	3.28E-04	0.00E+00	0.00E+00	0.000
			5.71E-04	5.71E-04	3.28E-04	0.00E+00	0.00E+00	0.000
122931-48-0	Rimsulfuron	0.1	2.50E-01	2.50E-01	5.80E-03	9.45E-01	0.00E+00	0.951
			1.00E-01	1.00E-01	4.99E-03	0.00E+00	0.00E+00	0.005
123-91-1	1,4-Dioxane	50	2.50E-02	3.10E-02	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
			2.50E-02	3.10E-02	0.00E+00	0.00E+00	0.00E+00	0.000
124-48-1	Dibromochloromethane	100	5.00E-03	5.00E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-03	5.00E-03	0.00E+00	0.00E+00	0.00E+00	0.000
126535-15-7	Triflusulfuron-methyl	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
126-71-6	Triisobutyl phosphate	7455	3.35E-05	8.45E-05	0.00E+00	0.00E+00	0.00E+00	0.000
			3.35E-05	8.45E-05	0.00E+00	0.00E+00	0.00E+00	0.000
126-73-8	Tributyl phosphate	280	1.79E-03	1.79E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			1.79E-04	3.57E-04	0.00E+00	0.00E+00	0.00E+00	0.000
126833-17-8	Fenhexamid	0.1	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
128639-02-1	Carfentrazone-ethyl	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
129-00-0	Pyrene	105	2.19E-04	4.48E-04	3.24E-04	1.84E-01	0.00E+00	0.184
			4.10E-04	8.57E-04	5.79E-04	2.47E-01	0.00E+00	0.247
131-11-3	Dimethyl phthalate	32900	1.52E-05	1.52E-05	0.00E+00	0.00E+00	0.00E+00	0.000
			1.52E-05	1.52E-05	0.00E+00	0.00E+00	0.00E+00	0.000
131341-86-1	Fludioxonil	1295	1.93E-05	3.86E-05	0.00E+00	0.00E+00	0.00E+00	0.000
			1.93E-05	3.86E-05	0.00E+00	0.00E+00	0.00E+00	0.000
131860-33-8	Azoxystrobin	0.1	2.50E-01	4.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-01	4.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
131983-72-7	Triticonazole	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
1330-20-7	Xylene (mixed isomers)	500	2.00E-03	2.00E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			2.00E-03	2.00E-03	0.00E+00	0.00E+00	0.00E+00	0.000
133-06-2	Captan	0.1	2.50E-01	1.25E+00	1.85E-02	5.78E-01	4.00E-02	0.636
			2.50E-01	1.25E+00	1.85E-02	5.78E-01	4.00E-02	0.636
133-07-3	Folpet	0.1	2.50E-01	5.00E-01	4.35E-03	6.37E-01	0.00E+00	0.642

CAS	Substance	PNEC (µg/L	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
			2.50E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
1330-78-5	Tricresyl Phosphate	245	3.71E-05	5.63E-05	0.00E+00	0.00E+00	0.00E+00	0.000
			3.71E-05	5.63E-05	0.00E+00	0.00E+00	0.00E+00	0.000
133855-98-8	Epoxiconazole	28	1.79E-03	1.79E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			1.79E-03	1.79E-03	0.00E+00	0.00E+00	0.00E+00	0.000
134-62-3	Diethyltoluamide (DEET)	2625	3.35E-05	5.33E-05	0.00E+00	0.00E+00	0.00E+00	0.000
			3.35E-05	5.33E-05	0.00E+00	0.00E+00	0.00E+00	0.000
13684-56-5	Desmedipham	0.1	1.50E+00	1.50E+00	4.95E-02	9.41E-01	4.00E-02	1.031
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
13684-63-4	Phenmedipham	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
138261-41-3	Imidacloprid	0.1	3.00E-01	7.00E-01	2.02E-02	3.26E-01	7.00E-02	0.416
			9.00E-01	2.50E+00	2.74E-02	3.35E-01	1.10E-01	0.473
139-13-9	Nitrilotriacetic acid	200	2.02E-02	3.81E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			2.02E-02	3.81E-02	0.00E+00	0.00E+00	0.00E+00	0.000
139-40-2	Propazine	0.1	2.50E-01	2.50E-01	7.93E-04	3.41E-01	0.00E+00	0.342
			2.50E-01	2.50E-01	5.17E-04	2.61E-01	0.00E+00	0.262
141517-21-7	Trifloxystrobin	350	1.43E-04	1.43E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			1.43E-04	1.43E-04	0.00E+00	0.00E+00	0.00E+00	0.000
141776-32-1	Sulfosulfuron	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
142-28-9	1,3-Dichloropropane	70	1.43E-01	1.43E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			3.57E-03	3.57E-03	0.00E+00	0.00E+00	0.00E+00	0.000
142459-58-3	Flufenacet	14	3.57E-03	3.57E-03	1.31E-03	3.93E-01	0.00E+00	0.394
			1.79E-03	1.79E-03	1.38E-03	1.00E+00	0.00E+00	1.001
143390-89-0	Kresoxim-methyl	0.1	2.50E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
144550-36-7	Iodosulfuron	0.1	3.50E-01	3.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
			3.50E-01	3.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
145701-23-1	Florasulam	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			n/a	n/a	n/a	n/a	n/a	n/a
14797-65-0	Nitrite (NO2)	3000	2.94E-02	4.83E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			2.97E-02	4.87E-02	0.00E+00	0.00E+00	0.00E+00	0.000
14816-18-3	Phoxim	0.1	5.00E-01	5.00E-01	1.20E-02	6.20E-01	0.00E+00	0.632
			n/a	n/a	n/a	n/a	n/a	n/a
150-68-5	Monuron	0.1	2.50E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			n/a	n/a	n/a	n/a	n/a	n/a
152019-73-3	Metolachlor OA	0.1	4.50E-01	6.30E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			4.50E-01	6.30E-01	0.00E+00	0.00E+00	0.00E+00	0.000
15299-99-7	Napropamide	0.1	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
15307-86-5	Diclofenac	5600	1.04E-04	3.04E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			1.04E-04	3.04E-03	0.00E+00	0.00E+00	0.00E+00	0.000
153719-23-4	Thiamethoxam	0.1	1.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			1.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
15545-48-9	Chlorotoluron	30	1.67E-03	2.10E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			1.67E-03	1.90E-03	0.00E+00	0.00E+00	0.00E+00	0.000
1563-66-2	Carbofuran	7	3.57E-03	3.57E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			1.79E-03	1.79E-03	0.00E+00	0.00E+00	0.00E+00	0.000
15687-27-1	Ibuprofen	385	2.84E-04	4.42E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			2.84E-04	4.42E-04	0.00E+00	0.00E+00	0.00E+00	0.000
15950-66-0	2,3,4-Trichlorphenol	10.5	2.38E-02	2.38E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			2.38E-02	2.38E-02	0.00E+00	0.00E+00	0.00E+00	0.000
1610-18-0	Prometon	52.5	3.81E-04	3.81E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			3.81E-04	3.81E-04	0.00E+00	0.00E+00	0.00E+00	0.000
1634-04-4	Methyl-tert-butyl ether (MTBE)	1050	4.76E-03	4.76E-03	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
			4.76E-03	4.76E-03	0.00E+00	0.00E+00	0.00E+00	0.000
1646-88-4	Aldicarb sulfone	3.5	1.43E-02	1.43E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			1.43E-02	1.43E-02	0.00E+00	0.00E+00	0.00E+00	0.000
16752-77-5	Methomyl	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
16887-00-6	Chloride	250000	5.04E-04	2.84E-02	2.38E-03	1.00E+00	0.00E+00	1.002
			5.04E-04	2.84E-02	2.38E-03	1.00E+00	0.00E+00	1.002
1689-84-5	Bromoxynil	0.1	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
16984-48-8	Fluoride	1500	2.27E-01	3.20E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.27E-01	3.20E-01	0.00E+00	0.00E+00	0.00E+00	0.000
1698-60-8	Chloridazon	0.1	5.00E-01	2.50E+00	3.18E-02	5.49E-01	7.00E-02	0.651
			5.00E-01	2.50E+00	3.18E-02	5.49E-01	7.00E-02	0.651
1702-17-6	Clopyralid	0.1	5.00E-01	5.00E-01	2.50E-02	6.12E-01	4.00E-02	0.677
			5.00E-01	5.00E-01	2.50E-02	6.12E-01	4.00E-02	0.677
17040-19-6	Demeton-S-methylsulfon	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
171118-09-5	Metolachlor ESA	0.1	1.05E+00	1.49E+00	2.78E-02	2.91E-01	4.00E-02	0.358
			1.05E+00	1.49E+00	2.78E-02	2.91E-01	4.00E-02	0.358
17254-80-7	Chloridazon methyl-desphenyl	0.1	2.50E+00	3.09E+00	1.06E-01	7.61E-01	7.00E-02	0.937
			2.50E+00	3.09E+00	1.06E-01	7.61E-01	7.00E-02	0.937
173159-57-4	Foramsulfuron	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			n/a	n/a	n/a	n/a	n/a	n/a
1746-81-2	Monolinuron	0.1	2.50E-01	2.50E-01	2.36E-03	8.12E-01	0.00E+00	0.815
			2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
175013-18-0	Pyraclostrobine	105	4.76E-04	4.76E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			4.76E-04	4.76E-04	0.00E+00	0.00E+00	0.00E+00	0.000
18691-97-9	Methabenzthiazuron	0.1	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
			2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
188425-85-6	Boscalid	0.1	2.50E-01	7.19E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-01	7.19E-01	0.00E+00	0.00E+00	0.00E+00	0.000
1897-45-6	Chlorothalonil	0.1	2.00E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.00E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
1918-00-9	Dicamba	105	4.76E-04	4.76E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			4.76E-04	4.76E-04	0.00E+00	0.00E+00	0.00E+00	0.000
19666-30-9	Oxadiazon	12.6	1.98E-03	1.98E-03	1.70E-03	4.97E-01	0.00E+00	0.499
			1.98E-03	1.98E-03	1.70E-03	8.47E-01	0.00E+00	0.849
1982-47-4	Chloroxuron	0.1	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
19937-59-8	Metoxuron	0.1	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
2008-58-4	2,6-Dichlorobenzamide	0.1	2.50E-01	3.11E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-01	3.11E-01	0.00E+00	0.00E+00	0.00E+00	0.000
2032-65-7	Methiocarb	0.1	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			8.00E-02	1.40E-01	8.03E-03	5.31E-01	0.00E+00	0.539
208-96-8	Acenaphthylene	175	1.43E-04	2.86E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			1.43E-04	2.86E-04	0.00E+00	0.00E+00	0.00E+00	0.000
21087-64-9	Metribuzin	0.1	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
210880-92-5	Clothianidin	0.1	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
2163-68-0	2-Hydroxyatrazine	200	2.50E-04	5.00E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-04	5.00E-04	0.00E+00	0.00E+00	0.00E+00	0.000
#2164-08-1	Lenacil	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
21725-46-2	Cyanazine	0.6	4.17E-02	4.17E-02	8.12E-04	7.98E-01	0.00E+00	0.799

CAS	Substance	PNEC (µg/L	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
			4.17E-02	4.17E-02	3.56E-04	9.34E-01	0.00E+00	0.934
2212-67-1	Molinate	6	8.33E-03	8.33E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			8.33E-03	8.33E-03	0.00E+00	0.00E+00	0.00E+00	0.000
2303-17-5	Triallate	0.1	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			n/a	n/a	n/a	n/a	n/a	n/a
23103-98-2	Pirimicarb	0.1	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
23135-22-0	Oxamyl	87.5	5.71E-04	5.71E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			5.71E-04	5.71E-04	0.00E+00	0.00E+00	0.00E+00	0.000
2385-85-5	Mirex	0.7	7.14E-03	3.57E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			n/a	n/a	n/a	n/a	n/a	n/a
23950-58-5	Propyzamide	0.1	2.50E-01	2.50E-01	4.14E-03	1.12E-01	0.00E+00	0.116
			2.50E-01	2.50E-01	4.14E-03	1.12E-01	0.00E+00	0.116
24017-47-8	Triazophos	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			n/a	n/a	n/a	n/a	n/a	n/a
24579-73-5	Propamocarb	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
25057-89-0	Bentazone	0.1	3.00E-01	5.90E-01	7.24E-03	1.93E-01	4.00E-02	0.240
			3.00E-01	5.90E-01	7.24E-03	1.93E-01	4.00E-02	0.240
26225-79-6	Ethofumesate	0.1	2.50E-01	6.00E-01	1.81E-02	4.45E-01	7.00E-02	0.533
			2.50E-01	6.00E-01	1.81E-02	4.45E-01	7.00E-02	0.533
26259-45-0	Secbumeton	0.1	2.00E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.00E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
2642-71-9	Azinphos-ethyl	0.1	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			3.00E-01	5.00E-01	2.87E-03	2.50E-01	0.00E+00	0.253
29232-93-7	Pirimiphos-methyl	0.1	2.00E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-02	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.000
298-04-4	Disulfoton	0.14	1.79E-01	3.57E-01	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
			n/a	n/a	n/a	n/a	n/a	n/a
298-46-4	Carbamazepine	56	6.79E-03	1.21E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			6.79E-03	1.21E-02	0.00E+00	0.00E+00	0.00E+00	0.000
301-12-2	Oxydemeton-methyl	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			n/a	n/a	n/a	n/a	n/a	n/a
30125-63-4	Desethylterbuthylazine	14	1.79E-03	1.79E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			1.79E-03	1.79E-03	0.00E+00	0.00E+00	0.00E+00	0.000
30125-63-4	Desethylterbuthylazine	14	1.79E-03	1.79E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			1.79E-03	1.79E-03	0.00E+00	0.00E+00	0.00E+00	0.000
302-17-0	Chloral hydrate	350	1.43E-03	1.43E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			1.43E-03	1.43E-03	0.00E+00	0.00E+00	0.00E+00	0.000
3060-89-7	Metobromuron	0.1	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
307-24-4	Perfluorohexanoic acid (PFHxA)	0.1	2.80E-01	6.50E-01	8.74E-03	3.48E-01	4.00E-02	0.396
			2.80E-01	6.50E-01	8.74E-03	3.48E-01	4.00E-02	0.396
314-40-9	Bromacil	0.1	5.00E-01	5.00E-01	8.53E-04	1.23E-01	0.00E+00	0.124
			1.00E-01	1.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
32809-16-8	Procymidone	0.1	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
330-55-2	Linuron	0.1	2.50E-01	2.50E-01	9.22E-03	2.76E-01	0.00E+00	0.285
			2.50E-01	2.50E-01	2.84E-03	1.46E-01	0.00E+00	0.149
333-41-5	Diazinon	0.7	3.57E-02	5.71E-02	1.19E-03	7.60E-01	0.00E+00	0.761
			1.43E-02	1.43E-02	3.30E-04	3.23E-01	0.00E+00	0.323
335-67-1	Perfluorooctanoic acid (PFOA)	0.35	1.91E-01	4.00E-01	3.38E-03	2.89E-01	0.00E+00	0.292
			1.89E-01	4.00E-01	3.31E-03	2.89E-01	0.00E+00	0.292
3380-34-5	Triclosan	17.5	2.29E-03	2.66E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			2.00E-03	2.97E-03	0.00E+00	0.00E+00	0.00E+00	0.000
3397-62-4	Desisopropyldesethylatrazine	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
			n/a	n/a	n/a	n/a	n/a	n/a
3424-82-6	2,2-(2-Chlorophenyl-4'-chlorophenyl)-1,1-dichloroethene (DDE, o,p')	2	2.50E-03	3.13E-03	1.37E-03	8.05E-01	0.00E+00	0.807
			2.50E-03	2.50E-03	2.45E-04	4.56E-01	0.00E+00	0.457
34256-82-1	Acetochlor	70	3.57E-04	3.57E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			1.79E-04	1.79E-04	0.00E+00	0.00E+00	0.00E+00	0.000
35367-38-5	Diflubenzuron	0.1	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			n/a	n/a	n/a	n/a	n/a	n/a
35554-44-0	Imazalil	87.5	8.57E-04	8.57E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			8.57E-04	8.57E-04	0.00E+00	0.00E+00	0.00E+00	0.000
36734-19-7	Iprodione	210	1.19E-04	2.38E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			1.19E-04	2.38E-04	0.00E+00	0.00E+00	0.00E+00	0.000
37350-58-6	Metoprolol	9.8	4.59E-02	6.63E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			4.59E-02	6.63E-02	0.00E+00	0.00E+00	0.00E+00	0.000
375-73-5	Perfluorobutanesulfonate (PFBS)	3	9.96E-03	1.91E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			9.96E-03	1.91E-02	0.00E+00	0.00E+00	0.00E+00	0.000
40487-42-1	Pendimethalin	20	1.25E-03	1.25E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			6.25E-04	6.25E-04	0.00E+00	0.00E+00	0.00E+00	0.000
41394-05-2	Metamitron	0.1	5.00E-01	5.00E-01	5.37E-03	1.71E-01	4.00E-02	0.217
			5.00E-01	5.00E-01	5.32E-03	1.72E-01	4.00E-02	0.217
41859-67-0	Bezafibrate	35	2.77E-03	4.29E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			2.77E-03	4.29E-03	0.00E+00	0.00E+00	0.00E+00	0.000
43121-43-3	Triadimefon	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
50-00-0	Formaldehyde	700	3.57E-03	1.43E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			3.57E-03	3.57E-03	0.00E+00	0.00E+00	0.00E+00	0.000
50-28-2	17-beta-Estradiol	0.175	2.86E-03	2.86E-03	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
			5.71E-03	1.11E-02	0.00E+00	0.00E+00	0.00E+00	0.000
50471-44-8	Vinclozolin	87.5	2.86E-04	2.86E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			2.86E-04	2.86E-04	0.00E+00	0.00E+00	0.00E+00	0.000
51218-45-2	Metolachlor	10	2.50E-03	5.00E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-03	5.00E-03	0.00E+00	0.00E+00	0.00E+00	0.000
51235-04-2	Hexazinone	0.1	2.50E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
52645-53-1	Permethrin	175	1.43E-04	1.43E-04	1.18E-03	1.00E+00	0.00E+00	1.001
			5.71E-05	1.14E-04	0.00E+00	0.00E+00	0.00E+00	0.000
52-68-6	Trichlorfon	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			n/a	n/a	n/a	n/a	n/a	n/a
52888-80-9	Prosulfocarb	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
52918-63-5	Deltamethrin	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			n/a	n/a	n/a	n/a	n/a	n/a
53112-28-0	Pyrimethanil	0.1	2.50E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
53-19-0	DDD, o,p'	2	2.50E-03	5.00E-03	7.40E-04	7.83E-01	0.00E+00	0.783
			2.50E-04	2.50E-04	8.34E-04	4.79E-01	0.00E+00	0.480
534-52-1	Dinitro-o-cresol (DNOC)	0.1	2.50E-01	4.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-01	4.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
53-70-3	Dibenz(a,h)anthracene	1.75	2.86E-03	2.86E-03	1.12E-03	4.18E-01	0.00E+00	0.419
			8.57E-04	4.01E-03	4.07E-03	1.00E+00	0.00E+00	1.004
540-59-0	1,2-Dichloroethene	50	2.50E-01	4.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			1.00E-01	1.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
541-73-1	1,3-Dichlorobenzene	10.5	4.76E-02	9.52E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			4.76E-02	4.76E-02	0.00E+00	0.00E+00	0.00E+00	0.000
542-75-6	1,3-Dichloropropene	20	5.00E-02	7.50E-02	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
			5.00E-02	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.000
55179-31-2	Bitertanol	10.5	2.38E-03	2.38E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			2.38E-03	2.38E-03	0.00E+00	0.00E+00	0.00E+00	0.000
55219-65-3	Triadimenol	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
55335-06-3	Triclopyr	0.1	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
55-38-9	Fenthion	0.1	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			3.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
5598-13-0	Chlorpyriphos-methyl	35	5.71E-04	7.14E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			2.86E-04	5.71E-04	0.00E+00	0.00E+00	0.00E+00	0.000
563-12-2	Ethion	1.75	5.71E-03	1.43E-02	4.27E-03	5.62E-01	0.00E+00	0.566
			1.14E-02	1.14E-02	0.00E+00	0.00E+00	0.00E+00	0.000
56-38-2	Parathion	21	1.19E-03	1.19E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			2.38E-04	2.38E-04	0.00E+00	0.00E+00	0.00E+00	0.000
56-55-3	Benzo(a)anthracene	0.175	8.57E-02	1.60E-01	7.73E-03	8.13E-01	1.80E-01	1.001
			1.71E-01	3.03E-01	8.08E-03	5.70E-01	0.00E+00	0.578
56-72-4	Coumaphos	0.1	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			n/a	n/a	n/a	n/a	n/a	n/a
57018-04-9	Tolclofos-methyl	224	1.12E-04	2.23E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			1.12E-04	2.23E-04	0.00E+00	0.00E+00	0.00E+00	0.000
57-12-5	Cyanides (as total CN)	50	1.00E-01	1.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			1.00E-01	1.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
57-74-9	Chlordane	0.2	5.00E-02	1.25E-01	9.64E-04	4.19E-01	0.00E+00	0.420
			n/a	n/a	n/a	n/a	n/a	n/a
57837-19-1	Metalaxyl	0.1	2.50E-01	2.50E-01	2.18E-03	2.13E-01	0.00E+00	0.216
			2.50E-01	2.50E-01	2.18E-03	2.13E-01	0.00E+00	0.216
5915-41-3	Terbuthylazine	7	3.57E-03	9.43E-03	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
			3.57E-03	9.30E-03	0.00E+00	0.00E+00	0.00E+00	0.000
59-50-7	Chlorocresol	0.1	1.25E+00	2.50E+00	6.72E-02	5.76E-01	7.00E-02	0.713
			1.25E+00	2.50E+00	4.90E-02	5.80E-01	7.00E-02	0.699
60-00-4	Edetic acid (EDTA)	600	1.83E-02	2.83E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			1.83E-02	2.83E-02	0.00E+00	0.00E+00	0.00E+00	0.000
60168-88-9	Fenarimol	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			n/a	n/a	n/a	n/a	n/a	n/a
60207-90-1	Propiconazole	140	3.57E-04	3.57E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			3.57E-04	3.57E-04	0.00E+00	0.00E+00	0.00E+00	0.000
60-51-5	Dimethoate	6	4.17E-03	8.33E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			1.67E-03	1.67E-03	0.00E+00	0.00E+00	0.00E+00	0.000
6190-65-4	Desethylatrazine	70	7.14E-04	1.16E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			7.14E-04	1.14E-03	0.00E+00	0.00E+00	0.00E+00	0.000
62-53-3	Aniline	5.04	9.92E-02	9.92E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			9.92E-02	9.92E-02	0.00E+00	0.00E+00	0.00E+00	0.000
630-20-6	1,1,1,2-Tetrachloroethane	105	2.38E-02	2.38E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			2.38E-02	2.38E-02	0.00E+00	0.00E+00	0.00E+00	0.000
63-25-2	Carbaril	0.1	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			1.00E-01	1.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
66230-04-4	Esfenvalerate	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			n/a	n/a	n/a	n/a	n/a	n/a
66246-88-6	Penconazole	105	2.38E-04	4.76E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			2.38E-04	4.76E-04	0.00E+00	0.00E+00	0.00E+00	0.000
668-34-8	Triphenyltin	0.1	1.70E-01	1.70E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			1.35E-01	1.85E-01	7.22E-04	0.00E+00	0.00E+00	0.001
67129-08-2	Metazachlor	0.1	2.50E-01	2.80E-01	7.49E-03	1.08E-01	4.00E-02	0.156
			2.50E-01	2.80E-01	7.28E-03	1.08E-01	4.00E-02	0.155
67306-00-7	Fenpropidin	0.1	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
			n/a	n/a	n/a	n/a	n/a	n/a
67564-91-4	Fenpropimorph	10.5	2.38E-03	2.38E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			1.19E-03	1.19E-03	0.00E+00	0.00E+00	0.00E+00	0.000
67-72-1	Hexachloroethane	2.45	1.02E-01	1.02E-01	4.20E-03	1.00E+00	0.00E+00	1.004
			1.02E-01	1.02E-01	1.38E-04	0.00E+00	0.00E+00	0.000
67747-09-5	Prochloraz	35	1.00E-03	1.43E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			1.00E-03	1.43E-03	0.00E+00	0.00E+00	0.00E+00	0.000
68359-37-5	Cyfluthrin	0.1	2.50E-01	1.00E+00	0.00E+00	0.00E+00	0.00E+00	0.000
			n/a	n/a	n/a	n/a	n/a	n/a
69377-81-7	Fluroxypyr	0.1	2.50E-01	5.00E-01	4.11E-03	1.36E-01	0.00E+00	0.140
			2.50E-01	5.00E-01	4.07E-03	1.36E-01	0.00E+00	0.140
709-98-8	Propanil	0.1	5.00E-01	5.00E-01	3.02E-03	9.18E-01	0.00E+00	0.921
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
71-55-6	1,1,1-Trichloroethane	980	2.55E-04	5.10E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			2.55E-04	5.10E-04	0.00E+00	0.00E+00	0.00E+00	0.000
723-46-6	Sulfamethoxazole	455	4.40E-04	2.57E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			4.40E-04	2.67E-03	0.00E+00	0.00E+00	0.00E+00	0.000
72-43-5	Methoxychlor	20	1.25E-03	1.25E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-05	2.50E-05	0.00E+00	0.00E+00	0.00E+00	0.000
7286-69-3	Sebuthylazine	0.1	2.00E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			1.00E-01	1.00E-01	1.44E-03	5.97E-01	0.00E+00	0.599
7287-19-6	Prometryn	14	1.79E-03	1.79E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			1.79E-03	1.79E-03	0.00E+00	0.00E+00	0.00E+00	0.000
731-27-1	Tolylfluanid	350	1.43E-04	1.43E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			1.43E-04	1.43E-04	0.00E+00	0.00E+00	0.00E+00	0.000
738-70-5	Trimethoprim	14.7	2.72E-03	4.59E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			2.72E-03	4.59E-03	0.00E+00	0.00E+00	0.00E+00	0.000
74223-64-6	Metsulfuron-methyl	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
			1.00E-01	1.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
7429-90-5	Aluminium	200	2.15E+00	3.95E+00	2.70E-01	3.36E-01	1.10E-01	0.715
			2.15E+00	3.95E+00	2.70E-01	3.36E-01	1.10E-01	0.715
7439-89-6	Iron	200	5.50E+00	9.00E+00	4.71E-01	5.44E-01	1.80E-01	1.195
			5.50E+00	9.00E+00	4.71E-01	5.44E-01	1.80E-01	1.195
7439-95-4	Magnesium	672000	8.54E-03	1.49E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			8.54E-03	1.49E-02	0.00E+00	0.00E+00	0.00E+00	0.000
7439-96-5	Manganese	50	2.84E+00	4.52E+00	5.88E-01	4.78E-01	1.80E-01	1.247
			2.84E+00	4.51E+00	5.88E-01	4.78E-01	1.80E-01	1.246
7439-98-7	Molybdenum	17.5	1.43E-01	2.65E-01	1.12E-03	2.53E-01	0.00E+00	0.254
			1.43E-01	2.65E-01	1.12E-03	2.53E-01	0.00E+00	0.254
7440-22-4	Silver	17.5	7.14E-02	1.43E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.86E-02	4.29E-02	0.00E+00	0.00E+00	0.00E+00	0.000
7440-23-5	Sodium	200000	1.90E-02	2.10E-01	3.68E-03	9.49E-01	0.00E+00	0.952
			1.90E-02	2.10E-01	3.68E-03	9.49E-01	0.00E+00	0.952
7440-24-6	Strontium	2100	2.14E-01	2.48E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.14E-01	2.48E-01	0.00E+00	0.00E+00	0.00E+00	0.000
7440-28-0	Thallium	0.245	5.10E+00	1.02E+01	5.03E-01	8.77E-01	1.80E-01	1.560
			2.04E-01	4.90E-01	1.04E-01	5.42E-01	2.80E-01	0.926
7440-31-5	Tin	700	7.14E-03	3.57E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			7.14E-04	1.00E-03	0.00E+00	0.00E+00	0.00E+00	0.000
7440-36-0	Antimony	20	7.50E-02	1.25E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			7.50E-02	1.25E-01	0.00E+00	0.00E+00	0.00E+00	0.000
7440-38-2	Arsenic	10	2.74E-01	4.80E-01	6.43E-03	2.63E-01	4.00E-02	0.309
			2.67E-01	4.40E-01	4.97E-03	3.29E-01	4.00E-02	0.374
7440-39-3	Barium	700	1.15E-01	1.36E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			1.16E-01	1.37E-01	0.00E+00	0.00E+00	0.00E+00	0.000
7440-41-7	Beryllium	7	1.79E-01	3.57E-01	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
			1.71E-02	3.43E-02	1.15E-02	9.63E-01	4.00E-02	1.014
7440-42-8	Boron	2400	5.00E-02	7.92E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-02	7.88E-02	0.00E+00	0.00E+00	0.00E+00	0.000
7440-47-3	Chromium	50	4.02E-02	7.23E-02	5.78E-04	9.46E-02	0.00E+00	0.095
			3.80E-02	5.92E-02	3.57E-04	9.48E-02	0.00E+00	0.095
7440-48-4	Cobalt	4.9	2.55E-01	5.10E-01	2.15E-02	3.66E-01	4.00E-02	0.428
			1.82E-01	2.86E-01	1.37E-02	3.46E-01	4.00E-02	0.400
7440-50-8	Copper	2000	2.60E-03	4.05E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-03	3.65E-03	0.00E+00	0.00E+00	0.00E+00	0.000
7440-61-1	Uranium	30	8.33E-02	3.33E+00	3.19E-02	9.14E-01	2.80E-01	1.226
			6.67E-02	1.43E-01	1.97E-02	9.20E-01	2.80E-01	1.220
7440-62-2	Vanadium	3.5	8.00E-01	1.29E+00	1.13E-01	4.25E-01	7.00E-02	0.608
			7.43E-01	1.14E+00	7.20E-02	3.75E-01	7.00E-02	0.517
7440-66-6	Zinc	1050	2.53E-02	4.41E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			2.51E-02	4.37E-02	0.00E+00	0.00E+00	0.00E+00	0.000
75-01-4	Chloroethene	0.3	4.17E+00	1.67E+01	1.46E-01	6.00E-01	1.80E-01	0.926
			1.67E-01	3.33E-01	1.82E-02	5.67E-01	7.00E-02	0.655
75-25-2	Bromoform	100	5.00E-03	5.00E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-03	5.00E-03	0.00E+00	0.00E+00	0.00E+00	0.000
75-27-4	Dichlorobromomethane	60	4.17E-03	8.33E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			4.17E-03	8.33E-03	0.00E+00	0.00E+00	0.00E+00	0.000
75-34-3	1,1-Dichloroethane	700	7.14E-03	1.43E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			7.14E-03	1.43E-02	0.00E+00	0.00E+00	0.00E+00	0.000
76-03-9	Trichloroacetic acid	200	9.00E-04	1.20E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			1.05E-03	1.40E-03	0.00E+00	0.00E+00	0.00E+00	0.000
7664-41-7	Ammonia	500	4.20E-01	7.53E-01	4.05E-02	4.92E-01	7.00E-02	0.603
			4.20E-01	7.53E-01	4.05E-02	4.92E-01	7.00E-02	0.603
76674-21-0	Flutriafol	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
7782-49-2	Selenium	40	6.25E-02	6.25E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			4.75E-02	7.50E-02	0.00E+00	0.00E+00	0.00E+00	0.000
7786-34-7	Mevinphos	0.1	2.00E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			1.00E-01	2.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
78587-05-0	Hexythiazox	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
78-87-5	1,2-Dichloropropane	40	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
79-00-5	1,1,2-Trichloroethane	14	8.93E-02	1.79E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			8.93E-02	1.79E-01	0.00E+00	0.00E+00	0.00E+00	0.000
79-11-8	Chloroacetic acid	20	2.50E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			n/a	n/a	n/a	n/a	n/a	n/a
79241-46-6	Fluazifop-P-butyl	0.1	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
79277-27-3	Thifensulfuron methyl	0.1	5.00E-01	5.00E-01	3.81E-03	5.09E-01	0.00E+00	0.513
			5.00E-01	5.00E-01	3.81E-03	5.09E-01	0.00E+00	0.513
79622-59-6	Fluazinam	0.1	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
80-05-7	Bisphenol A	14	1.79E-02	2.25E-02	1.42E-03	7.16E-01	0.00E+00	0.717
			8.57E-03	1.61E-02	1.51E-03	7.36E-01	0.00E+00	0.737
80-09-1	Bisphenol S	1750	2.86E-05	4.40E-05	0.00E+00	0.00E+00	0.00E+00	0.000
			2.86E-05	4.40E-05	0.00E+00	0.00E+00	0.00E+00	0.000
8065-48-3	Demeton	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
82097-50-5	Triasulfuron	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			n/a	n/a	n/a	n/a	n/a	n/a
82558-50-7	Isoxaben	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
82-68-8	Quintozene	0.1	1.25E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			1.25E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
83121-18-0	Teflubenzuron	0.1	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			n/a	n/a	n/a	n/a	n/a	n/a
83164-33-4	Diflufenican	700	3.57E-05	3.71E-05	0.00E+00	0.00E+00	0.00E+00	0.000
			7.71E-05	1.43E-04	0.00E+00	0.00E+00	0.00E+00	0.000
83-32-9	Acenaphthene	210	5.95E-05	1.19E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			5.95E-05	1.19E-04	4.44E-05	6.11E-01	0.00E+00	0.611
834-12-8	Ametryn	0.1	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
84-66-2	Diethyl phthalate	2625	1.90E-04	1.90E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			1.90E-04	1.90E-04	0.00E+00	0.00E+00	0.00E+00	0.000
84-74-2	Di-n-butylphthalate	182	2.75E-03	2.75E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			2.75E-03	2.75E-03	0.00E+00	0.00E+00	0.00E+00	0.000
85-01-8	Phenanthrene	140	1.50E-04	3.57E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			1.36E-04	2.14E-04	0.00E+00	0.00E+00	0.00E+00	0.000
85509-19-9	Flusilazole	7	7.14E-03	7.14E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			7.14E-03	7.14E-03	0.00E+00	0.00E+00	0.00E+00	0.000
86-50-0	Azinphos-methyl	0.1	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-02	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.000
86-73-7	Fluorene	140	7.14E-05	8.93E-05	0.00E+00	0.00E+00	0.00E+00	0.000
			7.14E-05	7.14E-05	0.00E+00	0.00E+00	0.00E+00	0.000
87-65-0	2,6-Dichlorophenol	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
87674-68-8	Dimethenamid	0.1	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
88-06-2	2,4,6-Trichlorophenol	200	6.25E-04	6.25E-04	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
			6.25E-04	6.25E-04	0.00E+00	0.00E+00	0.00E+00	0.000
88-72-2	o-Nitrotoluene	35	7.14E-03	7.14E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			7.14E-03	7.14E-03	0.00E+00	0.00E+00	0.00E+00	0.000
88-85-7	Dinoseb	3.5	7.14E-03	7.14E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			7.14E-03	7.14E-03	0.00E+00	0.00E+00	0.00E+00	0.000
90-12-0	1-Methylnaphthalene	140	7.14E-05	7.14E-05	0.00E+00	0.00E+00	0.00E+00	0.000
			7.14E-05	7.14E-05	0.00E+00	0.00E+00	0.00E+00	0.000
90717-03-6	Quinmerac	0.1	2.50E-01	3.40E-01	1.51E-02	1.25E-01	4.00E-02	0.180
			2.50E-01	3.40E-01	1.51E-02	1.25E-01	4.00E-02	0.180
91465-08-6	lambda-Cyhalothrin	2	2.50E-02	2.50E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-03	2.50E-02	0.00E+00	0.00E+00	0.00E+00	0.000
919-86-8	Demeton-S-methyl	0.1	5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-01	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
92-52-4	Biphenyl	175	2.86E-04	2.86E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			2.86E-04	2.86E-04	0.00E+00	0.00E+00	0.00E+00	0.000
933-75-5	2,3,6-Trichlorphenol	10.5	2.38E-02	2.38E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			4.76E-03	4.76E-03	0.00E+00	0.00E+00	0.00E+00	0.000
933-78-8	2,3,5-Trichlorphenol	10.5	1.19E-02	1.19E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			4.76E-03	4.76E-03	0.00E+00	0.00E+00	0.00E+00	0.000
93-65-2	Mecoprop	10	2.50E-03	4.00E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-03	4.00E-03	0.00E+00	0.00E+00	0.00E+00	0.000
93-72-1	Fenoprop	9	2.78E-03	2.78E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			2.78E-03	2.78E-03	0.00E+00	0.00E+00	0.00E+00	0.000
93-76-5	2,4,5-Trichlorophenoxyacetic acid	9	2.78E-03	2.78E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			2.78E-03	2.78E-03	0.00E+00	0.00E+00	0.00E+00	0.000
94361-06-5	Cyproconazole	0.1	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
94-74-6	2-Methyl-4-chlorophenoxyacetic acid (aka MCPA)	2	1.25E-02	2.56E-02	4.17E-04	2.06E-01	0.00E+00	0.207
			1.25E-02	2.50E-02	0.00E+00	0.00E+00	0.00E+00	0.000
94-75-7	2,4-Dichlorophenoxyacetic acid (aka 2,4-D)	0.1	2.50E-01	4.00E-01	5.50E-03	1.48E-01	4.00E-02	0.193
			2.50E-01	3.70E-01	0.00E+00	0.00E+00	0.00E+00	0.000
94-81-5	2-Methyl-4-chlorophenoxybutyric acid (aka MCPB)	0.1	2.50E-01	2.50E-01	5.17E-03	8.95E-01	0.00E+00	0.900
			2.50E-01	2.50E-01	5.17E-03	8.95E-01	0.00E+00	0.900
94-82-6	4-(2,4-Dichlorophenoxy)butyric acid (aka 2,4-DB)	90	2.22E-04	2.78E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			2.22E-04	2.78E-04	0.00E+00	0.00E+00	0.00E+00	0.000
950-37-8	Methidathion	3.5	7.14E-03	7.14E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			n/a	n/a	n/a	n/a	n/a	n/a
95-50-1	1,2-Dichlorobenzene	1000	5.00E-04	1.00E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-04	5.00E-04	0.00E+00	0.00E+00	0.00E+00	0.000
95-51-2	2-Chloroaniline	0.0315	3.17E+00	7.94E+00	2.49E-01	9.50E-01	1.10E-01	1.309
			1.59E+00	1.59E+00	1.50E-01	9.57E-01	7.00E-02	1.177
95-57-8	2-Chlorophenol	17.5	2.86E-03	5.71E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			2.86E-03	5.71E-03	0.00E+00	0.00E+00	0.00E+00	0.000
95-94-3	1,2,4,5-Tetrachlorobenzene	0.735	6.80E-01	6.80E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			1.36E-03	1.36E-03	0.00E+00	0.00E+00	0.00E+00	0.000
95-95-4	2,4,5-Trichlorophenol	350	1.86E-04	3.57E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			1.86E-04	1.86E-04	0.00E+00	0.00E+00	0.00E+00	0.000
96-12-8	1,2-Dibromo-3-chloropropane	1	6.50E-01	6.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			6.50E-01	6.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
96-18-4	1,2,3-Trichloropropane	28	8.93E-02	8.93E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			8.93E-02	8.93E-02	0.00E+00	0.00E+00	0.00E+00	0.000
96525-23-4	Flurtamone	0.1	2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
			2.50E-01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.000
98-82-8	Isopropylbenzene	350	1.43E-03	2.86E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			7.14E-04	1.43E-03	0.00E+00	0.00E+00	0.00E+00	0.000
98-95-3	Nitrobenzene	1.75	1.43E-01	1.43E-01	1.85E-02	9.36E-01	0.00E+00	0.955
			5.71E-02	5.71E-02	8.95E-04	2.53E-01	0.00E+00	0.253
99-87-6	p-Cymene	140	7.14E-03	7.14E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			7.14E-03	7.14E-03	0.00E+00	0.00E+00	0.00E+00	0.000

Table IV-5. STEdw, hh results - inland water (dissolved fraction) monitoring data for metals, $PNEC_{dw, hh}$.

For each substance, two scenarios are presented. Top/shaded: Sc2 (all monitoring records; non-quantified records set as half LOD/Q); Bottom/white: Sc2-PNEC QC (quantified records plus non-quantified samples excluding those for which ½LOD/Q > PNEC).

[1] RQ_P90 is the risk quotient between the 90th percentile of all monitoring records and the selected PNEC.
[2] RQ_P95 is the risk quotient between the 95th percentile of all monitoring records and the selected PNEC.
[3] Fspat, Ftemp and Fext stand for the spatial, temporal and extend of PNEC exceedance factors in the STE approach, calculated as described in Section 2.1, while the Final STE score is the sum of the individual factors.
[4] Only STE scores using Sc2-PNEC QC were used for the risk-based ranking of substances.

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
7429-90-5	Aluminium	200	8.40E-01	1.39E+00	2.86E-02	3.09E-01	7.00E-02	0.407
			1.30E+00	1.98E+00	8.76E-02	4.23E-01	7.00E-02	0.581
7439-89-6	Iron	200	4.35E+00	7.10E+00	1.57E-01	5.66E-01	1.10E-01	0.833
			4.35E+00	7.10E+00	1.57E-01	5.66E-01	1.10E-01	0.833
7439-96-5	Manganese	50	2.20E+00	3.36E+00	3.27E-01	4.94E-01	1.10E-01	0.931
			2.20E+00	3.36E+00	3.27E-01	4.94E-01	1.10E-01	0.931
7439-98-7	Molybdenum	17.5	1.15E-01	3.24E-01	6.59E-03	4.32E-01	0.00E+00	0.439
			1.15E-01	3.14E-01	6.59E-03	4.31E-01	0.00E+00	0.437
7440-38-2	Arsenic	10	5.00E-01	1.00E+00	3.49E-03	2.82E-01	4.00E-02	0.325
			5.00E-01	1.00E+00	3.13E-03	2.79E-01	4.00E-02	0.323
7440-39-3	Barium	700	1.04E-01	1.20E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			1.04E-01	1.20E-01	0.00E+00	0.00E+00	0.00E+00	0.000
7440-42-8	Boron	2400	6.25E-02	1.04E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			6.25E-02	9.23E-02	0.00E+00	0.00E+00	0.00E+00	0.000
7440-47-3	Chromium	50	1.00E-01	2.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-02	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.000
7440-48-4	Cobalt	4.9	5.10E+00	5.10E+00	1.76E-01	9.44E-01	1.10E-01	1.230
			1.07E-01	1.69E-01	5.03E-03	2.85E-01	0.00E+00	0.290

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
7440-50-8	Copper	2000	4.37E-03	1.50E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			2.50E-03	3.00E-03	0.00E+00	0.00E+00	0.00E+00	0.000
7440-62-2	Vanadium	3.5	1.43E+00	1.43E+00	1.40E-01	5.67E-01	4.00E-02	0.747
			4.00E-01	6.57E-01	4.48E-02	3.78E-01	4.00E-02	0.463
7440-66-6	Zinc	1050	4.76E-02	4.76E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			2.67E-02	4.62E-02	0.00E+00	0.00E+00	0.00E+00	0.000
7782-49-2	Selenium	40	1.35E-01	3.13E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			8.75E-02	1.28E-01	0.00E+00	0.00E+00	0.00E+00	0.000

Table IV-6. STEwater, hh food results - inland water monitoring data, $PNEC_{water, hh\ food}$.

For each substance, two scenarios are presented. Top/shaded: Sc2 (all monitoring records; non-quantified records set as half LOD/Q); Bottom/white: Sc2-PNEC QC (quantified records plus non-quantified samples excluding those for which ½LOD/Q > PNEC).

[1] RQ_P90 is the risk quotient between the 90th percentile of all monitoring records and the selected PNEC.
[2] RQ_P95 is the risk quotient between the 95th percentile of all monitoring records and the selected PNEC.
[3] Fspat, Ftemp and Fext stand for the spatial, temporal and extend of PNEC exceedance factors in the STE approach, calculated as described in Section 2.1, while the Final STE score is the sum of the individual factors.
[4] Only STE scores using Sc2-PNEC QC were used for the risk-based ranking of substances.

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
1031-07-8	Endosulfan sulfate	2.041	4.90E-03	1.22E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			2.45E-03	2.45E-03	0.00E+00	0.00E+00	0.00E+00	0.000
107534-96-3	Tebuconazole	23.411	2.14E-03	2.14E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			2.14E-03	2.14E-03	0.00E+00	0.00E+00	0.00E+00	0.000
1085-98-9	Dichlofluanid	295.894	6.76E-05	6.76E-05	0.00E+00	0.00E+00	0.00E+00	0.000
			6.76E-05	6.76E-05	0.00E+00	0.00E+00	0.00E+00	0.000
116-29-0	Tetradifon	0.587	8.52E-02	8.52E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			8.52E-02	8.52E-02	0.00E+00	0.00E+00	0.00E+00	0.000
118134-30-8	Spiroxamine	17.491	2.86E-03	2.86E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			5.72E-04	1.51E-03	0.00E+00	0.00E+00	0.00E+00	0.000
119446-68-3	Difenoconazole	1.845	5.42E-02	5.42E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			5.42E-02	5.42E-02	0.00E+00	0.00E+00	0.00E+00	0.000
129-00-0	Pyrene	20.201	1.14E-03	2.33E-03	1.12E-03	4.17E-01	0.00E+00	0.418
			2.13E-03	4.46E-03	1.85E-03	5.13E-01	0.00E+00	0.515
131341-86-1	Fludioxonil	61.535	4.06E-04	8.13E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			4.06E-04	8.13E-04	0.00E+00	0.00E+00	0.00E+00	0.000
1330-78-5	Tricresyl Phosphate	5.367	1.70E-03	2.57E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			1.70E-03	2.57E-03	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
133855-98-8	Epoxiconazole	486.957	1.03E-04	1.03E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			1.03E-04	1.03E-04	0.00E+00	0.00E+00	0.00E+00	0.000
141517-21-7	Trifloxystrobin	14.123	3.54E-03	3.54E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			3.54E-03	3.54E-03	0.00E+00	0.00E+00	0.00E+00	0.000
142459-58-3	Flufenacet	2.556	1.96E-02	1.96E-02	1.41E-03	9.40E-01	0.00E+00	0.941
			9.78E-03	9.78E-03	1.43E-03	9.39E-01	0.00E+00	0.940
15687-27-1	Ibuprofen	230.885	4.74E-04	7.36E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			4.74E-04	7.36E-04	0.00E+00	0.00E+00	0.00E+00	0.000
175013-18-0	Pyraclostrobine	2.591	1.93E-02	1.93E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			1.93E-02	1.93E-02	0.00E+00	0.00E+00	0.00E+00	0.000
19666-30-9	Oxadiazon	0.181	1.38E-01	1.38E-01	4.78E-03	3.27E-01	0.00E+00	0.332
			1.38E-01	1.38E-01	4.56E-03	3.58E-01	0.00E+00	0.362
208-96-8	Acenaphthylene	11.230	2.23E-03	4.45E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			2.23E-03	4.45E-03	2.66E-04	1.00E+00	0.00E+00	1.000
333-41-5	Diazinon	0.170	1.47E-01	2.35E-01	3.17E-03	6.69E-01	0.00E+00	0.672
			5.87E-02	5.87E-02	6.05E-04	3.12E-01	0.00E+00	0.313
35554-44-0	Imazalil	27.029	2.77E-03	2.77E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			2.77E-03	2.77E-03	0.00E+00	0.00E+00	0.00E+00	0.000
36734-19-7	Iprodione	10.868	2.30E-03	4.60E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			2.30E-03	4.60E-03	0.00E+00	0.00E+00	0.00E+00	0.000
41859-67-0	Bezafibrate	2.364	4.10E-02	6.35E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			4.10E-02	6.35E-02	0.00E+00	0.00E+00	0.00E+00	0.000
52645-53-1	Permethrin	6.793	3.68E-03	3.68E-03	1.18E-03	1.00E+00	0.00E+00	1.001
			1.47E-03	2.94E-03	0.00E+00	0.00E+00	0.00E+00	0.000
53-70-3	Dibenz(a,h)anthracene	0.023	2.20E-01	2.20E-01	5.07E-03	4.72E-01	0.00E+00	0.477
			6.59E-02	3.09E-01	4.14E-02	5.90E-01	7.00E-02	0.701
55179-31-2	Bitertanol	1.074	2.33E-02	2.33E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			2.33E-02	2.33E-02	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
5598-13-0	Chlorpyriphos methyl	0.338	5.91E-02	7.39E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			2.96E-02	5.91E-02	0.00E+00	0.00E+00	0.00E+00	0.000
56-55-3	Benzo(a)anthracene	0.012	1.28E+00	2.39E+00	2.35E-01	3.44E-01	5.60E-01	1.138
			2.56E+00	4.53E+00	5.27E-01	4.51E-01	1.10E-01	1.088
57018-04-9	Tolclofos-methyl	5.411	4.62E-03	9.24E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			4.62E-03	9.24E-03	0.00E+00	0.00E+00	0.00E+00	0.000
60207-90-1	Propiconazole	13.527	3.70E-03	3.70E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			3.70E-03	3.70E-03	0.00E+00	0.00E+00	0.00E+00	0.000
66246-88-6	Penconazole	5.707	4.38E-03	8.76E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			4.38E-03	8.76E-03	0.00E+00	0.00E+00	0.00E+00	0.000
67564-91-4	Fenpropimorph	0.176	1.42E-01	1.42E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			7.10E-02	7.10E-02	0.00E+00	0.00E+00	0.00E+00	0.000
67-72-1	Hexachloroethane	0.084	2.99E+00	2.99E+00	2.46E-01	9.63E-01	7.00E-02	1.279
			2.99E+00	2.99E+00	2.24E-01	9.62E-01	7.00E-02	1.255
67747-09-5	Prochloraz	2.254	1.55E-02	2.22E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			1.55E-02	2.22E-02	0.00E+00	0.00E+00	0.00E+00	0.000
72-43-5	Methoxychlor	0.966	2.59E-02	2.59E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			5.17E-04	5.17E-04	0.00E+00	0.00E+00	0.00E+00	0.000
731-27-1	Tolylfluanid	82.256	6.08E-04	6.08E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			6.08E-04	6.08E-04	0.00E+00	0.00E+00	0.00E+00	0.000
80-05-7	Bisphenol A	5.559	4.50E-02	5.68E-02	1.90E-03	6.08E-01	0.00E+00	0.610
			2.16E-02	4.05E-02	1.95E-03	6.62E-01	0.00E+00	0.664
83164-33-4	Diflufenican	8.531	2.93E-03	3.05E-03	9.74E-04	6.90E-01	0.00E+00	0.691
			6.33E-03	1.17E-02	2.97E-03	1.00E+00	0.00E+00	1.003
84-74-2	Di-n-butylphthalate	18.954	2.64E-02	2.64E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			2.64E-02	2.64E-02	0.00E+00	0.00E+00	0.00E+00	0.000
85509-19-9	Flusilazole	0.487	1.03E-01	1.03E-01	1.76E-04	1.09E-01	0.00E+00	0.109
			1.03E-01	1.03E-01	0.00E+00	0.00E+00	0.00E+00	0.000

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
86-73-7	Fluorene	4.635	2.16E-03	2.70E-03	5.42E-04	2.78E-01	0.00E+00	0.279
			2.16E-03	2.16E-03	6.04E-04	7.94E-01	0.00E+00	0.795
90-12-0	1-Methylnaphthalene	10.418	9.60E-04	9.60E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			9.60E-04	9.60E-04	0.00E+00	0.00E+00	0.00E+00	0.000
92-52-4	Biphenyl	69.722	7.17E-04	7.17E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			7.17E-04	7.17E-04	0.00E+00	0.00E+00	0.00E+00	0.000
93-72-1	Fenoprop	0.989	2.53E-02	2.53E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			2.53E-02	2.53E-02	0.00E+00	0.00E+00	0.00E+00	0.000
94-82-6	4-(2,4-Dichlorophenoxy)butyric acid (2,4-DB)	7.441	2.69E-03	3.36E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			2.69E-03	3.36E-03	0.00E+00	0.00E+00	0.00E+00	0.000
95-94-3	1,2,4,5-Tetrachlorobenzene	0.005	1.09E+02	1.09E+02	6.32E-01	9.90E-01	5.60E-01	2.182
			2.17E-01	2.17E-01	1.88E-02	6.00E-01	0.00E+00	0.619
95-95-4	2,4,5-Trichlorophenol	11.418	5.69E-03	1.09E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			5.69E-03	5.69E-03	0.00E+00	0.00E+00	0.00E+00	0.000
98-82-8	Isopropylbenzene	171.554	2.91E-03	5.83E-03	0.00E+00	0.00E+00	0.00E+00	0.000
			1.46E-03	2.91E-03	0.00E+00	0.00E+00	0.00E+00	0.000
99-87-6	p-Cymene	9.983	1.00E-01	1.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			1.00E-01	1.00E-01	0.00E+00	0.00E+00	0.00E+00	0.000

Table IV-7. STEsw, eco results - coastal and transitional whole water, $PNEC_{sw, eco}$.

For each substance, two scenarios are presented. Top/shaded: Sc2 (all monitoring records; non-quantified records set as half LOD/Q); Bottom/white: Sc2-PNEC QC (quantified records plus non-quantified samples excluding those for which ½LOD/Q > PNEC).

[1] RQ_P90 is the risk quotient between the 90th percentile of all monitoring records and the selected PNEC
[2] RQ_P95 is the risk quotient between the 95th percentile of all monitoring records and the selected PNEC
[3] Fspat, Ftemp and Fext stand for the spatial, temporal and extend of PNEC exceedance factors in the STE approach, calculated as described in Section 2.1, while the Final STE score is the sum of the individual factors.
[4] Only STE scores using Sc2-PNEC QC were used for the risk-based ranking of substances.

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
108-88-3	Toluene	74	6.76E-04	6.76E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			6.76E-04	6.76E-04	0.00E+00	0.00E+00	0.00E+00	0.000
129-00-0	Pyrene	0.04	1.25E+00	1.88E+00	9.36E-02	8.65E-01	4.00E-02	0.998
			1.17E+00	2.08E+00	1.37E-02	3.04E-01	7.00E-02	0.388
218-01-9	Chrysene	1	5.00E-02	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			5.00E-02	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.000
330-55-2	Linuron	0.3	1.67E-02	3.33E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			1.67E-02	3.33E-02	0.00E+00	0.00E+00	0.00E+00	0.000
56-55-3	Benzo(a)anthracene	0.3	1.67E-01	1.67E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			1.67E-01	1.67E-01	0.00E+00	0.00E+00	0.00E+00	0.000
85-01-8	Phenanthrene	0.1	5.00E-01	5.00E-01	6.22E-03	1.23E-01	0.00E+00	0.129
			5.00E-01	5.00E-01	6.22E-03	1.23E-01	0.00E+00	0.129

Table IV-8. STEsw, eco results - coastal and transitional waters (dissolved fraction), $PNEC_{sw,\ eco}$.

For each substance, two scenarios are presented. Top/shaded: Sc2 (all monitoring records; non-quantified records set as half LOD/Q); Bottom/white: Sc2-PNEC QC (quantified records plus non-quantified samples excluding those for which ½LOD/Q > PNEC).

[1] Two PNEC values have been compared in the Sc2 given the discrepancy between the accepted values from the MS and Stakeholders.
[2] RQ_P90 is the risk quotient between the 90th percentile of all monitoring records and the selected PNEC.
[3] RQ_P95 is the risk quotient between the 95th percentile of all monitoring records and the selected PNEC.
[4] Fspat, Ftemp and Fext stand for the spatial, temporal and extend of PNEC exceedance factors in the STE approach, calculated as described in Section 2.1, while the Final STE score is the sum of the individual factors.
[5] Only STE scores using Sc2-PNEC QC were used for the risk-based ranking of substances.

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
7440-47-3	Chromium	0.6	1.67E+00	2.92E+00	4.12E-01	5.77E-01	1.80E-01	1.170
			8.80E-01	1.17E+00	2.75E-01	1.79E-01	1.10E-01	0.564
7440-50-8	Copper	3.76	6.65E-01	8.19E-01	2.90E-02	1.30E-01	4.00E-02	0.199
			6.65E-01	8.19E-01	2.45E-02	1.30E-01	4.00E-02	0.195
7440-66-6	Zinc	3	4.08E+00	5.00E+00	6.35E-01	6.22E-01	1.10E-01	1.367
			3.93E+00	5.08E+00	5.50E-01	4.78E-01	1.10E-01	1.138

Table IV-9. STEsed, eco results – sediment monitoring data, $PNEC_{sed, eco}$.

For each substance, two scenarios are presented. Top/shaded: Sc2 (all monitoring records; non-quantified records set as half LOD/Q); Bottom/white: Sc2-PNEC QC (quantified records plus non-quantified samples excluding those for which ½LOD/Q > PNEC). The data contains only inland water sediments (rivers; lakes). The records for transitional and coastal water were excluded because they were few. In addition to the outlier procedure applied, some additional non-realistic high concentrations were excluded (as 1kg/kg dd).

[1] RQ_P90 is the risk quotient between the 90th percentile of all monitoring records and the selected PNEC

[2] RQ_P95 is the risk quotient between the 95th percentile of all monitoring records and the selected PNEC

[3] Fspat, Ftemp and Fext stand for the spatial, temporal and extend of PNEC exceedance factors in the STE approach, calculated as described in Section 2.1, while the Final STE score is the sum of the individual factors.

[4] Only STE scores using Sc2-PNEC QC were used for the risk-based ranking of substances.

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
1002-53-5	Dibutyltin (dichloride)	7	2.79E+00	2.79E+00	4.11E-02	9.92E-01	7.00E-02	1.103
			5.58E-01	1.22E+00	6.99E-03	8.18E-01	4.00E-02	0.865
1163-19-5	Decabromodiphenyl ether (BDE-209)	384000	6.51E-04	6.51E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			6.51E-04	6.51E-04	0.00E+00	0.00E+00	0.00E+00	0.000
1461-25-2	Tetrabutyltin	0.202	8.46E+01	8.46E+01	1.91E-01	1.00E+00	4.10E-01	1.601
			n/a	n/a	n/a	n/a	n/a	n/a
207122-16-5	Heptabromodiphenyl ether (BDE-183)	266	3.76E-04	3.76E-04	0.00E+00	0.00E+00	0.00E+00	0.000
			3.76E-04	3.76E-04	0.00E+00	0.00E+00	0.00E+00	0.000
53-19-0	DDD, o,p'	0.99	1.26E+01	1.26E+01	6.65E-02	9.99E-01	1.80E-01	1.245
			5.05E-01	1.84E+00	7.66E-03	7.86E-01	7.00E-02	0.863
56-55-3	Benzo(a)anthracene	27.7	2.52E+01	4.38E+01	2.05E-01	9.58E-01	2.80E-01	1.443
			2.52E+01	4.38E+01	2.05E-01	9.58E-01	2.80E-01	1.443
668-34-8	Triphenyltin	20	8.45E-01	8.45E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			8.45E-01	8.45E-01	0.00E+00	0.00E+00	0.00E+00	0.000
7440-38-2	Arsenic	17000	1.19E+00	1.69E+00	5.89E-02	7.18E-01	4.00E-02	0.817

CAS	Substance	PNEC (µg/L)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
			1.19E+00	1.69E+00	5.89E-02	7.18E-01	4.00E-02	0.817
7440-47-3	Chromium	90000	6.90E-01	8.62E-01	3.34E-03	6.20E-01	0.00E+00	0.623
			6.90E-01	8.62E-01	3.34E-03	6.20E-01	0.00E+00	0.623
7440-50-8	Copper	87000	5.17E-01	8.63E-01	3.72E-02	5.37E-01	4.00E-02	0.615
			5.17E-01	8.63E-01	3.72E-02	5.37E-01	4.00E-02	0.615
7440-66-6	Zinc	119000	1.88E+00	2.66E+00	5.83E-02	7.69E-01	7.00E-02	0.898
			1.88E+00	2.66E+00	5.83E-02	7.69E-01	7.00E-02	0.898
78763-54-9	Monobutyltin	1.17	2.84E+01	2.84E+01	7.43E-01	9.89E-01	2.80E-01	2.012
			2.80E+01	5.65E+01	4.20E-01	5.68E-01	4.10E-01	1.398
85-01-8	Phenanthrene	2708	2.40E-01	3.88E-01	0.00E+00	0.00E+00	0.00E+00	0.000
			2.40E-01	3.88E-01	0.00E+00	0.00E+00	0.00E+00	0.000

Table IV-10. STEbiota, secpois – biota results: fish monitoring data, $PNEC_{biota,\ secpois}$.

For each substance, two scenarios are presented. Top/shaded: Sc2 (all monitoring records; non-quantified records set as half LOD/Q); Bottom/white: Sc2-PNEC QC (quantified records plus non-quantified samples excluding those for which ½LOD/Q > PNEC). The data contains only coastal and transitional waters. Data given in dry weight have been converted to wet weight. In addition to the outlier procedure applied, some additional non-realistic high concentrations were excluded.

[1] RQ_P90 is the risk quotient between the 90th percentile of all monitoring records and the selected PNEC

[2] RQ_P95 is the risk quotient between the 95th percentile of all monitoring records and the selected PNEC

[3] Fspat, Ftemp and Fext stand for the spatial, temporal and extend of PNEC exceedance factors in the STE approach, calculated as described in Section 2.1, while the Final STE score is the sum of the individual factors.

[4] Only STE scores using Sc2-PNEC QC were used for the risk-based ranking of substances.

CAS	Substance	PNEC (µg/kg)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
7440-47-3	Chromium	5700	5.26E-02	7.30E-02	0.00E+00	0.00E+00	0.00E+00	0.000
			5.26E-02	7.30E-02	0.00E+00	0.00E+00	0.00E+00	0.000

Table IV-11. STEbiota, secpois – biota results: mollusc monitoring data, $PNEC_{biota,\ secpois}$.

For each substance, two scenarios are presented. Top/shaded: Sc2 (all monitoring records; non-quantified records set as half LOD/Q); Bottom/white: Sc2-PNEC QC (quantified records plus non-quantified samples excluding those for which ½LOD/Q > PNEC). The data contains only coastal and transitional waters. Data given in dry weight have been converted to wet weight. In addition to the outlier procedure applied, some additional non-realistic high concentrations were excluded.

[1] RQ_P90 is the risk quotient between the 90th percentile of all monitoring records and the selected PNEC

[2] RQ_P95 is the risk quotient between the 95th percentile of all monitoring records and the selected PNEC

[3] Fspat, Ftemp and Fext stand for the spatial, temporal and extend of PNEC exceedance factors in the STE approach, calculated as described in Section 2.1, while the Final STE score is the sum of the individual factors.

[4] Only STE scores using Sc2-PNEC QC were used for the risk-based ranking of substances.

CAS	Substance	PNEC (µg/kg)	RQ_P90 [1]	RQ_P95 [2]	Fspat	Ftemp	Fext	STE score [3,4]
129-00-0	Pyrene	1	1.81E+01	3.49E+01	8.79E-01	9.44E-01	2.80E-01	2.103
			1.86E+01	3.51E+01	8.72E-01	9.42E-01	2.80E-01	2.094
218-01-9	Chrysene	0.5	3.29E+01	6.39E+01	9.17E-01	9.21E-01	4.10E-01	2.248
			3.42E+01	6.53E+01	9.07E-01	9.12E-01	4.10E-01	2.229
53-70-3	Dibenzo(a,h)anthracene	0.5	2.82E+00	1.00E+01	3.53E-01	7.45E-01	4.10E-01	1.508
			2.46E+00	6.04E+00	2.08E-01	6.48E-01	4.10E-01	1.266
56-55-3	Benzo(a)anthracene	0.5	1.74E+01	3.41E+01	8.18E-01	8.92E-01	2.80E-01	1.991
			1.84E+01	3.60E+01	8.05E-01	8.81E-01	2.80E-01	1.966
7440-38-2	Arsenic	5454.55	6.28E-01	7.66E-01	2.81E-03	3.31E-01	0.00E+00	0.333
			6.28E-01	7.66E-01	2.81E-03	3.31E-01	0.00E+00	0.333
7440-47-3	Chromium	1090.91	5.94E-01	8.83E-01	1.70E-02	3.43E-01	4.00E-02	0.400
			5.94E-01	8.83E-01	1.70E-02	3.43E-01	4.00E-02	0.400
85-01-8	Phenanthrene	1	1.15E+01	1.82E+01	9.63E-01	9.41E-01	2.80E-01	2.183
			1.17E+01	1.86E+01	9.61E-01	9.36E-01	2.80E-01	2.177

Annex V: Factsheets for substances short-listed in the monitoring-based exercise

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